Influence of the Shape and Size of a Quantum Structure on its Energy Levels

By

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*For my Heavenly Father and
my family*

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- My parents, family and friends for their love, support and understanding.

'Glory to God who gave me the privilege to touch the hem of His garment'

-Isaac Newton after one of his discoveries

Abstract

In this study the importance of the luminescent properties of low-dimensional quantum structures are investigated focusing on the change in the exciton binding energy with a change in the size of the low dimensional Quantum Well or Wire.

With a reduction in dimensionality, moving from bulk semiconductor materials through Quantum Wells, Wires and ultimately Quantum Dots, the band structure as well as the density of states for these low-dimensional structures change appreciably going from quasi-continuous in bulk semiconductors to discrete in Quantum Dots. This leads to an increase in the energy gap (compared to the bulk material), with a decrease in size for a low-dimensional structure.

An interacting electron-hole pair in a Quantum Well-Wire is studied within the framework of the Effective-Mass Approximation. A mathematical technique is presented which investigates the quasi-two-dimensional, quasi-one-dimensional behavior of a confined exciton inside a semiconductor as the bulk material is reduced in dimensions to form a Quantum Well and Wire. The technique is applied to an infinite Well-Wire confining potential. The Envelope Function Approximation is employed in the approach, involving a three parameter variational calculation in which the symmetry of the component of the wave function representing the relative motion is allowed to vary from the one- to the two- and three-dimensional limits. A quasi–two-dimensional behavior occurs on reducing the well width as the average electron-hole distance decrease leading to an increase in the binding energy. However, when the well width is smaller than a critical value, the leakage of the wave function into the barriers becomes more important and the binding energy is reduced until it reaches the value appropriate to the bulk barrier material for which $L = 0$.

As the electronic industry progress from micro-technologies to nanotechnologies whereby devices are designed in the nanometer range, it becomes increasingly necessary to address the concern of the exciton losing its enhanced effects in the ultra- small

quantum structures, due to the increased penetration of the exciton wave function into the barrier regions in the direction of diminishing spatial confinement.

A trial wave function is employed; written as a product of three wave functions. The first two are corresponding to the single particle wave function of an electron and a hole in the Quantum Well-Wire and the third represents a *free* exciton whose radius is adjusted as a variational parameter. This method can be suitably adapted for any particular choice of variational wave function. The choice of this wave function is only limited by the users' qualitative knowledge of the system under consideration and how this knowledge is imbedded into this trial wave function.

Results to this numerical calculation are presented. Quantitative comparisons with previous calculations for quantum wells was made (in the wire limit where $Lz \rightarrow \infty$) and it was found that there exists a good agreement between this infinite- and other finite- as well as infinite - potential models up to a point of *100 Å*.

A plot of the binding energy vs. the variational parameter λ revealed that the electron in the exciton has a very similar behavior than the electron in the Hydrogen atom (or for that matter any particle trapped inside a radial decreasing (i.e. *V~1/r*) potential field). However on reducing the size and dimensions of the quantum structure, it seems that the screening of the other electrons surrounding the hole start to play a very important role and the shape of a plot of binding energy versus λ is very similar to that of an alpha particle trapped in an atomic nucleus.

It is concluded from this that for accurately predicting the behavior of systems like these it is important to include in such a model not only the different dielectric constants for the barrier and the well-wire materials, but also to include *the change in dielectric constant due to a change in size*, *i.e. $\varepsilon = \varepsilon$ (L),* i.e. to take into account the decrease in the amount of electrons in the valence band due to a decrease in size of the Quantum Well-Wire.

Keywords

Band gap

Conduction Band

Continuous

Density of States

Discrete

Effective Mass Approximation

Energy Level

Envelope Function Approximation

Exciton

Exciton Bohr Radius

Hole

Oscillator Strength

Quantum Dot

Quantum Confinement

Quantum Structure / Low Dimensional Structure

Quantum Well

Quantum Wire

Valence Band

Acronyms

E_G Band gap

CB Conduction Band

DOS Density of States

EMA Effective Mass Approximation

E_n Energy Level

EFA Envelope Function Approximation

a_b/a_0 Exciton Bohr Radius

f Oscillator Strength

VB Valence Band

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"If I were asked for an area of science and engineering that will most likely produce the breakthroughs of tomorrow, I would point to nanoscale science and engineering."

- Neal Lane

Assistant to the President of the USA

for Science and Technology

Chapter 1

Introduction

'There's plenty of room at the bottom!'   - Richard P. Feynman, 1959

Nowadays nanoscale physics is one of the most topical research subjects having two major areas of focus, one being the important field of potential applications. This bears the promise of a great assortment of materials having explicit properties advantageous in every day life. However, to the researcher in physics, the fundamental aspects where quantum mechanics is seen at work, is even more enthralling. Most macroscopic phenomena of nanoscale physics can only be understood and described using quantum mechanics. The exquisite tools by which quantum behaviour can be probed an a scale significantly larger that the atomic scale, that is, on the nanometer scale, are Quantum dots, often denoted as artificial atoms due to their atomic-like properties. In this way, the physics of the devices is closer to classical physics than that of atomic physics but they are still sufficiently small to clearly exhibit quantum phenomena.

1.1   History of Quantum Structures

'What has been will be again, what has been done will be done again; there is nothing new under the sun. Is there anything of which one can say, "Look! This is something new"? It was here already, long ago;   it was here before our time.'

                              - Ecclesiastes 1:9-10

Early in the twentieth century, encounters with physical phenomena, such as electron motion, for which Newtonian mechanics could not at all provide an adequate explanation, prompted the advent of quantum mechanics, as it required detailed analyses on the

nanoscale. Electron tunnelling through nanoscale barriers is the most direct consequence of the laws of quantum mechanics. The Esaki tunnel diode gave most convincing experimental evidence for this phenomenon in 1957. However even before then nanoscale science has played a significant role in the evolution of science and humanity as a whole. A brief description of the evolutionary path of nanoscience follows.

Colloidal dispersed pigments uses are so old that it is essentially a history of humankind's pursuit of colour. Such pigments were used by Stone Age peoples in paintings dating from the dawn of civilization itself. Ancient Egyptians prepared colloidal dispersions as inks. Though not understood as such, these technologies were already widespread by the Middle Ages. Such understanding would not come until the 1850s and 1860s when visionaries such as Michael Faraday began to unravel the reasons behind the remarkable properties of nanocrystalline systems. [2]

Nano-sized particles have been used in pottery for thousands of years. The oldest known such object is thought to be the **Lycurgus chalice**, dating back to the late fourth century AD, Rome, and which can be seen in the National British Museum of History. The Roman chalice has a raised fresco showing the myth of King Lycurgus, and is made from glass which appears green in reflected light, but red in transmitted light.

This curious optical effect is caused by 70nm particles of silver and gold contained within the glass. The understanding that glass could be coloured red by adding small amounts of gold is often credited to **Johann Kunckel**, who worked in Germany in the late seventeenth century.

Johann KUNCKEL (1638-1703)

The chalice, however, is not a unique example of nanoparticles being used in centuries past; pottery from the ninth century AD also contains nanoparticles in glazed films applied to ceramic pottery. In medieval times the technique was brought to Spain as Arabian culture spread, and then migrated to Italy, where Renaissance pottery made much use of the effect in polychrome lustres on pottery [3]

The twentieth century was characterized by the fact that science and technology have made remarkable progress. The establishment of quantum mechanics, the development of semiconductor devices with the invention of the transistor and the evolution of computers and telecommunications were some of the significant highlights. In the early century, the advent of quantum mechanics was driven by encounters with physical phenomena such as electron's motion or photon's behaviour for which Newtonian mechanics could not possibly provide a satisfactory explanation. The framework of quantum mechanics was established in the superb work of Werner Heisenberg, Erwin Schrödinger, Paul Dirac and Max Born in the period 1925-1926.

It was de Broglie that introduced a new fundamental hypothesis during the infancy of the quantum theory: matter was endowed with a dualistic nature – particles may also have the characteristics of waves! Finding expression in the hands of Schrödinger a mathematical equation emerged to be known as the Schrödinger wave equation. This hypothesis stated that an electron is assumed to be represented by a solution to this equation. The continuous non-zero nature of such solutions, even in classically forbidden regions of negative kinetic energy, implies an ability to penetrate such forbidden regions and a probability of tunnelling from one classically allowed region to another. The concept of tunnelling itself arises from this quantum-mechanical result, and has no analogy in classical mechanics. The subsequent experimental manifestations of that concept can be regarded as one of the early triumphs of the quantum theory. In 1928, Fowler and Nordheim [3] explained, on the basis of electron tunnelling, the main features of the phenomenon of electron emission from cold metals by high external electric fields, which had been unexplained since its observation by Lilienfeld in 1922.

In 1969 research on artificially structured materials was initiated when Esaki and Tsu. They proposed to use a semiconductor superlattice based on a periodic structure of alternating layers of semiconductor materials with wide and narrow band gaps. The first superlattices were fabricated using an AlGaAs/GaAs material system (Figure 1.1)
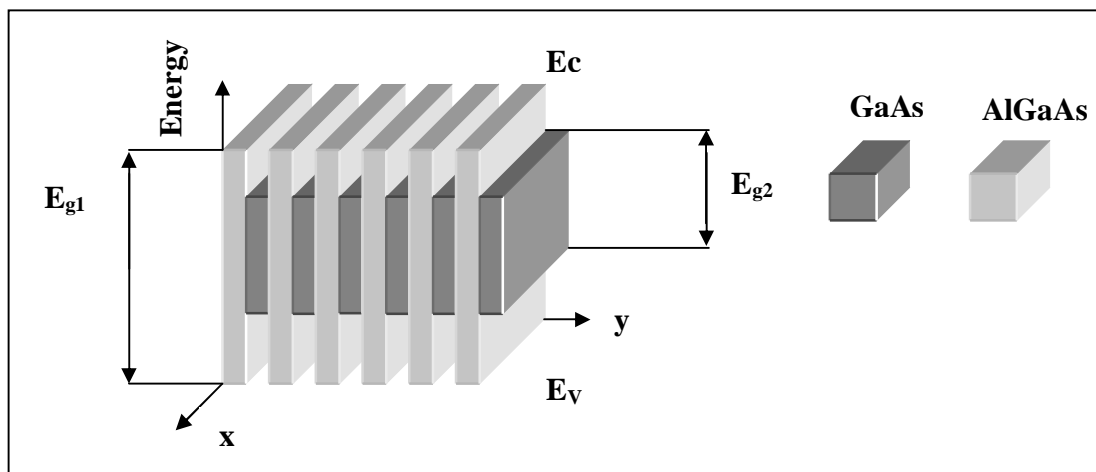
Figure 1.1: AlGaAs-GaAs superlattice

1970's and beyond

Early in the 1970s, the first quantum wells (QWs) which were also the first low dimensional heterostructures, were developed. Almost thirty years later, in 2000, the Nobel Prize in Physics was rewarded to Zhores Alferov and Herbert Kroemer for developing semiconductor heterostructures used in high-speed- and opto-electronics, recognizing the importance of quantum wells. Today quantum wells form the basis of most of the optoelectronic devices and their importance must therefore not be underestimated.

Zhores I. Alferov and Herbert Kroemer

In these quantum well structures the electrical carriers (electrons and holes) are confined in a two dimensional (2D) plane. For this reason they are often referred to as being "two dimensional" though in the strictest sense they are not completely two dimensional since the thickness of the quantum wells are usually in the order of nanometers and do not completely vanish. The first advantage of such a design involves the optical properties of these quantum wells. Optical properties can be tuned by changing the structural parameters: typically thickness and composition. This is known as band-gap engineering. The reduced dimensionality also leads to improved optical performances: by reducing the size of one dimension the probability of electron-hole recombination increases.

Led by the insights to this discovery, scientists investigated the possibility of reducing the dimensionality of heterostructures even further in order to create one dimensional (1D - quantum wire) and zero dimensional (0D - quantum dot) structures. An interesting consequence of changing the density of states for quantum dots is that this change leads to a discrete DOS for QDs. For this reason QDs are often described as **artificial atoms**, making them exceedingly fascinating for fundamental studies.

The quest to find new solutions to meet the worldwide energy demand stimulated the development of modern quantum dot technology even further. The advantage of the surface area-to-volume ratio of nanocrystal particles for energy generation was realized and photo-electrochemistry research (e.g. solar energy conversion) was tapping the semiconductor/liquid interface to utilize this. Then in the early 1980s two very influential and independent developments from two labs arose. Drs. Alexander Efros and A.I Ekimov of the Yoffe Institute in St. Petersburg (then Leningrad) in the former Soviet Union and Dr. Louis Brus at Bell Laboratories. Bell Labs scientists were studying the optical phenomena that occur when the properties of bulk semiconductor materials change. Their work contributed to the understanding of the quantum confinement effect that explains the correlation between size and colour for these nanocrystals.
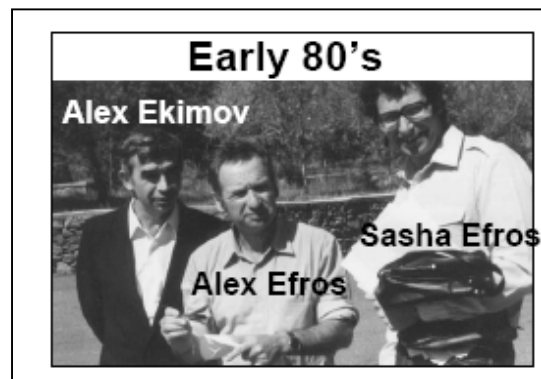
Drs. Alex Ekimov, Alex Efros and Sasha Efros

Dr. Ekimov discovered quantum dots with his colleague, Dr. Efros, while working at the Ioffe Institute in St. Petersburg, Russia. Dr. Ekimov's discovery of quantum dots occurred at nearly the same time as the discoveries by Dr. Brus at AT&T Bell Labs. Dr. Ekimov is the recipient of the prestigious State Prize of the USSR in Physics and Technology and the Alexander Von Humboldt Award for his work in semiconductor

nanocrystals. He has been a visiting professor at Ecole Polytechnique and University Clode Bernade in France, Max Planck Institute in Germany and Osaka University in Japan. He is internationally renowned in the scientific community and has more than 100 publications and several patents [4].

Louis E. Brus,

"Thomas A. Edison" - Professor of Chemical Engineering, Brus is one of the founders of a new branch of solid state physics and chemistry: inorganic nanostructures. He pioneered the study of physical, electronic and chemical properties of semiconductor nanocrystals as a function of their size [5].

Experimenting with nanocrystal semiconductor materials, Dr. Brus and his collaborators observed solutions of astonishingly different colours made from the same substance. This observation led to the discovery that there is a very clear transition when a structure becomes smaller than a fundamental scale, intrinsic to the substance. The Bohr radius of the electron-hole pair determines this scale length.

Ever since then ways to make the quantum dots water-soluble were discovered by two of these Bell Labs scientists (Dr. Moungi Bawendi and Dr. Paul Alivisatos). They moved to MIT and UC Berkeley, respectively, were they continued their investigation of quantum dots' optical properties. Another significant discovery by these two scientists showed that by adding a passivating inorganic "shell" around the nanocrystals, and then shining blue light on them, caused the quantum dots to shine brightly [6].

Even though it was predicted in 1982 that QDs could be used as the active region of lasers, providing a reduced threshold current and improved temperature dependence, it has taken nearly a decade to develop reliable growth techniques to produce QDs of a quality suitable for commercial applications. QD devices have now been demonstrated in

many research laboratories, and commercial products are now starting to be available on the market [7].

The advances we see reported today in nanotechnology owe their origins to scientific research that has been going on for over a hundred years, some of which has been conducted by some very famous and respected scientists, including Michael Faraday, Irving Langmuir and Albert Einstein.

As time has gone on, further advances have been built upon this and other research and new techniques have been developed to allow matter at the nanoscale to be seen and studied. These include the development of the Scanning Tunneling Microscope (STM), which allows individual atoms to be moved, and high-resolution electron microscopes. These machines have used a wealth of previous research and have in turn fuelled further advances in science.

The time milestones below show the progress of some of the scientific and especially technological advances that have been important in the advancement of nanotechnology.

During this time period there has been a trend for the different disciplines of science to converge towards the nanoscale: physics and engineering have been considering smaller and smaller objects, chemistry has been considering larger and larger groups of atoms, or molecules.

This convergence means that ideas in physics, chemistry and biology can be shared, and new advances can be made in materials science, medicine, electronics, environmental technology, and many other areas, that might not have occurred otherwise. [3]

   1857 - This year marks the introduction of 'colloidal gold ' samples to the Royal
            Society by Michael Faraday. This suspension of gold nanoparticles in solution
            was totally transparent in some lighting, but in other lighting conditions could
            produce differently coloured solutions of 'ruby, green, violet or blue'. [8]

1905 – A thoroughly quantitative theory for the colloid dispersion state was provided by Albert Einstein wherin he considered colloids to behave as 'large atoms' and explained their movement in terms of Brownian motion. Jean-Baptiste Perrin confimed this theory experimentally and this contributed toward Perrin's 1926 Nobel prize.

1932 - Langmuir established the existence of monolayers (layers of atoms or molecules one atom thick). These monolayers have peculiar two-dimensional qualities, and led to the development of a totally transparent glass produced by forming a thin film of fluorine compound on the surface. He was awarded the Nobel prize in 1932 for this work on thin films.

1958 - Richard P. Feynman gave a ground-breaking speech: 'There's plenty of room at the bottom'. He discussed the possibility of controlling materials at the level of atoms and molecules. The vision of the possibilities of science and technology at the nanoscale was born. He became a Nobel laureate in 1965.

1974 – Norio Taniguchi of the University of Tokyo coined the term 'nanotechnology' in this year. He used the word to refer to 'production technology to get the extra high accuracy and ultra fine dimensions, i.e. the preciseness and fineness on the order of 1 nm (nanometre)'(On the Basic Concept of "NanoTechnology", [9]

1981 – The Scanning Tunneling Microscope (STM) was invented by IBM scientists, Gerd Binning and Heinrich Rohrer, for which they were awarded the Nobel prize in 1986. This microscope allows atomic-scale three-dimensional profiles of surfaces to be obtained. The microscope relies on a tip that is positioned within 2 nm of the surface and measures the electron density of the surface.

1985 – C_{60}, known as buckminsterfullerene, was discovered by Richard Smalley, Robert Curl and Harold Kroto while investigating the outer atmosphere of stars, for which they were awarded the Nobel Prize in 1996. C_{60} is more commonly known as a buckyball as the 60 carbon atoms are arranged into a sphere made of 12 pentagons and 20 hexagons (exactly like a football).

1990 – Don Eigler, also from IBM, showed that the position of atoms could be controlled precisely. Using the STM he manoeuvred 35 xenon atoms on a nickel surface so that they spelled out 'IBM'. This was achieved at high vacuum and in the supercooled temperature of liquid helium.

1991 – The process to make 'graphitic carbon needles ranging from 4 nm to 30 nm in diameter and 1 micron in length' (*Nature* 354, 1991, 56) was discovered by Sumino Iijima in this year. The needle-like tubes he described consisted of multiple sheets of graphite rolled into hollow tubes, which have now become known as carbon nanotubes. In 1993 the first single-walled nanotubes (SWNT) were produced.

1993 – The first high quality quantum dots were synthesised by Murray, Norris and Bawendi. These dots consisted of nearly monodisperse CdS, CdSe and CdTe (*Journal of the American Chemical Society*, 1993, 115). Quantum dots are very small particles with interesting optical properties: they absorb normal white light and, depending on their size, emit a range of bright colours. This property arises directly from the very small size of the particle.

1997 - In this year the first 'nanotransistor' – a complete metal oxide semiconductor transistor was invented by Lucent Technologies. Being only 60 nm wide and consisting of a source, drain, gate and gate oxide, it improved the key measures of performance. The key advance was being able to fabricate a 1.2 nm thick gate oxide layer. Other companies have since built smaller nanotransistors.

2000 – Lucent technologies in collaboration with Oxford University fabricated the first DNA motor. These devices are similar to motorised tweezers and have the potential to make computers 1 000 more powerful than today's machines. The hope is that DNA motors can be attached to electrically conducting molecules to assemble rudimentary circuits by acting as switches [10].

2001 - Nanohorns, irregularly shaped nanotubes, were developed as fuel cells for hydrogen-based fuel such as methanol. They group together creating a high

surface area ideal for catalysts. NEC Corporation announced that the latest generation weigh less than 2 pounds, when fully fuelled, and power a laptop for 5 hours before needing refuelling.

2002 – Nanoparticles that produce a stain-repellent coating, embedded in clothing, have been developed. Nano-care™ khakis have the fabric fibres coated with nanowhiskers 10–100nm in length. This new stain-repellent fabric is available from a number of high street retailers and is available in trousers, shirts and ties.

2003 – Nanosolar Inc in California fabricated prototype solar cells which use conducting polymers and nano-based particles. This technology has great advantages, compared to that for traditional silicon-based solar cells, including making the products much cheaper and easier to make. These cells are also produced in flexible sheets, making them suitable for many applications.

2004 - Research and development in many nanotechnology fields continues rapidly; some recent developments include the following: Nanospectra Bioscience has used gold-coated nanoshells to destroy cancer tumours in mice (*Cancer Letters*, 209, 171). NanoScale Materials Inc. has developed a family of non-toxic nano-engineered products that counteract a variety of chemical warfare agents and toxic chemicals.

The Future

A plot of the number of publications per year (in the nanotechnology field) over the last 20 years is shown below (Figure 2). It is interesting to note that there has been an almost exponential increase in the amount of papers published over this period of time, showing clearly the immense fascination that nanoscience holds and the increasing realization of the potency of this field of science.
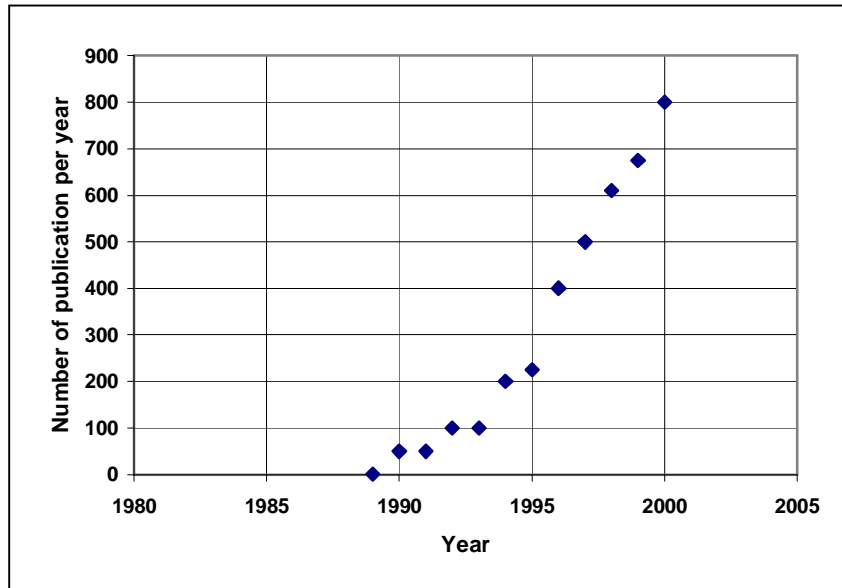
Figure 2: Plot of number of publications per year vs. year for publications in nanoscience.

However over a period of 7 years (Figure 3), the technological advancement whereby reaching smaller and smaller feature sizes has become possible, has only increased linearly.
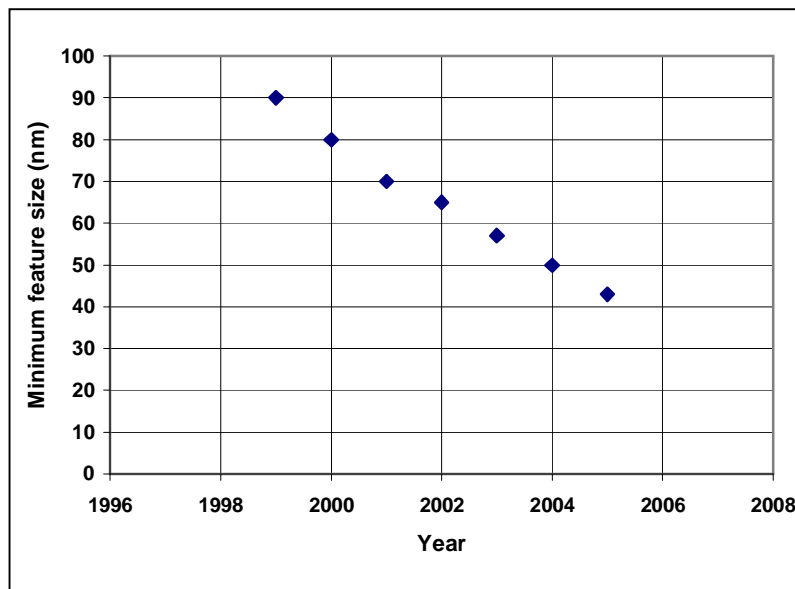
Figure 3: Plot of minimum feature size vs. year

1.2   Purpose of this study

This study's main focus is the development of a theoretical model to calculate an exciton's binding energy for a Quantum Well-Wire structure for different sizes. Although infinite confining potentials are used in this study, the model can easily be modified to account for finite confining potentials. A specific trial wave function is used to achieve comparable results; however any chosen trial wave function is easily compatible in this model. Thus the choice of the trial wave function is at the users' discretion where the economy as well as its qualitative correctness – i.e. how well it describes the physics of the system - of that wave function would be the main parameters to consider when making this choice.

1.3   Layout of the thesis

Chapter 2 introduces the reader to the theory behind low-dimensional structures focusing on the influence on the band structure, density of states and energy curves. Experimentally measured absorption curves for quantum structures are discussed.

Chapter 3 lays the foundation for the mathematical techniques that are used in this dissertation in order to calculate the binding energy of an exciton in a Quantum Well-Wire structure. In particular focus falls on the Variational Approach, the Effective Mass – and Envelope Function Approximations. Insight is also given into atomic units, since these units facilitate an easier approach to the programming aspect of very small numbers.

Chapter 4 shows the theory behind and calculation of the exciton binding energy in a Quantum Well-Wire structure. Emphasis falls on the Hamiltonian of the system, the expectation value of the binding energy, the chosen trial wave function and the solution to the Hamiltonian and thus expectation value when the infinite confining potential boundary conditions are considered. All the relevant mathematical equations are shown, which are solved via numerical techniques. Justification for introducing some

simplifying terms is given in terms of vectors and simplification is done via substitution and differentiation.

Chapter 5 discusses the results of the variational calculation done in Chapter 4 and compares these results with results of calculations done by other authors. A discussion on the effect of the dielectric constants that stems from the results also follows.

A brief conclusion is given in *Chapter 6*.

Appendix A gives all the mathematical details needed to do the calculations of Chapter 4.

Appendix B gives a glossary and definitions of all the terms that are used and relevant to this dissertation.

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Chapter 2

Theory

'Poets say that science takes away from the beauty of the stars. I, too, can see the stars on a desert night, and feel them. But do I see less or more? The vastness of the heavens stretches my imagination – stuck on this carousel my eye can catch one-million-year old light. It does no harm to the mystery to know a little about it.'

- Richard P. Feynman
  The Feynman Lectures on
  Physics

2.1   The Band structure of Quantum Structures

Ever since the invention of the first semiconductor heterostructure-devices there has been a great increase in the variety of applications for these structures for example the first semiconductor lasers were band-engineered by doping (i.e., they were p-n junctions). Since then low-dimensional structures like quantum wells, wires and dots have become very important. They come in various forms: they can be grown by compositional variations in epitaxially grown semiconductor layers by MBE/MOCVD techniques. Nanowires/nanotubes/nanocrystals can be grown by bottom-up approaches (by CVD techniques, or by solution chemistry). [1]

What makes nanostructures so useful is the fact that their band structure (that is the band structure of the constituent bulk semiconductor) can be precisely engineered. The result of such precise engineered band structures are materials with a wide range of applications having the potential to perform functions that are difficult (if not impossible) to achieve in bulk materials such as the semiconductor (diode) laser, to name but one example. Thus an understanding of the band structure of these artificially engineered materials is of great interest.

In order to study the behaviour of an electron in a crystalline solid, the Schrödinger equation is used:

$$H\Psi(\boldsymbol{r}) = E\Psi(\boldsymbol{r})$$

$$\left[-\frac{\mathbf{h}^2}{2m}\nabla^2 + V(\boldsymbol{r}) \right]\Psi(\boldsymbol{r}) = E\Psi(\boldsymbol{r}) \qquad (2.1.1)$$

Here $V(\boldsymbol{r})$ is the crystal potential experienced by the electron, and $\psi(\boldsymbol{r})$ and E are respectively, the state-function/eigenfunction and energy/eigenvalue of this electron. The potential $V(\boldsymbol{r})$ includes the interaction of the electron with all atoms in the solid, as well as its interaction with other electrons. It is important to note that the potential $V(\boldsymbol{r})$ is periodic. Such a potential is shown schematically in Figure 2.1.1
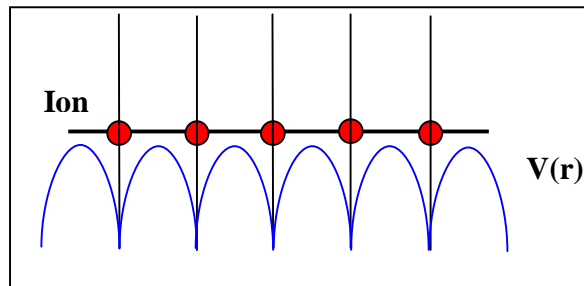
Figure 2.1.1: The periodic crystal potential as experienced by an electron [2]

The **Bloch theorem** gives the solution of (2.1.1) for a periodic potential $V(\boldsymbol{r})$ as [2]

$$\Psi_k(\boldsymbol{r}) = e^{ik\cdot r}u_k(\boldsymbol{r}) \qquad (2.1.2)$$

with $e^{ik\cdot r}$ the envelope function and $u_k(\boldsymbol{r})$ the carrier function. In understanding the band structure in these semiconductor materials the *Effective Mass Equation* for carriers in

bulk semiconductors in the envelope-function approximation needs to be obtained. It thus follows that the *Effective Mass Equation* is:

$$\left[-\frac{\mathbf{h}^2}{2m^*}\nabla^2 + V(\boldsymbol{r}) \right] f(\boldsymbol{r}) = \left[E - E_c(\boldsymbol{r}) \right] f(\boldsymbol{r}) \tag{2.1.3}$$

where the envelope function of carriers in the band under consideration is given by $f(\boldsymbol{r})$. In this form the Schrödinger equation represents an electron in a total potential $V(r) + E_c(r)$, (the band-edge behaviour included) and the difficult problem of an electron moving through a crystal experiencing very complicated potentials is reduced to a textbook-type "particle-trapped-in-a-box" problem.

Now, the true wavefunction (state function/eigenfunction) modelling the particle-like nature of the electrons is given by $\Psi(\boldsymbol{r}) \approx q_{n0}(\boldsymbol{r})f(\boldsymbol{r})$. The periodic crystal potential resulting in periodic Bloch eigenstates is represented by $q_{n0}(\boldsymbol{r})$. However; only the envelope function is needed to find the band structure of the low-dimensional structure! In this lies the power of the envelope function approximation.

2.1.1   Bulk band structure

I)   Pure Semiconductors

To obtain precise results the Schrödinger equation / *Effective Mass Equation* (2.1.1) must be solved for the actual potential *V(r)* in the particular solid of interest. However the process of solving the Schrödinger equation for any but the simplest potentials is a difficult and time-consuming task, submerged with mathematical details. Although this is essential for obtaining results that may be compared with experiments, it is preferable to start the discussion of explicit solutions by using rather simplified potentials. The advantage is that the Schrödinger equation can be solved with only minimal mathematical effort and thus the focus can fall on the new physical concepts involved.

When no external fields are present in the bulk semiconductor, thus having $V(r) + E_c(r) = constant$, the solution to the Shrödinger equation / *Effective Mass Equation* gives **envelope functions** [7]

$$f(\boldsymbol{r}) = \frac{1}{\sqrt{V_{Volume}}} e^{i\bar{\boldsymbol{k}}\cdot\bar{\boldsymbol{r}}} \qquad (2.1.4)$$

and energies

$$E(\boldsymbol{k}) = E_{c0}(\boldsymbol{r}) + \frac{\mathbf{h}^2 \boldsymbol{k}^2}{2m^*} = E_{c0}(\boldsymbol{r}) + \frac{\mathbf{h}^2}{2}\left(\frac{k_x^2}{m_{xx}^*} + \frac{k_y^2}{m_{yy}^*} + \frac{k_z^2}{m_{zz}^*}\right) \qquad (2.1.5)$$

The energy $E(k_x)$ (in one dimension) is plotted versus k_x in Figure 2.1.2 and exhibits a curve in the familiar parabolic shape.
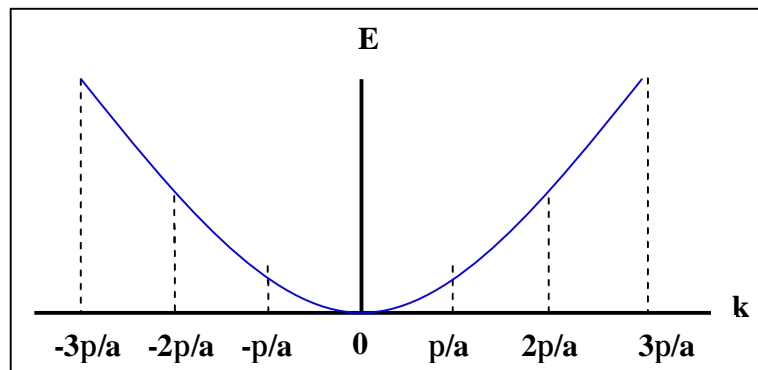
Figure 2.1.2: The parabola representing the dispersion curve for a free particle [2]

It is important to remember that the wavenumbers (k_x, k_y and k_z) are quantized even though they are written as continuous variables. That is

$$k_x = k_y = k_z = \frac{2p}{L_x}m = \frac{2p}{L_y}m = \frac{2p}{L_z}m = \frac{2p}{L}m \qquad (2.1.6)$$

where m = 0, ±1,±2,….

However this quantization is very fine because L is a macroscopic length. Thus for all practical purposes, k can be assumed continuous.

I.I) Density of States (DOS)

When considering electronic processes, like transport phenomena, it is important to find the *number of available states in a certain energy range* in a given band. This is known as the density of states. Denote the density-of-states-function by g(E). Then it is defined as:

g(E)dE = number of electron states per unit volume in the energy range (E, E+dE)

To evaluate *g(E)* the definition is applied: a shell in *k*-space is drawn whose inner and outer surfaces are determined by the energy contours *E(k) = E* and *E(k) = E + dE*, respectively, as shown in Figure 2.1.3. The number of states is then given by the number of allowed *k* values lying inside this shell. When dividing this by the thickness of the shell, *dE*, the desired function *g(E)* is obtained.[2]
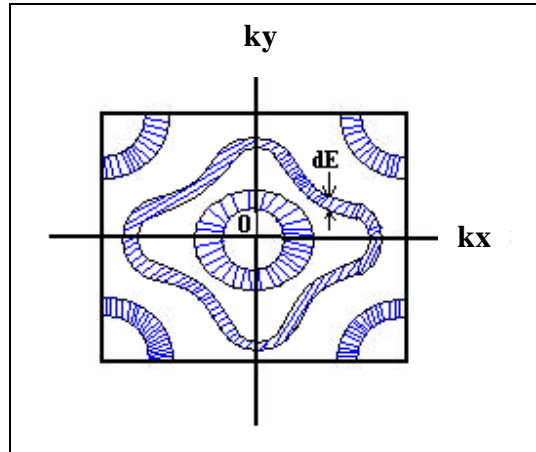
Figure 2.1.3: Concentric shells in k-space used to evaluate the DOS, g(E)[2]

Clearly *g(E)* is closely related to the shape of the energy contours, and hence the band structure. The complexities of this structure are reflected in the form taken by *g(E)*.

I.II)   Calculation of the Density of States

The following discussion is based on general arguments and common assumptions as detailed in Gerald Burns's *Solid State Physics* [4].

In order to calculate the density of states for a semiconductor, begin by assuming that semiconductors can be modelled as an infinite quantum well (not to be confused with Quantum Wells - the heterojunction) and that the material under consideration is a cube with side *L*. Suppose electrons with an effective mass, *m**, are free to move inside this potential well with the energy set to zero inside.

It is important to note that the assumption of a cube with sides L do not affect the result since the DOS per unit volume should not depend on the actual *size* or *shape* of the semiconductor [3].

Now, going back to the textbook-like problem described above, the solution to the wave equation: [4]

$$\frac{d^2y}{dx^2} + \frac{2m^*}{\mathbf{h}^2}(E - V(x))y = 0 \qquad (2.1.7)$$

(where $V(x) = 0$) are sine and cosine functions:

$$\Psi = A \sin(k_x x) + B \cos(k_x x) \qquad (2.1.8)$$

Here A and B are the normalizing terms to be determined. Now the solution is subjected to the boundary conditions that the wave function must have a zero amplitude for $x = 0$ and $x = L$. However, since the cosine function cannot be equal to zero at $x = 0$, it is concluded that $B = 0$. With these boundary conditions, the following possible values for the wavenumber k_x are yielded:

$$k_x = \frac{np}{L}, n = 1, 2, 3.... \qquad (2.1.9)$$

By now repeating this analysis for the y- and z- directions, each possible solution is found corresponding to a cube in $\mathbf{k}$-space with a volume $(n\pi/L)^3$ as indicated in Figure (2.1.4)
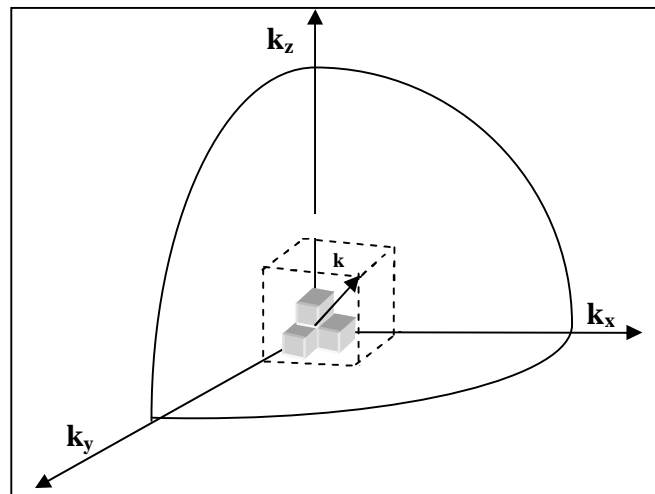
***Figure 2.1.4: Calculating the number of states with wavenumber less than k.
[3]***

With this result it is possible to find the total number of solutions with a different value for k_x, k_y and k_z and with a magnitude of the wave vector less than $\mathbf{k}$. This is done by calculating the volume of one eighth of a sphere with radius k. This result is then divided by the volume corresponding to a single solution $(\pi/L)^3$, giving:

$$N = 2 \times \frac{1}{8} \times \left(\frac{L}{p} \right)^3 \times \frac{4}{3} \times p \times k^3 \tag{2.1.10}$$

Now, keeping in mind that two possible spins exist for each solution, a factor of 2 is added. By using the chain rule the density per unit energy is found as:

$$\frac{dN}{dE} = \frac{dN}{dk} \frac{dk}{dE} = \left(\frac{L}{p} \right)^3 p k^2 \frac{dk}{dE} \tag{2.1.11}$$

Hence dN/dk can easily be found. The kinetic energy E of a particle with mass m^* is related to the wave number, k, by:

$$E(k) = \frac{\mathbf{h}^2 k^2}{2m^*} \tag{2.1.12}$$

So, having $E(k)$ the density of states per unit volume and per unit energy, $g(E)$, becomes:

$$g(E) = \frac{1}{L^3} \frac{dN}{dE} = \frac{8p\sqrt{2}}{h^3} m^{*3/2} \sqrt{E}, \; for \; E \geq 0 \tag{2.1.13}$$

Interesting to note as that the idea of "zero-point energy" is expressed in this equation as the DOS is zero at the bottom of the well (obviously there are no available states for negative energies). Thus there is no available state at $E = 0$. The effective mass takes into account the effect of the periodic potential on the electron. The minimum energy of the electron is the energy at the bottom of the conduction band, E_c (ground state energy), so that the density of states for electrons in the conduction band is given by:

$$g_c(E) = \frac{1}{L^3}\frac{dN}{dE} = \frac{8p\sqrt{2}}{h^3}m^{*3/2}\sqrt{E-E_c}, \, for \, E \geq E_c \qquad (2.1.14)$$

or simplified:

$$g_{3D}(E) = \frac{1}{2p^2}\left(\frac{2m^*}{\mathbf{h}^2}\right)^{3/2}\sqrt{E-E_{c0}} \qquad (2.1.15)$$

Thus the density function, $g(E)$, has a square root dependence of the energy [3].

For the valence band (VB), similar results hold. Here the contributions from the Light and Heavy hole bands only add to give the total DOS.
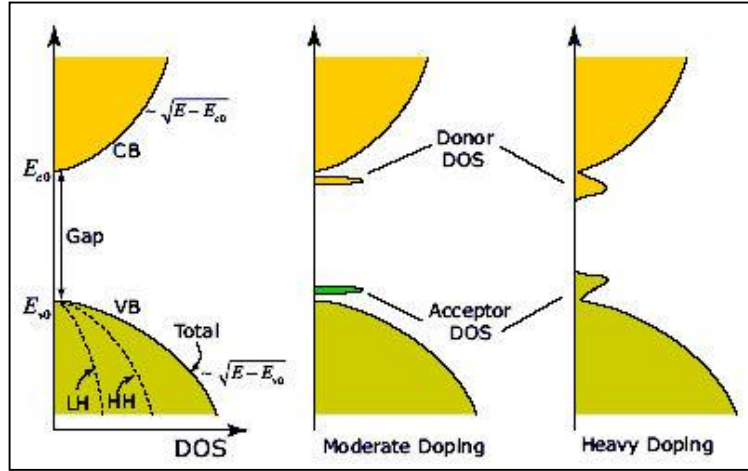
Figure 2.1.5: Density of states of bulk (undoped), moderately doped and heavily doped semiconductors. [1, 2]

II)   Doped Semiconductors

When doping a semiconductor material with impurity atoms, extra energy states are added in the band gap of the semiconductor.   New states close to the band-edges are introduced when a shallow dopant is used. Now, when a shallow donor is used, the effective mass equation is solved via the Hydrogenic model leading to eigenvalues very similar to that of a hydrogen atom. [8]

$$\left[-\frac{\mathbf{h}^2}{2m^*}\nabla^2 - \frac{e^2}{4per} \right] f(r) = (E - E_c)f(r) \tag{2.1.16}$$

The hydrogen atom's eigenvalues are given by $E_n = E_{c_0} - Ry^* / n^2$, where

$$Ry^* = 13.6 \times (m^*)/e_r^{\,2} \tag{2.1.17}$$

is the modified hydrogenic energy levels, and in a similar way, for all practical purposes the donor states are also assumed to be "atomic like", i.e. discrete. Energy separations between these individual atomic-like states are very small.

However during heavier doping, the changes that occur are more significant since the radii of adjacent electrons associated with adjacent donors can overlap. This leads to the formation of impurity bands. When this occurs the semiconductor acquires metal-like properties, because thermal activation of carriers into the bands is no longer necessary for transport. The effects of moderate and heavy doping on the density of states (DOS) of bulk semiconductors are shown in Figure 2.1.5.

2.1.2   Quantum Wells
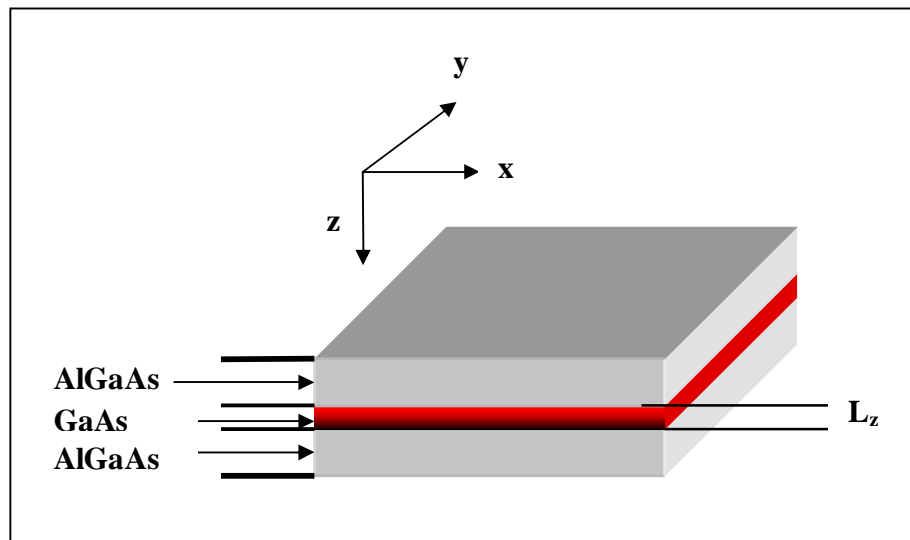
Figure 2.1.6: Quantum Well with x y dimensions infinite and Lz finite [30].

In order to understand the band structure of quantum wells it is important to first realize how these structures are formed. By using at least two different types of semiconductor materials, one of these having a wider band gap, quantum wells are formed upon sandwiching a thin layer of semiconductor between wider band gap barrier layers. When this is the case electrons are free to move unrestricted in the *x-y*-plane but they are

restricted in the z-direction. Hence the conduction band profile will imitate a one-dimensional quantum well. Now in reference to the conduction band edge, E_{c0}, the square-well potential is

$$V(x,y,z) = 0, \ z < 0 \tag{2.1.18}$$

$$V(x,y,z) = 0, \ z > L_z \tag{2.1.19}$$

$$V(x,y,z) = -\Delta E_c, \ 0 \le z \le L_z \tag{2.1.20}$$

From this it is clear that the ***envelope function*** need to be separated into a planar part (x,y - dependant) and a confined part (z - dependant)

$$f_{n_x}(x,y,z) = q(x,y)x_{n_z}(z) = \left[\frac{1}{\sqrt{A_{Area}}} e^{i(k_x x + k_y y)} \right] \bullet [x_{n_z}(z)] \tag{2.1.21}$$

Assuming an infinitely deep potential well, then only waves that satisfy $n_z(\lambda/2) = L_z$ fit into the well of width Lz. So

$$k_{n_z} = \frac{2p}{l} = \frac{p}{L_z} n_z \tag{2.1.22}$$

with $n_z = 1,2,3\ldots$.

This means the z-component of the electron wave number is quantized. Now the z-component of the envelope function (normalized) can be deduced from the textbook-type "particle-in-a-box" problem in quantum physics. This leads to [5]

28

$$z_{n_z}(z) = \frac{2}{\sqrt{L_z}} \sin \frac{p n_z z}{L_z} \qquad (2.1.23)$$

Now, having the envelope function as defined in (2.1.21), the eigenvalues for the *Effective Mass Equation* is easily obtained. The physical interpretation of these eigenvalues is of course the band structure itself

$$E(k) = E_{c0} + \underbrace{\frac{\mathbf{h}^2}{2}\left(\frac{k_x^2}{m^*} + \frac{k_y^2}{m^*}\right)}_{E_{2D}(k_x,k_y)} + \underbrace{\frac{\mathbf{h}^2}{2m^*}\left(\frac{p n_z}{L}\right)^2}_{E_{1D}(n_z)} \qquad (2.1.24)$$

From equation (2.1.24) it is clear that the growth direction of the quantum well (z-direction) plays a significant role, in the characteristics of the energy band. A quantized component in the z-direction exists, contrast to the "free" electron component in the x-y-plane. The influence of this is very significant in the band structure. It decomposes the band structure into multiple bands, E_{2D} (k_z, k_y) (quasi-continuous in the x-y – plane and discrete in the z-direction). These bands are indexed by the quantum number n_z, as shown in Figure 2.1.7.
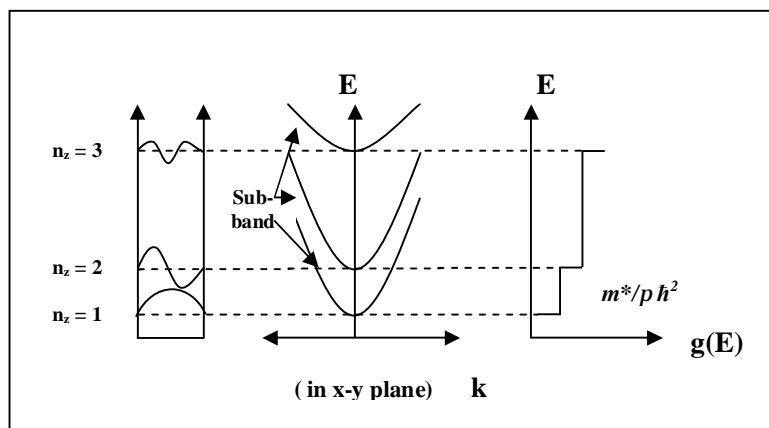
Figure 2.1.7: Band structure and DOS of realistic hetero-structure quantum wells [1].

I)   DOS

When electrons confined in an ideal two dimensional plane (2D - plane) are considered, the DOS is constant and given by: [3]

$$g_{c,2D}(E) = \frac{dN_{2D}}{dE} = \frac{4pm^*}{h^2} = \frac{m^*}{p\mathbf{h}^2} \qquad (2.1.25)$$

Now, knowing this, and knowing that each sub band (corresponding to the quantum number n_z) in the quantum well is an ideal 2D system (thus each sub band has a $g_{c,2D}(E)$ contribution to the total DOS) the DOS of the quantum well is:

$$g_{QW}(E) = \frac{m^*}{p\mathbf{h}^2} \sum_{n_z} q(E - E_{n_z}) \qquad (2.1.26)$$

As shown schematically in Figure 2.1.7

Here $q\left(E - E_{n_z}\right)$ is the Heaviside unit step function.

In light of the above, a discussion on the influence of the confining potential $V(z)$ is appropriate. Via modern epitaxial techniques the spatial changes in the material composition can be engineered almost at will. Thus different forms of confining potentials can easily be applied. For example the parabolic potential ($V(z) \sim z^2$) leads to E_{n_z} values spaced in equal energy intervals which is a characteristic of a square or Harmonic Oscillator potential. For triangular potentials ($V(z) \sim z$) the E_{n_z} values are given by Airy functions. However the band structure and DOS is not influenced by the specific

choice of a confining potential, i.e. is not dependent on the *shape* of the confining potential, as it remains similar to the square well, case [1]. Thus the only modification will be on the E_{n_z} E_{nz} values and the corresponding subband separations.

2.1.3   Quantum Wires
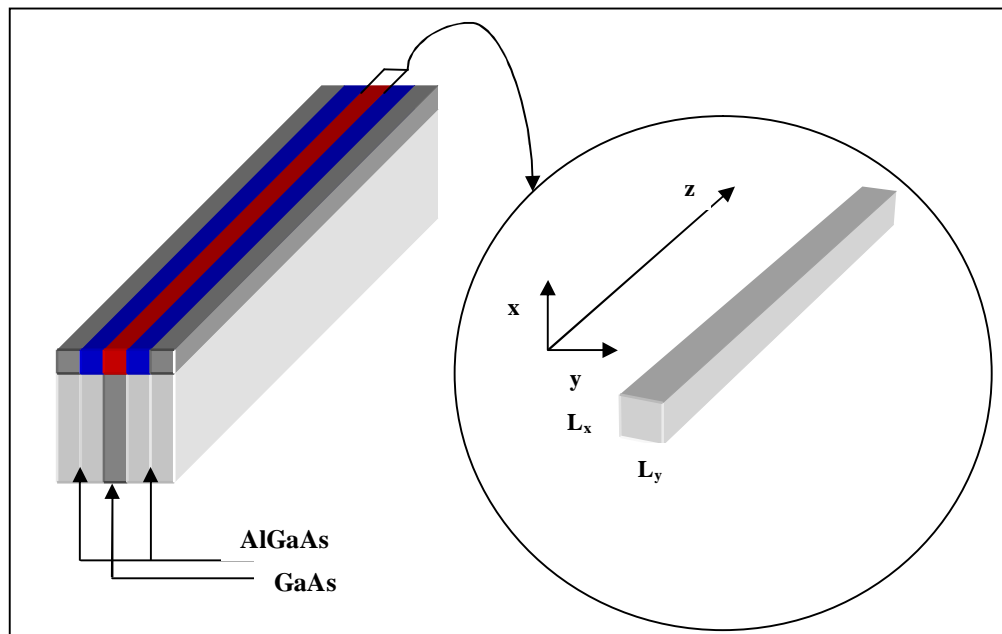
Figure 2.1.8: Quantum Wire with Dimensions z infinite and L_x, L_y finite [30].

There are two approaches for forming quantum wires (as is also the case with quantum wells): the top-down approach or the bottom-up approach. In the top-down approach quantum wires are formed lithographically. In the bottom-up approach quantum wires are formed via direct growth in the form of semiconductor nanowire/nanotubes. Whichever approach is preferred, both have the same goal*:   to confine the real space movement of carriers in two dimensions, leaving only one dimension free for carrier movement* – hence the name "wire".

With this in mind, assume that the length of the wire (L_z) along the *z*-axis is the one degree of freedom where carriers are unconfined/free to move unrestricted. Let the

x-y – plane be the two degrees of freedom where the carriers are quantum confined. Thus (L_z, L_y << L_z). Then it is easy to see that the ***envelope function*** must decompose into:

$$f(x, y, z) = z_{n_x}(x) \bullet z_{n_y}(y) \bullet \left(\frac{1}{\sqrt{L_z}} e^{ik_z z} \right) \qquad (2.1.27)$$

with the z-part of the envelope function the same as that given by equation (2.1.4) and the x and y parts representing the quantum confinement in the x-y – plane. From this the energy eigenvalues are

$$E(n_x, n_y, k_z) = E(n_x, n_y) + \frac{\mathbf{h}^2 k_z^2}{2m_{zz}^*} \qquad (2.1.28)$$

If again an infinite confining potential is assumed in the x-y – plane (as is often done in quantum wire calculations) then the condition holds that the only waves that will satisfy $n_{x,y}(\lambda_{x,y}/2)=L_{x,y}$ (respectively) will fit into the wire of length L_z. This naturally leads to

$$k_{n_x} = \frac{p}{L_x} n_x \qquad (2.1.29)$$

$$k_{n_y} = \frac{p}{L_y} n_y \qquad (2.1.30)$$

where $n_x, n_y = 1, 2, 3, \ldots$ independently.

So now, as before, by using the simple "particle-in-a-box" – problem in quantum physics the functions $z_{n_x}(x)$ and $z_{n_y}(y)$ are easily obtained and hence the eigenfunctions are:

$$f_{n_x,n_y}(x,y,z) = \underbrace{\left[\sqrt{\frac{2}{L_x}}\sin\left(\frac{pn_x}{L_x}x\right)\right]\cdot\left[\sqrt{\frac{2}{L_y}}\sin\left(\frac{pn_y}{L_y}y\right)\right]}_{2D\ \text{Confined Part}}\cdot\underbrace{\left[\frac{1}{\sqrt{L}}e^{ik_x x}\right]}_{1D\ \text{Free Part}} \qquad (2.1.31)$$

Consequently the corresponding band structure is given by:

$$E(n_x,n_y,k_z) = \underbrace{\left[\frac{\mathbf{h}^2}{2m_{xx}}\left(\frac{pn_x}{L_x}\right)^2\right]+\left[\frac{\mathbf{h}^2}{2m_{yy}}\left(\frac{pn_y}{L_y}\right)^2\right]}_{E(n_x,n_y)}+\underbrace{\left[\frac{\mathbf{h}^2 k_z^2}{2m^*}\right]}_{E(k_z)} \qquad (2.1.32)$$

Again, similar to quantum wells, subbands are formed, however in quantum wires *multiple* subbands are formed at each eigenvalue $E(n_x, n_y)$, spread out as $\hbar^2 k_z^2/2m_{zz}$. This is shown in Figure 2.1.9.
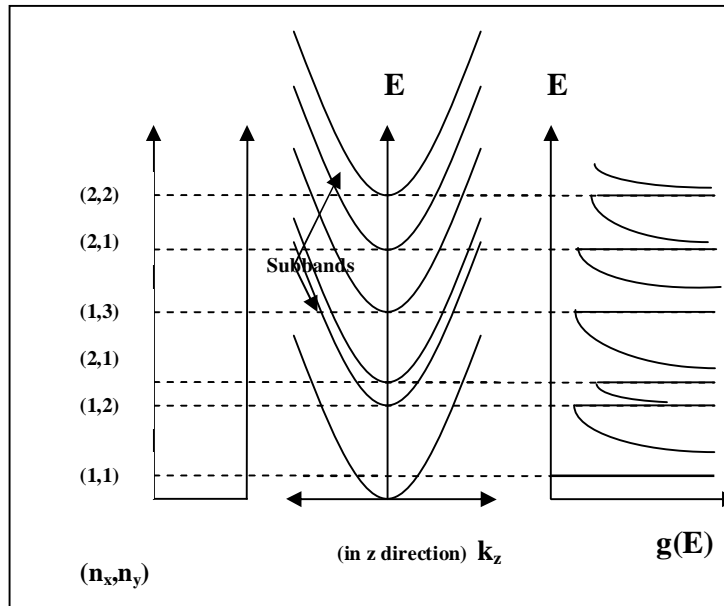
Figure 2.1.9: Band structure and density of states of Quantum Wires [1]

I)   DOS

When electrons confined in an ideal one dimensional line (*1D* -line) are considered, the DOS is given by:

$$g_{c,1D}(E) = \frac{dN_{1D}}{dE} = \sqrt{\frac{2pm^*}{h^2}}\frac{1}{\sqrt{E-E_{min}}} = \sqrt{\frac{m^*}{2p\mathbf{h}^2}}\frac{1}{\sqrt{E-E_{min}}} \qquad (2.1.33)$$

with E_{min} being the ground state energy. Thus the general DOS for a quantum wire can be written as:

$$g_{QWire}(E) = \sqrt{\frac{m^*}{2p\mathbf{h}^2}}\sum_{n_x,n_y}\frac{1}{\sqrt{E-E(n_x,n_y)}} \qquad (2.1.34)$$

Now because of the multiple subbands, the DOS has peaks at every eigenvalue $E(n_x,n_y)$. Eigenvalues can also be degenerate due to there being two quantum numbers involved. This is where the difference between Quantum Wells and Wires lie; since this can lead to peaks occurring at irregular intervals, different to Quantum Wells. This is also shown in Figure 2.1.9

2.1.4   Quantum Dots
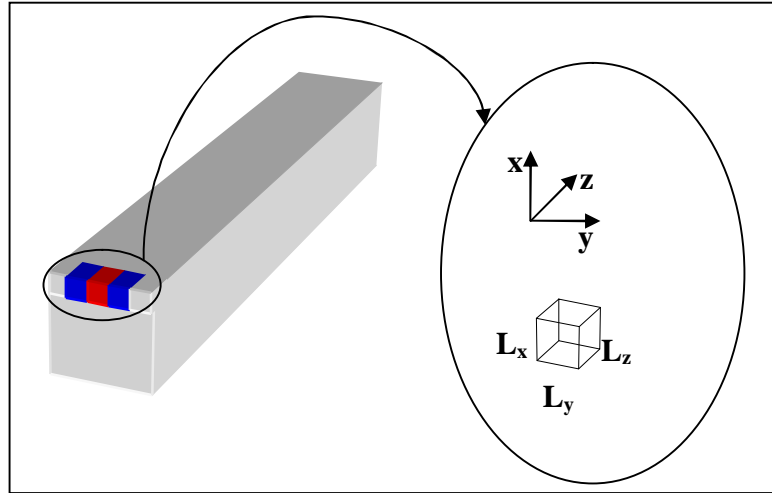
Figure 2.1.10: Quantum Dot with dimensions L_x, L_y and L_z finite [1,7]

In a quantum dot, all three degrees of freedom are quantum confined. Thus the *envelope function* can be written as

$$f(x, y, z) = z_{n_x}(x) \bullet z_{n_y}(y) \bullet z_{n_z}(z) \tag{2.1.35}$$

Now suppose that the three sides of the "quantum box" are given by L_x, L_y and L_z, and that the confining potential is infinite, as was the case for the Quantum Well and Wire. This leads to only waves satisfying the following condition that are allowed in the "quantum box":

$$k_{n_i} = \left(\frac{p}{L_i}\right) n_i \text{ for } i = x, y, z \tag{2.1.36}$$

With this in mind and again using the "particle trapped in an infinite well potential" –
problem in quantum physics, the ***envelope function*** is found to be:

$$f(x, y, z) = \left[\sqrt{\frac{2}{L_x}} \sin\left(\frac{p n_x}{L_x}\right) \right] \bullet \left[\sqrt{\frac{2}{L_y}} \sin\left(\frac{p n_y}{L_y}\right) \right] \bullet \left[\sqrt{\frac{2}{L_z}} \sin\left(\frac{p n_z}{L_z}\right) \right] \quad (2.1.37)$$

This leads to the energy eigenvalues having the form:

$$E(n_x, n_y, n_z) = \frac{\mathbf{h}^2}{2m_{xx}} \left(\frac{p n_x}{L_x}\right)^2 + \frac{\mathbf{h}^2}{2m_{yy}} \left(\frac{p n_y}{L_y}\right)^2 + \frac{\mathbf{h}^2}{2m_{zz}} \left(\frac{p n_z}{L_z}\right)^2 \quad (2.1.38)$$

From equation (2.1.36) it is clear that the quasi-continuous nature of the semiconductor
(and therefore also the band structure) is no longer present at all in quantum dots, since
the energy eigenvalues are now indexed by three quantum numbers (n_x, n_y and n_z).

I)   DOS

Since band structure is no longer a term that has any relevance in a quantum dot, the DOS
is now a sum of delta functions, written as:

$$g_{QDot} = \sum_{n_x, n_y, n_z} d(E - E_{n_x, n_y, n_z}) \quad (2.1.39)$$

This is clear if we consider the following: There is *no* direction of free motion within the
quantum dot and therefore *no* transport *within* a quantum dot. Hence there are no quasi-
continuous momentum components. All this can be seen in Figure 2.1.11.
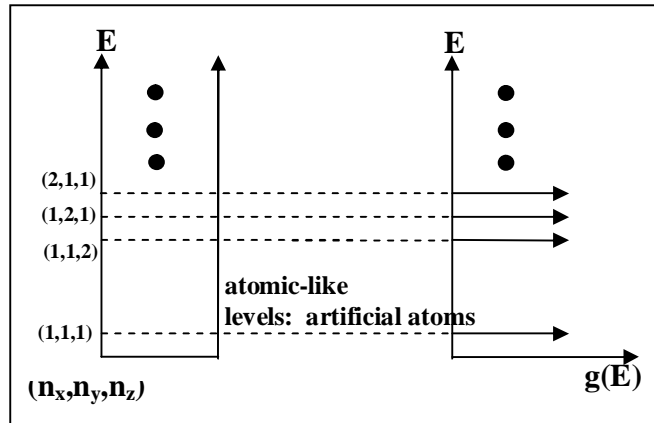
Figure 2.1.11: Energy levels and DOS of a Quantum Dot [1]

To summarize a comparison between the DOS for a bulk semiconductor, quantum well, quantum wire and quantum dot is presented in figure 2.1.12.
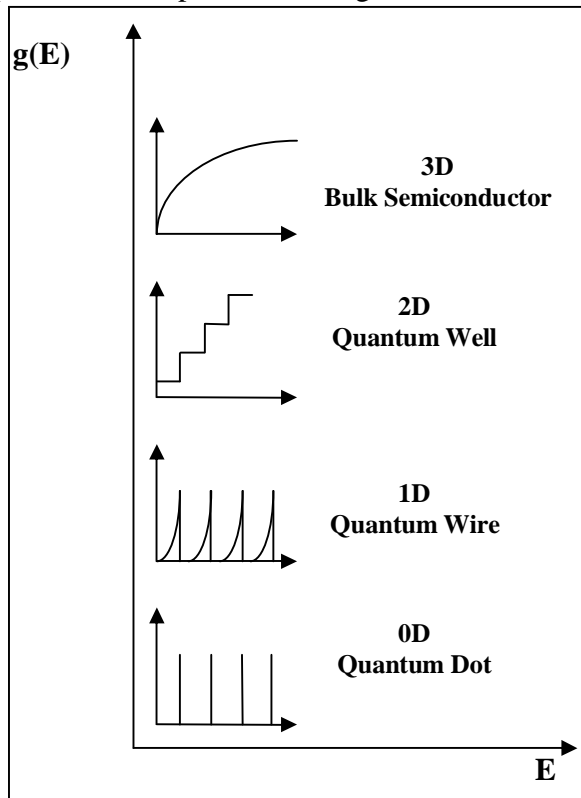
Figure 2.1.12: Comparison between DOS for Low-Dimensional structures [6]

2.2 Size Dependant Behaviour of Quantum Structures/Optical Properties of Quantum Structures

In order to understand that which will follow this section more clearly, a discussion on the energy levels of a quantum structure, in specific a zero-dimensional solid, i.e. a semiconductor Quantum Dot, will now follow. Though the results here can be equally applied to the semiconductor Quantum Well and Wire cases, this section focuses on the extreme case where all 3 spatial dimensions are diminished in order to arrive at an oversimplified model for the energy levels of a Quantum Dot in order to understand the most relevant physics best and so that it may act as a guide to the understanding of these low-dimensional structures.

It is a well known fact that the dispersion relations for the energy of electrons and holes in a semiconductor are parabolic at first approximation [see for example [2] and other similar sources]. This approximation is true only for electrons and holes that occupy the levels that lie at the bottom and top of the conduction and valence bands respectively. It is important to remember that these parabola are really a *quasi-continuous* set of electron (hole) states along a given direction in k-space and that the lowest occupied level in the CB and the highest occupied level in the VB are separated by an energy gap, which for bulk materials are usually in the order of a fraction of an eV to a few eV.

When the dimensionality of the semiconductor bulk material is reduced in size to a zero-dimensional Quantum Dot the quasi-continuous nature is emphasized, since (as was shown in Section 2.1) only discrete energy levels can exist in the dot. So now each of the original parabolic bands of the bulk case is fragmented into an ensemble of points.

Bulk Semiconductor
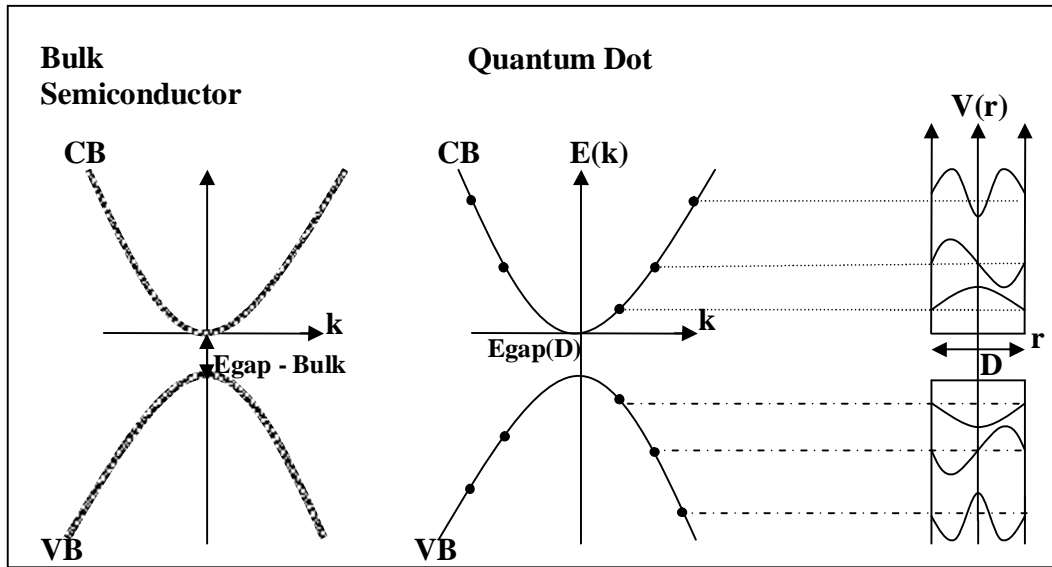
Quantum Dot

Figure 2.2.1: Energy Dispersion for the 3D bulk semiconductor case compared to that of the 0D Quantum Dot case [28]

In order to find a relatively good estimate for these energy levels in a Quantum Dot the textbook type "particle-in-a-box" – model is used. By applying the proper boundary conditions to a Schrödinger equation for a particle in a 1D box (trapped in an infinite potential well where $V(x) = 0$ inside the well and $V(x=L) = \infty$ at the boundaries), the solutions are stationary-waves with energies [19,20]

$$E_{n_x} = \frac{\mathbf{h}^2 k_x^{\ 2}}{2m} = \frac{h^2 k_x^{\ 2}}{8p^2 m} = \frac{h^2 n_x^{\ 2}}{8mL_x^{\ 2}} \quad \text{with } n_x = 1, 2, 3 \tag{2.2.1}$$

Thus the ground state energy for an electron in a 1D potential well is:

$$E_{1D-Well} = \frac{1}{8} \frac{h^2}{mL_x^{\ 2}} \tag{2.2.2}$$

Now applying similar boundary condition for infinite 3D potential wells remain. However the shape of this confining potential now influences the solution of the appropriate 3D Schrödinger-equation. If a cubic shape is assumed, the Schrödinger equation can be solved independently for each of the three translational degrees of freedom. Thus the overall ground state energy will simply be the sum of the individual zero point energies for each degree of freedom [19,22]:

$$E_{3D-Cube} = 3 \times E_{1D-Well} = \frac{3}{8} \frac{h^2}{mL^2} \qquad (2.2.3)$$

If however, the 3D potential well is a sphere with a diameter D, then the solution to the Schrödinger-equation involves the introduction of spherical coordinates and the separation of the radial- and angular momentum- parts. The ground state energy (corresponding to an angular momentum = 0) will now be given by:

$$E_{3D-Well} = \frac{1}{2} \frac{h^2}{mD^2} \qquad (2.2.4)$$

And so from this it is clear that the *shape* (or put more accurately: the volume) of the confinement potential will play a significant role in the energy-dispersion: *the smaller the confinement-volume, the higher the ground state/zero point energy will be*. (Note that in this oversimplified model, the effects of a finite confining potential, i.e. *V(x,y,z)≠∞*, has not even been considered!) So this gives the zero-point energy for a particle trapped in confined space.

Now the following need to be considered: the only way an electron can fill up an energy state in the conduction band (CB) is if it is excited to the CB from the valence band (VB). This leaves behind a hole in the VB. Now due to the fact that both these carriers have charges, they will interact via the Coulomb force. However, even before that is considered the amount of energy needed to excite the electron to the CB (which is equal to the energy gap) must also be taken into account. And then it must be considered that both carriers are confined in the 3D potential well, thus requiring that equation (2.2.4) for a spherical Quantum Dot be written as [28]:

$$E_{3D-Well} = \frac{1}{2}\frac{h^2}{mD^2} \qquad (2.2.5)$$

Where μ is now the reduced mass of the exciton (see section 2.3). Now considering the Coulomb interaction between the electron and the hole and also taking into account the screening by the rest of the crystal, a binding energy term can be *estimated* as:

$$E_B = -1.8\frac{e^2}{2pee_0D} \qquad (2.2.6)$$

where the dielectric constant, ε, gives and indication of the strength of the screening coefficient.

From equation (2.2.6) it is clear that the binding energy is size dependant. For very large Quantum Dots ($D \rightarrow \infty$) the E_b plays an almost insignificant role. However, the smaller the diameter of the Dot, the larger the role of the binding energy term will be. It is this role that will be investigated more fully further in this dissertation.

So now an estimate of the size dependence of the **energy gap** of a *spherical* Quantum Dot can be made [22 - 27]:

$$E_{G-Dot} = E_{G-Bulk} + E_{3D-Well} + E_B$$

$$E_{G-Dot} = E_{G-Bulk} + \frac{h^2}{2mD^2} - 1.8 \frac{e^2}{2pee_0 D} \qquad (2.2.7)$$

It was already pointed out the *shape* of the confining potential plays a significant role (as it will be the key factor contributing to the confinement volume). From equation (2.2.7) it can be seen that the *size* of the confining particle (in this case a Quantum Dot) also plays a very significant role in the band gap energy. However it must be clearly stated that equation (2.2.7) is only a first approximation as many effects, such as crystal anisotropy and the spin-orbit coupling have been neglected, to name but a few [28].

It is interesting to note the play off between the binding energy, E_B, and the confinement energy, $E_{3D\text{-}Well}$, in these low-dimensional systems. The confinement energy is always positive and thus the ground state's energy is always *raised* with respect to the bulk situation. The binding energy is however always negative and therefore tends to *lower* the ground state energy. The scaling for the confinement and binding energies are *1/D²* and *1/D* respectively. [28]
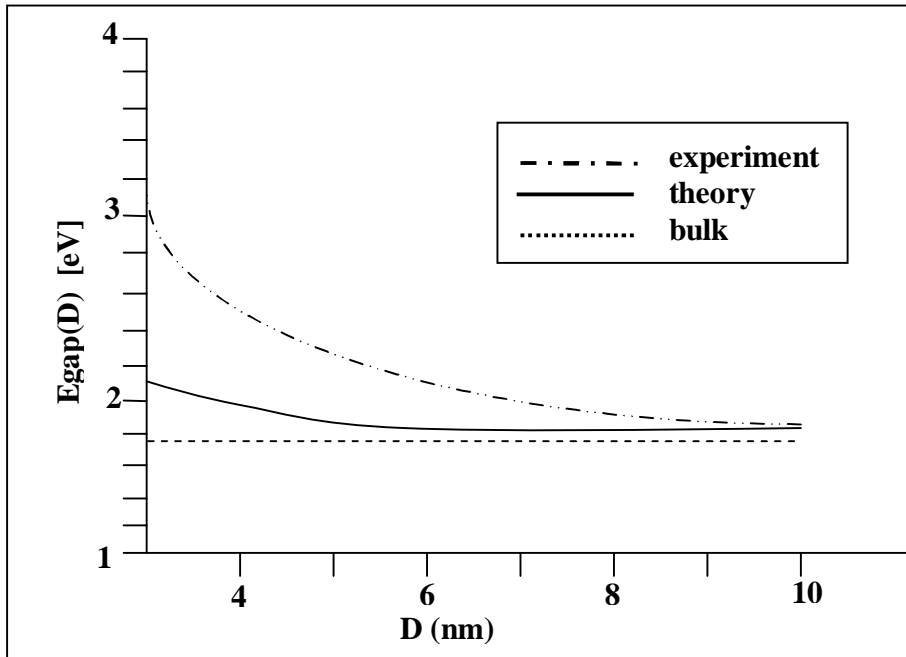
Figure 2.2.2.: Energy gap as a function of size for a colloidal CdSe quantum dot with a diameter D [28].

2.3   Excitons in Quantum Structures

Even though excitonic states have been known to exist since 1931, the last three decades have seen extensive investigation on excitonic states in *low-dimensional systems* [9 - 11]. Pioneers in this field are Frenkel, Wannier, Pikus, Lozovik, Peierls and Elliot [e.g. 12]. The main reason for the investigation into excitonic states in low-dimensional structures is as follows: for bulk materials the binding energy is very low and such states can only be observed in very pure materials. Hence it is usually used for characterization. In poorer quality samples these states merge with band-to-band transitions. However, in low-dimensional structures, the binding energy increases due to the quantum confinement effect. The oscillator strength also increases. This leads to sharp excitonic transitions. [13] *The excitonic effect thus **dominates** the absorption spectrum around the band gap for these low-dimensional systems* [14].

2.3.1 What is an Exciton?

An exciton is a composite of an electron and a hole due to the mutual Coulomb attraction. These objects are rare and rather unstable due to their extremely short lifetime. When energy is absorbed in a bulk semiconductor by an electron, an exciton is formed /created when a covalent bond is broken. This is usually achieved via incoming light (normally by laser)

2.3.2 Optical Properties of Excitons

The creation process of the electron-hole-pair is *local*: one photon is giving its energy to one localized electron (between two atomic sites) and the empty place where the electron was sitting would formally be treated as a hole. The energy needed to break the covalent bond is exactly the band gap energy E_G. Now once the electron has left the valence band by being excited into the conduction band, the remaining hole has a net positive charge. Hence a Coulombic interaction between these two components can be expected [13]. This is the exciton binding energy, E_B, and is *negative* as it should be for any bound system. Now, considering the fact that the electron need to be excited across the band gap (from the VB to the CB in a semiconductor), the required photon energy must be at least equal to E_G. However since the electron will now be bound to the hole (and vice versa) this required energy is *lowered* by the exciton binding energy. Thus the required transition energy, E, for the photon to create a bound exciton in a bulk material is given by:

$$E = h\nu = E_G + E_B(n) \tag{2.3.1}$$

where the binding energy, E_B, is a function of the principal quantum number
$n = 1,2,3...$
This energy would correspond to the position of an absorption peak in optical experiments.
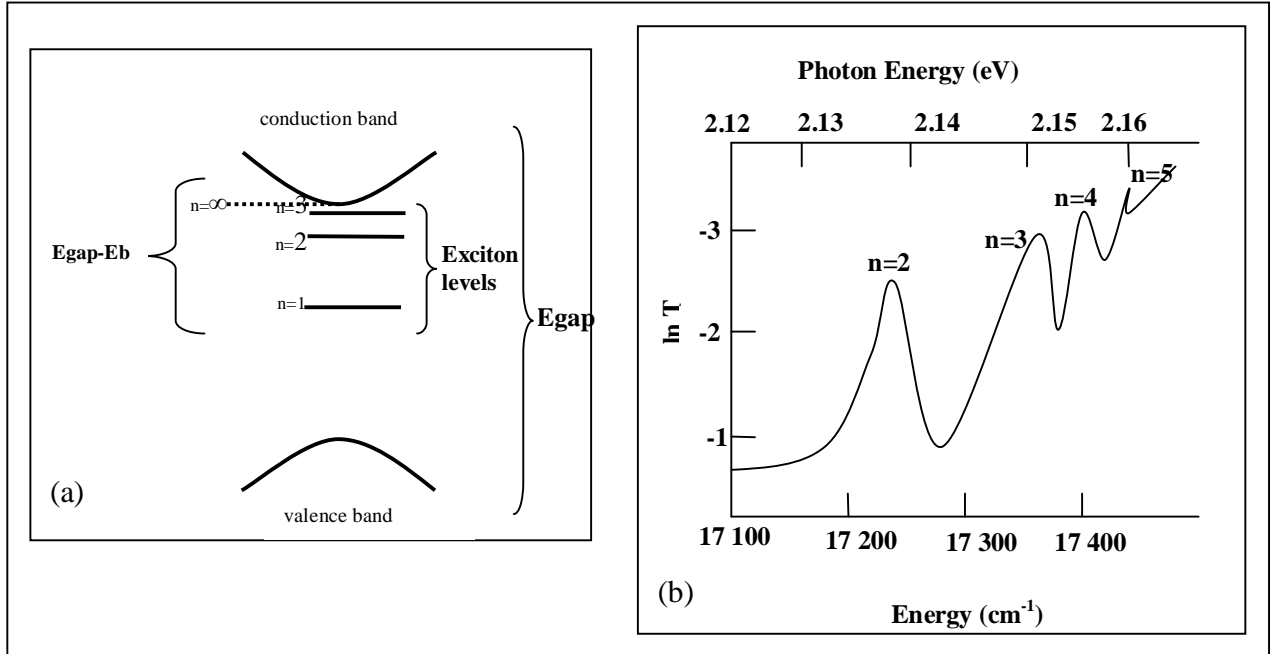
Figure 2.3.1: (a) The energy level diagram of an exciton in a direct band gap material. (b) Excitons in Cu_2O (T is the transmission) [15,16]

Thus, from figure 2.3.1., as in the Hydrogen atom, the Coulomb attraction forms bound levels of the exciton with the lowest-energy bound state characterized by the effective Rydberg energy Ry^* and the effective Bohr radius a_0*, which is for the 3D case:

$$a_0 = \frac{em_0}{m}\frac{4p\mathbf{h}^2e_0}{m_0e^2} = \frac{em_0}{m}a_B \tag{2.3.2}$$

(with ε the dielectric constant of the material, m_0 the electron mass and μ the reduced mass given by

$$m = \frac{m_e^*m_h^*}{(m_e^* + m_h^*)} \tag{2.3.3}$$

(m_e* and m_h* the effective masses of the electron and hole respectively) and a_B the Bohr radius of the Hydrogen atom [16]), and the Rydberg energy:

$$Ry^* = \frac{m}{e^2 m_0} Ry$$

(2.3.4)

with the Hydrogen Rydberg, $Ry = 13.6$ eV and the Hydrogen Bohr radius, $a_B = 52.9$ pm. So it follows that the exciton binding energy is given by.

$$E_B = -\frac{Ry^*}{n^2}$$

(2.3.5)

leading to the exciton energy levels given in the semiconductor given by:

$$E(n) = E_G + E_B$$

(2.3.6)

Now to see the importance of the excitonic effect in semiconductor absorption effect, remember that the absorption coefficient is usually given by [2]:

$$a(hn) = A\sqrt{(hn - E_G)}$$

(2.3.7)

Thus the absorption coefficient increases parabolically with the frequency (energy) above the fundamental edge.
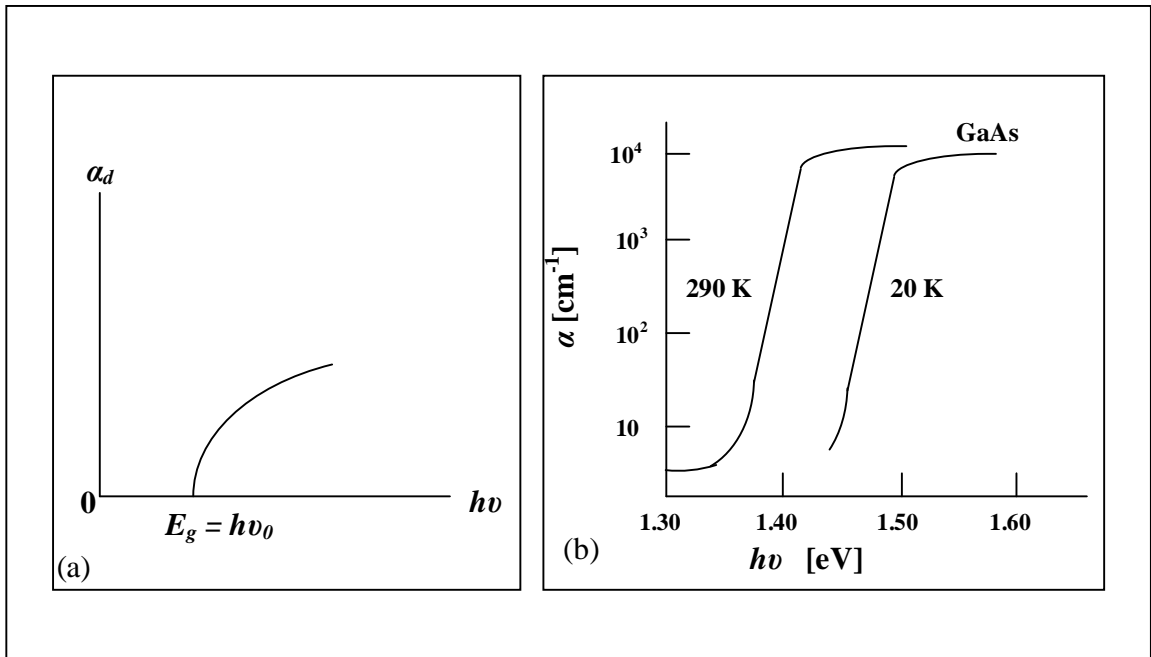
Figure 2.3.2 (a) The parabolic shape of an absorption spectrum in a semiconductor due to the square root dependence on energy (b) The absorption coefficient versus the photon energy as measured for GaAs [2]

However, once the excitonic effect is taken into account a modification to the absorption coefficient as given by equation (2.3.7), is in order. This is done by multiplying with a Sommerfeld factor which takes the Coulomb interaction of the electron-hole pair into account:

$$a(hn) = A\sqrt{hn - E_G} \; F(hn - E_G) \qquad (2.3.8)$$

with $F(hv - E_G)$ the Sommerfeld factor defined as follows: [17]

$$F(E) = \frac{2p}{\sqrt{E/E_B}} \frac{1}{1 - \exp(-2p/\sqrt{E/E_B})} \tag{2.3.9}$$

which leads to

$$F(E) = \frac{2p}{\sqrt{E/E_B}} \quad \text{for} \ E \ll E_B \tag{2.3.10}$$

and

$$F(E) = 1 \ \text{ for } \ E \gg E_B \tag{2.3.11}$$

Thus following is a representation of the absorption spectra for a *3D* exciton with and without the excitonic effect
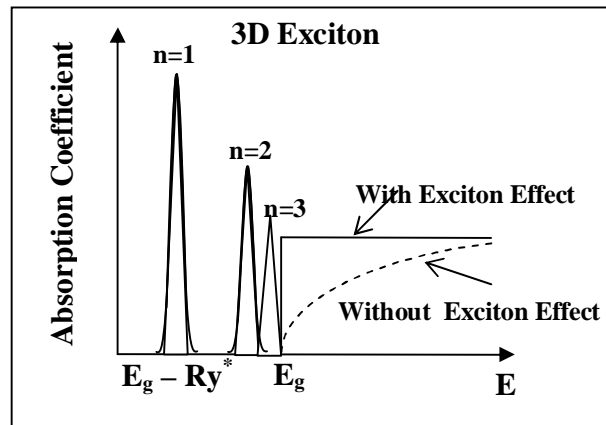
Figure 2.3.3: Absorption spectra for 3D (bulk) Excitons [14]

As can be seen from Figure 2.3.3, as a result of the Coulomb interaction between electrons and holes, the absorption coefficient is enhanced from its value by the Sommerfeld factor. The above is a representation of what happens in a bulk semiconductor material. It is thus clear that the exciton effect plays a very important role in the absorption spectra of semiconductors and therefore much attention need to be paid

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to it. But what happens once one dimension of the bulk material is made to "vanish", i.e. when the semiconductor becomes a Quantum Well?

Both the electron and the hole (therefore the exciton as a whole) become trapped inside a *2D* quantum "box". This means that their wave functions will be localized in a specific region in space, in 1 dimension and, depending on the confining potential, will not be likely to tunnel through to other regions. As a result of the electron and hole being "forced" together in a relatively small region in space (usually in the order on nm) their mutual attraction will also be increased as the discrete energy levels are "forced" to adapt to this confining potential which was not present in the bulk semiconductor case. Thus the binding energy of the exciton is increased with respect to the bulk semiconductor material. This binding energy can be estimated from the Hydrogen atom model to give a fair approximation of this value, however special emphasis should be placed on the fact that it is only an *approximation*! The true binding energy value for these excitons will be a function of the dimension parameters of the low-dimensional structure. Thus, by using the Hydrogen atom model, the required photon energy will be:

$$E(n,m) = E_G + E(n) - \frac{Ry^*}{(m+0.5)^2} \quad \text{with} \quad m = 0,1,2,3,.... \quad (2.3.12)$$
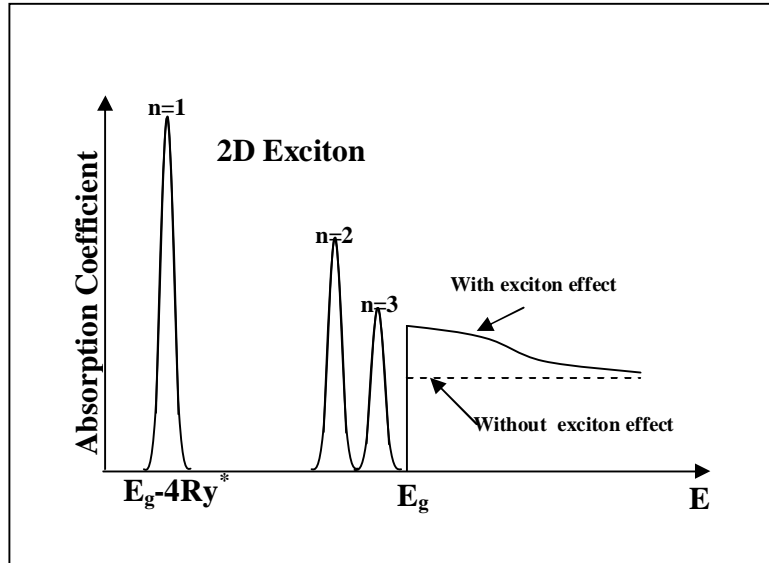
Figure 2.3.4: Absorption spectra for 2D excitons showing the presence and absence of the excitonic effect. [14]

What has happened now is this: The *2D* exciton wave function has shrunk in the 2D plane, making its radius $(\sqrt{3/4})a_0^*$. So, when this is compared to the *3D* case, there is an enhanced overlap between the electron- and hole- wave functions. Thus the oscillator strength of a *2D* exciton is larger that that of a *3D* exciton:

$$f_n^{2D} = \frac{n^3}{\left(n+0.5\right)^3} a_0^* f_n^{3D} \qquad\qquad (2.3.13)$$

Here f_n^{3D} is the oscillator strength of the nth *3D* exciton. *Now the enhancing of the binding energy and the oscillator strength leads to the stability of the excitons, causing them to be present even at room temperature* [14].

Thus far only semiconductor bulk material and semiconductor Quantum Wells have been discussed. However for the Quantum Wire, something very different happens. Unlike in the previously two mentioned cases the effect of the quantum confinement on the

Sommerfeld factor is to *lower* this value: the correlated absorption spectra of realistic Quantum Wires show a strong quenching of the *1D* single-particle singularity. The Sommerfeld factor, which is greater than unity in the bulk and in Quantum Wells (Coulomb enhancement), is instead smaller than unity in Quantum Wires (Coulomb-induced suppression), thus reducing the influence of dimensionality on the optical spectra. The excitonic-corrected absorption above the band edge is decreased from the non-interacting case, i.e., the Sommerfeld factor is negative here. This can be understood if it is considered that for strictly *1D* systems in the non-interacting case the absorption is diverging at the edge. Rather than considering the *1D* case as special with respect to the 2D or 3D case, interpret this as the excitonic effect leading the absorption coefficient (above the continuum edge) to behave in a way which is basically independent of the dimensionality [17].
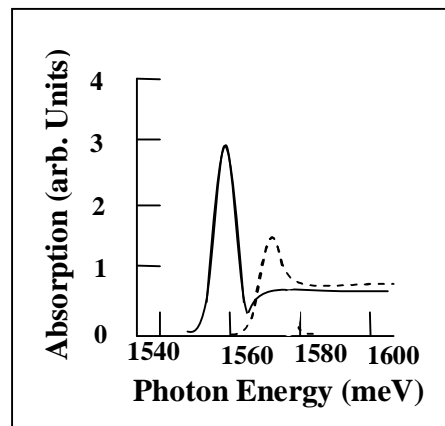
Figure 2.3.5: Calculated absorption spectra for a V-grooved Quantum Wire. The dashed line is for single-particle calculations. The full line is the results where the electron-hole correlations are included [18]

2.3.3 Effect of decrease in size and dimensionality on Excitons
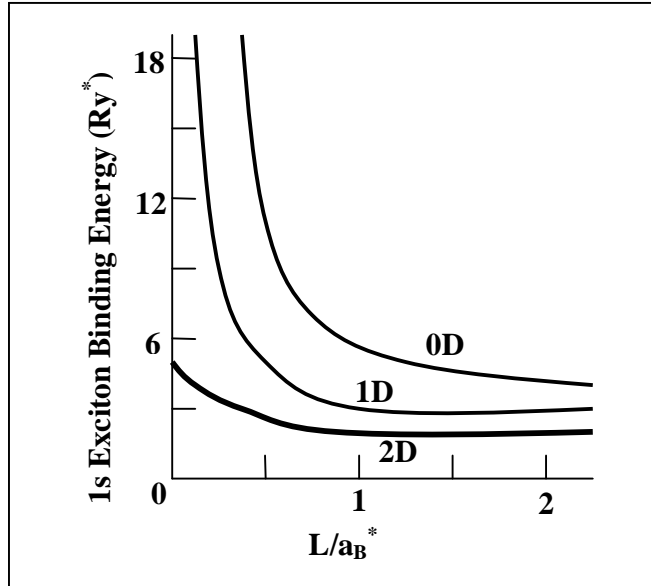
***Figure 2.3.6: A decrease in size and dimension of quantum structures lead to
an increase in binding energy [14]***

Figure 2.3.6 shows the effect of a decrease in the dimensional size for respectively a
Quantum Well (*2D*), Wire (*1D*) and Dot (*0D*). Both the binding energy and the oscillator
strength of an exciton increase with a decrease in size and dimensions. The effect on the
radiative lifetime ($\tau_{\text{Radiative}}$) for these different low-dimensional structures is as follows:

$$t_{Radiative} \propto \frac{1}{f} \tag{2.3.14}$$

with *f* the oscillator strength. Thus $\tau_{\text{Radiative}}$ decreases with a decrease in size and
dimensionality.
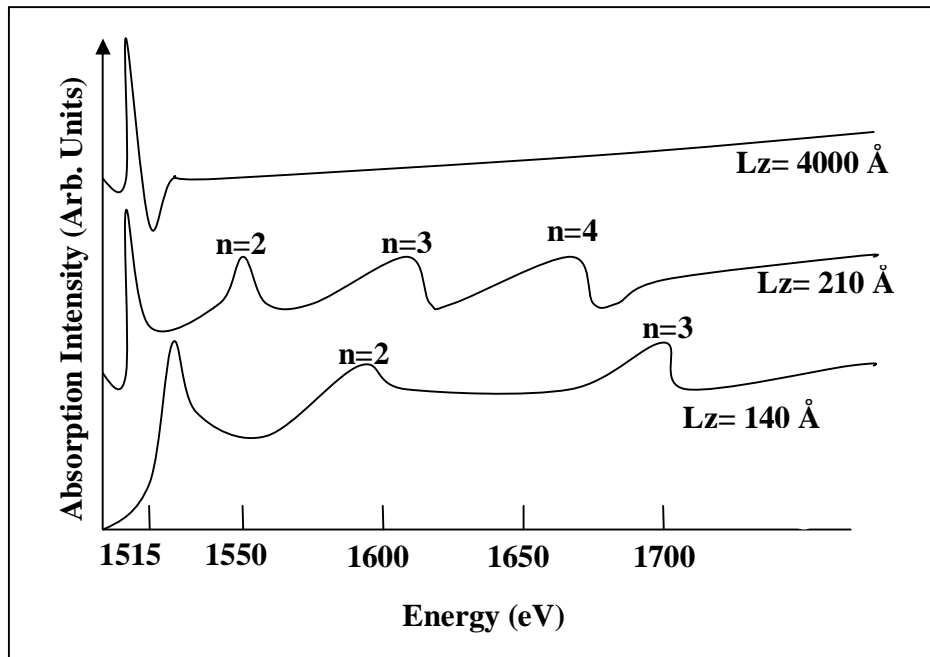
Figure 2.3.7: Absorption in GaAs-GaAlAs Quantum Wells of different thicknesses, L_z [29].

Figure 2.3.7 shows the absorption spectra for GaAs-GaAlAs Quantum Wells for different well thicknesses. In bulk GaAs excitons are very weak at room temperature. However, excitons are very prominent in Quantum Well structures. The upward shift in energy within the quantum well data reflects the quantum size effects within the wells, as the relevant energy is the separation between the minima and maxima in the electron and hole bands within the wells. Indeed much of the earliest work that confirmed the effects of quantum confinement were optical studies on wells of different thicknesses as shown in Figure 2.4.7

In summary, when the size and dimensionality of low-dimensional structures decreases the binding energy and oscillator strength of excitons increase which has a profound effect on the absorption spectra in optical experiments. The aim of this dissertation is to investigate the change of the binding energy in a Quantum Well-Wire structure to better understand this effect.

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Chapter 3

Mathematical Techniques

'... the whole procedure was an act of despair...'

- Max Planck on his Quantum Theory, 1900

3.1   Variational Approach

In situations where a physical system has a Hamiltonian that is not solvable either via an exact solution or to a perturbation treatment, a technique, called the *Variational Method* (also called the Rayleigh-Ritz method) comes in handy [1]. This technique is a very useful tool, allowing approximate calculations to be made in quantum mechanics. Usually when the Schrödinger equation is non-separable in nature some approximation technique must be used. In a similar situation for a confined system, the variational method might constitute an economical and physical appealing approach [2]. One of the advantages of the Variational technique is that the method requires only a qualitative knowledge of the behaviour of the system under study in order to choose adequately the trial wave functions [3].

The Variational Method is based on the simple fact that the average energy of a system, i.e. the *Expectation Value* of its Hamiltonian *H*, in a state represented by an arbitrary wave function, has got to be greater than or equal to the ground-state energy of the system [1]. To see this consider the following: the ground-state energy acts as a lower bound on an expectation value calculated with any arbitrary trial wave function. So, by choosing a trial wave function with a number of variational parameters, the expectation value of the Hamiltonian *H*, can be minimized as a function of these variational parameters! The lowest possible ground-state energy will be the solution to the Schrödinger equation that is sought after and this depends on the choice of the trial wave function, i.e. on the number of variational parameters introduced in the system.

This can be proven as follows:

Expand any arbitrary trial wave function ψ in terms of the complete set of eigenfunctions u_n of the Hamiltonian H belonging to the eigenvalues E_n:

$$y = \sum_n a_n u_n \tag{3.1.1}$$

This can also be written in Dirac notation:

$$|y\rangle = \sum_n a_n |u_n\rangle \tag{3.1.2}$$

Now the expectation value of the Hamiltonian, H, can be written as

$$\langle H \rangle = \frac{\langle y|H|y\rangle}{\langle y|y\rangle} = \frac{\sum_n |a_n|^2 E_n}{\sum_n |a_n|^2} \tag{3.1.3}$$

(Note that $|y\rangle$ may not be normalized)

An inequality is now obtained if all the energy values, E_n, are replaced by the ground-state energy, E_0, i.e. by the lowest eigenvalue of H:

$$\langle H \rangle \geq \frac{E_0 \sum\limits_{n} |a_n|^2}{\sum\limits_{n} |a_n|^2} = E_0 \qquad (3.1.4)$$

Hence to fully exploit the power of the Variational Method, choose a trial wave function that amply contains a whole lot of variational parameters, λ_i:

$$y = y(l_1, l_2, l_3 ....) \qquad (3.1.5)$$

Then vary those parameters, λ_i, as such until the expectation value of H is minimized [1]:

$$\frac{\partial \langle H \rangle}{\partial l_i} = 0 \qquad (3.1.6)$$

To demonstrate how this technique is used more clearly, consider the case for a quantum confined system. Assume that, for a given quantum system, the time-independent Schrödinger equation can be written as:

$$H y_n = E_n y_n \qquad (3.1.7)$$

Here set $\hbar = m = 1$. Then $H = -\frac{1}{2} \nabla^2 + V(q)$ is the associated Hamiltonian for this system with {q} the set of coordinates on which the potential V depends.

Now an approximate solution to equation (3.1.7) can be found by replacing the wave function, ψ_n, with a trial wave function, θ_n. It is however important that this trial wave function possess a similar behaviour at the "origin" as well as asymptotically at infinity. Now, with the expectation value being:

$$\langle H \rangle = \frac{\langle q_n^* | H | q_n \rangle}{\langle q_n^* | q_n \rangle} = \frac{\int q_n^* H q_n dt}{\int q_n^* q_n dt} \tag{3.1.8}$$

The estimate of the energy of the system can then be found by simply minimizing the function:

$$\int q_n^* H q_n dt \tag{3.1.9}$$

The following additional restriction also holds:

$$\int q_n^* q_n dt = d_{n,n'} \tag{3.1.10}$$

Therefore, as shown earlier, energy eigenvalues can be found which will be at least equal to the real eigenvalues (i.e. eigenvalues of the true wave function and not the postulated trial wave function) [3]:

$$e_n = \min \int q_n^* H q_n dt \geq E_n \tag{3.1.11}$$

From this it is clear that a bad postulation of the trial wave function, θ_n, leads to a bad estimate of the eigenvalues ε_n. And this means that all the qualitative knowledge of the system has not been properly included in the trial wave function [3].

In practice, however, the trial wave function depends on a set of spatial coordinates and on a set of unknown parameters, i.e.:

$$q_n = q_n(x, y, z....z_s) \text{ and } q_n = q_n(a_1, a_2, a_3...a_k) \tag{3.1.12}$$

This will mean that the eigenvalue will also be a function of these variational parameters, i.e.:

$$e_n = e_n(a_1, a_2, a_3...a_k) \tag{3.1.13}$$

Thus, in order to determine the set $\{\alpha_k\}$, the following system of equations must be solved:

$$\frac{\partial e_n}{\partial a_i} = 0, \text{ for } i = 1, 2, ..., k \tag{3.1.14}$$

From equation (3.1.14), the eigenvalues ε_n can be easily obtained. Thus an approximate set of eigenvalues ε_n for a trial eigenfunction θ_n, has been obtained and the accuracy (i.e. how close these set of eigenvalues are to the *real* eigenvalues of the *real* wave eigenfunction) is only dependent on the choice of the trial eigenfunction, in specific the amount of variational parameters included in it, and how much this reflects qualitatively the knowledge available of the system.

3.2 Effective Mass and Effective Mass Approximation

The following discussion is based on general arguments and common assumptions as detailed in Gerald Burns' *Solid State Physics* [4].

From Newton's second law, it is known that mass is defined as the constant of proportionality between force, *F*, and acceleration, *a*. However, when an electron interacts with other electrons in a metal or semiconductor, this interaction causes a change in the mass of the electron, i.e. the effective mass of the not free electron is different form that of a free electron.

For example: consider a spherical ball with charge *Z* and mass *M* being accelerated by an external electric field, *E*, in a frictionless fluid. It is clear that the force on the ball will be: $F = ZE$. However the ratio of $ZE/a \neq M$, simply because the ball will also push some of the fluid ahead of it. And thus Newton's second law will not give the correct proportionality constant, i.e. free mass, for this situation but instead will give an "effective mass" for the ball different from *M*. (This is so if the focus is on the ball only.) With this analogy in mind, it is clear to see that an electron moving in a crystal will experience the same result, however the effective mass m_e^* can be larger, smaller of even negative in comparison to the rest mass m_e [4].

To show this, let the group velocity of an electron in an energy band in a crystal under an applied electric field, *E*, be v_g. A wave packet, whose wave vector is cantered at *k*, represents the electron. It is known from optics that:

$$v_g = \frac{dw}{dk}$$
(3.2.1)

where ω is the angular frequency of the wave. But since from Planck's law, it is known that there exist a relation between angular frequency and energy, namely:

$$E = \mathbf{h}w \qquad (3.2.2)$$

leading to

$$v_g = \frac{1}{\mathbf{h}}\frac{dE}{dk} \qquad (3.2.3)$$

$$\frac{dv_g}{dt} = \frac{1}{\mathbf{h}}\frac{d^2E}{dt\,dk} = \frac{1}{\mathbf{h}}\frac{d^2E}{dk^2}\frac{dk}{dt} \qquad (3.2.4)$$

Thus, from equation (3.2.4) it is clear that the electron acceleration (dv_g/dt) is related to the energy dispersion (d^2E/dk^2), i.e. to the curvature of the band, and the variation of k with time under the influence of an external force (dk/dt). Now the applied electric field (applied for a time interval δt) does an amount of work on the electron of charge $-e$:

$$\partial E = (-eE \times v_g) \times dt \qquad (3.2.5)$$

However, this work can also be written as:

$$dE = \left(\frac{dE}{dk}\right)dk = \mathbf{h}v_g\,dk \qquad (3.2.6)$$

Stating that:

$$\frac{dk}{dt} = \frac{dk}{dt} \qquad (3.2.7)$$

it is clear that:

$$-eEdt = \mathbf{h}dk$$

$$\frac{dk}{dt} = -\frac{eE}{\mathbf{h}}$$

(3.2.8)

from equations (3.2.6) and (3.2.7).

Now, substitution of *dk/dt* in equation (3.2.4) leads to:

$$\frac{dv_g}{dt} = a = \frac{1}{\mathbf{h}^2}\frac{d^2E}{dk^2}(-eE)$$

(3.2.9).

This has the same form as Newton's second law (*a = F/m*) and hence an **effective mass** (*m**) can be defined as:

$$\frac{1}{m^*} = \frac{1}{\mathbf{h}^2}\frac{d^2E}{dk^2}$$

(3.2.10)

It is therefore clear that the effective mass is simply related to the curvature of the energy bands.

Although band diagrams are in general quite complex and difficult to calculate, in the ***effective mass approximation (EMA)*** the bands are assumed to have simple parabolic forms near extremes in the band diagram [5].
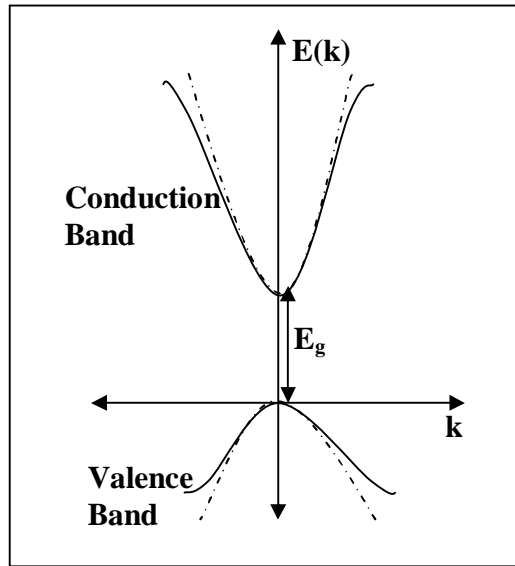
Figure 3.2.1: Simple two-band model for bulk direct gap semiconductors [5].

Figure 3.2.1 shows the band structure in the EMA for a bulk direct gap semiconductor. The solid lines, showing the real/true band structure, is approximated by parabolic bands (dashed lines) at $k = 0$ in the effective mass approximation. The curvature of the bands reflects the "mass" of the electrons in the conduction band and the holes in the valence band. In this approximation the carriers behave as free particles with an "effective mass" m^*.

Physically the effective mass attempts to incorporate the complicated periodic potential "felt" by the carriers in the lattice. This approximation completely ignores the semiconductor atoms in the lattice to treat the electron and hole as "free particles".

3.3   Envelope Function Approximation

By combining the effective mass approximation with appropriate boundary conditions

$$V(r) = \begin{cases} 0 \text{ for } r < a \\ \infty \text{ for } r > a \end{cases} \qquad (3.3.1)$$

(*a* being the boundaries of the confined system) each of the carriers in the quantum structure- /low-dimensional-system - problem can be viewed as being in a "particle-in-a-box" - form. Thus, this requires that the quantum structure is treated as a "bulk" sample, i.e. assume that the single particle (electron or hole) wave function can be written in terms of Bloch functions:

$$y_{nk}(\boldsymbol{r}) = u_{nk}(\boldsymbol{r})e^{(ik \cdot r)} \tag{3.3.2}$$

where u_{nk} is a function with the periodicity of the crystal lattice and the wave functions are labelled by the band index n and wave vector $\boldsymbol{k}$. *This* approximation is called the *Envelop Function Approximation (EFA)*. The single particle wave function can then be written as a linear combination of Bloch functions with expansion coefficients, C_{nk}:

$$y_{\text{single particle}}(\boldsymbol{r}) = \sum_{\boldsymbol{k}} C_{nk} u_{nk}(\boldsymbol{r}) e^{(ik \cdot r)} \tag{3.3.3}$$

Now, assuming that the functions u_{nk} have weak $\boldsymbol{k}$ dependence, this will lead to:

$$y_{\text{single particle}}(\boldsymbol{r}) = u_{n0}(\boldsymbol{r}) \sum_{\boldsymbol{k}} C_{nk} e^{(ik \cdot r)} = u_{n0}(\boldsymbol{r}) f_{\text{single particle}}(\boldsymbol{r}) \tag{3.3.4}$$

Here the single particle function, $f_{single\ particle}$, is the "envelope function". Now these u_{n0} functions are usually known from the bulk material. So the quantum structure- or low-dimensional - problem is reduced to determining the envelope functions for the single particle wave functions: $f_{single\ particle}$. Thus, if for example spherically shaped quantum dots are assumed, with infinitely high potential barriers at the dot boundary, then the

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envelope functions of these particles are given by the "particle-in-a-sphere" solutions with the free particle mass, m_0, replaced by an effective mass, m^*.

3.4   Atomic Units

When solving complicated systems of mathematical equations, even the simplest of mistakes can result in hours of debugging. For this reason it is vital to make software as clean and simple as possible. One thing that can be done in the physical sciences toward this end, is to use dimensional analysis.

The simplest form of dimensional analysis is to change to a new system of units tailored specifically to the problem at hand. This entails changing numerical values of physical constants in the equations used, but not changing the equations themselves at all. And then, once the calculations are completed, the results should be converted back to the standard units using the familiar rules for unit conversion. Such an adapted system of units can be very useful when the relevant physical constants have large or small values in terms of standard units [6].

As an example in atomic-physics so called atomic units are frequently adopted to make things easy. For the purposes of this dissertation, however, a slight modification is required to use the so called *effective atomic units*. When using this convention one measures quantities in units of some suitable atomic constants. For example one measures the mass in units of m^* and charge in units of e. This has the effect that, in effective atomic units

$$e = m^* = \hbar = 4\pi\varepsilon\varepsilon_r = a_B{}^* = 1$$

Note that the units change when changing the semiconductor material because ε_r and m^* then changes [7,8].

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Chapter 4

Theoretical Calculations for

Quantum Well-Wire

'As far as the laws of mathematics refer to reality, they are not certain;
and as far as they are certain, they do not refer to reality.'
> *- Albert Einstein, "Geometry and Experience", January 27, 1921*

'It is the mark of an educated mind to be able to entertain a thought without accepting it.'
> - Aristotle, Greek critic, philosopher, physicist, & zoologist (384 BC - 322 BC)

An interacting electron-hole pair in a Quantum Well-Wire is studied within the framework of the Effective-Mass Approximation. An expansion to a mathematical technique proposed by Harrison et. al. [12] is presented. The technique is applied to an infinite Well-Wire confining potential.   The Envelope Function Approximation is employed in the approach, involving a three parameter variational calculation in which the symmetry of the component of the wave function representing the relative motion is allowed to vary from the one- to the two- and three-dimensional limits.

4.1   Introduction

At the beginning of the 1980's, advances in technology, especially in very accurate lithographic techniques, made it possible to confine electrons in a quasi-one-dimensional structure known as the Quantum Wire [1-3].   Correlated electron-hole pairs form Wannier-excitons in semiconductor heterostructures. For the past two decades, the study of confined excitons in a Quantum Well as well as a Quantum Wire and Wire heterostructures has been a subject of great interest and an enormous amount of literature

has been devoted to this field [4-8]. It is well established that the confinement of excitons in Quantum Wells yields enhanced excitonic effects (such as the binding energy and oscillator strength). This can be exploited in the design of novel optoelectronic devices for example blue and ultraviolet light emitting diodes (LEDs) and blue laser diodes (LDs) have been developed recently using InGaN Quantum Wells (QWs) as the active layers [9-11].

As was seen in an earlier section (section 2.3), excitons are characteristic of the optical spectra of Quantum Wells and Wires [12]. In a real solid, many complicating effects inhibit a simple comparison of the experimental observation of the exciton emission energy with the theoretical estimate of this value, arising from the uncertainty in the knowledge of a range of parameters like the exact widths of the potential wells and barriers, the relevant effective mass parameters and the degenerate nature of the valence band states [13]. For excitons in most III-V Quantum Wells, for example, both the electron and the hole are strongly confined within the well region by the band gap discontinuities in the valence band (VB) and conduction band (CB). This is the case in GaAs/(Al,Ga)As among others [14]. A quasi–two-dimensional behaviour occurs on reducing the well width as the average electron-hole distance decrease leading to an increase in the binding energy. However, when the well width is smaller than a critical value, the leakage of the wave function into the barriers becomes more important and the binding energy is reduced until it reaches the value appropriate to the bulk barrier material for which $L = 0$.

As the electronic industry progresses from micro-technologies to nanotechnologies whereby devices are designed in the nanometre range, it becomes increasingly necessary to address the concern of the exciton losing its enhanced effects in the ultra- small quantum structures, due to the increased penetration of the exciton wave function into the barrier regions in the direction of diminishing spatial confinement [15].

In this chapter an expansion of a mathematical technique proposed by Harrison *et. al.* [12,13] is introduced to investigate the quasi-two-dimensional, quasi-one-dimensional

behaviour of a confined exciton inside a semiconductor as the bulk material is reduced in dimensions to form a Quantum Well and Wire. It is standard in literature to employ trial wave functions, written as a product of three wave functions: the first two are corresponding to the single particle wave function of an electron and a hole in the Quantum Well-Wire and the third represents a *free* exciton whose radius is adjusted as a variational parameter [16]. This method can be suitably adapted for any particular choice of variational wave function.

4.2   Exciton Hamiltonian and Expectation Value

The validity of the envelope function approximation (which takes the wave function of the interacting system of an electron and hole in a semiconductor to be written as the product of a Bloch function appropriate to the bottom of the associated (electron) conduction or (hole) valence band states together with an envelope function describing the relative electron – hole motion) is assumed [13] as well as the effective mass approximation, in the single band scheme, allowing the use of relevant effective masses for the charge carriers in the CB and VB respectively.

Consider a Wannier exciton in a rectangular Quantum Well-Wire of infinite extent in the *x*-direction but having a width, *Ly*, and height, *Lz*, in the *y*- and *z*- direction respectively. Using the variational scheme, the Hamiltonian of a correlated electron-hole pair can be written as:

$$H = H_e + H_h + H_r \tag{4.2.1}$$

$$H_e = -\frac{\mathbf{h}^2}{2m_e^*}\nabla^2_{z_e, y_e} + V_e$$

where $\hspace{8cm}$ (4.2.2)

$$H_e = \frac{-\mathbf{h}^2}{2m_e^*}\left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2}\right) + V_e$$

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and

$$H_h = -\frac{\mathbf{h}^2}{2m_h^*}\nabla^2_{z_h,y_h} + V_h$$

$$H_h = -\frac{\mathbf{h}^2}{2m_h^*}\left(\frac{\partial^2}{\partial z_h^2} + \frac{\partial^2}{\partial y_h^2}\right) + V_h$$

(4.2.3)

are the single-particle Hamiltonians of the electron (hole) and V_e (V_h) is the confining potential due to the valence- (conduction-) band offsets, m_e^* (m_h^*) is the effective mass of the electron (hole) appropriate to the VB (CB) of the semiconductor material under consideration, and

$$H_r = -\frac{\mathbf{h}^2}{2m}\nabla^2_x + V_{Coulomb}$$

$$H_r = -\frac{\mathbf{h}^2}{2m}\left(\frac{\partial^2}{\partial x^2}\right) + V_{Coulomb}$$

(4.2.4)

is the relative motion Hamiltonian for the electron-hole pair with μ the reduced mass of the electron-hole pair :

$$m = \frac{m_e^* m_h^*}{m_e^* + m_h^*}$$

(4.2.5)

and $V_{Coulomb}$ is the Coulombic interaction between the electron and the hole:

$$V_{Coulomb} = -\frac{e^2}{4per}$$

(4.2.6)

with r being the electron-hole separation distance and ε the dielectric constant for the semiconductor material under consideration.

The envelope function is now taken to have the form:

$$f = \varphi_e(y_e, z_e)\varphi_h(y_h, z_h)\varphi_r(x_e, y_e, z_e, x_h, y_h, z_h) \tag{4.2.7}$$

where φ_e (φ_h) is the eigenfunction of the Hamiltonian H_e (H_h) normalized over the confined region , i.e.

$$H_e\varphi_e = E_e\varphi_e \tag{4.2.8}$$

$$H_h\varphi_h = E_h\varphi_h \tag{4.2.9}$$

with E_e and E_h being the eigenvalues for these equations. *It is in these Hamiltonians that the quantum confinement potential will be present.*

It is now simply a matter of solving the expectation value

$$\mathbf{E} = \mathbf{E_g} + \frac{<f^*|\hat{\mathbf{H}}|f>}{<f^*|f>} \tag{4.2.10}$$

in order to calculate the total energy of the electron-hole system (where E_g is the semiconductor band gap energy).

Equation (4.2.10) can now be expanded to

$$E = E_g + \frac{<f^*|H_e|f>}{<f^*|f>} + \frac{<f^*|H_h|f>}{<f^*|f>} + \frac{<f^*|H_r|f>}{<f^*|f>} = E_g + \frac{A+B+C}{D} \qquad (4.2.11)$$

Consider now the normalizing term, **D**:

$$D = <f^*|f> = \int_{All\ Space} |j_e(y_e, z_e)|^2 |j_h(y_h, z_h)|^2 |j_r|^2 \, dx \, dy_e dy_h dz_e dz_h \qquad (4.2.12)$$

Now: φ_e and φ_h are both functions of y and z so, the integration over x involve only the relative motion term φ_r. Thus, the result of this integration will be a quantity that is a function of $z = |z_e - z_h|$ and $y = |y_e - y_h|$:

$$F(y,z) = \int |j_r|^2 \, dx \qquad (4.2.13)$$

The remainder of the integral over coordinates z_e, z_h and y_e, y_h defined between "effective infinities"[⊗] $\mu\ (=-\infty)$, $v(=+\infty)$ and $\rho(=-\infty)$, $\tau(=+\infty)$ gives

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[⊗] Since it is impossible to numerically/computationally integrate to $\pm \infty$ it is necessary to integrate only as far as "effective infinities". Thus the actual values for μ, v, τ and ρ are at the discretion of the user. However the benefits gained in accuracy must be weighed against the increased computational effort.[12]

$$D = \int\limits_{0}^{n-m}\int\limits_{0}^{t-r}\int\limits_{m}^{n}\int\limits_{r}^{t}\int\limits_{m}^{n}\int\limits_{r}^{t}\lfloor j_{e}(y_{e},z_{e})\rfloor^{2}\,\lfloor j_{h}(z_{h},y_{h})\rfloor^{2}\,F(y,z)\,dy_{e}dy_{h}dz_{e}dz_{h}$$
$$\times[d(z_{e}-z_{h}-z,y_{e}-y_{h}-y)+d(z_{h}-z_{e}-z,y_{h}-y_{e}-y)]dy\,dz \qquad (4.2.14)$$

If a probability term is defined as

$$p(y,z)=\int\limits_{m}^{u-z}\int\limits_{r}^{t-y}\lfloor j_{e}(z'+z,y'+y)\rfloor^{2}\lfloor j_{h}(z',y')\rfloor^{2}+\lfloor j_{e}(z',y')\rfloor^{2}\lfloor j_{h}(z'+z,y'+y)\rfloor^{2}\,dy'\,dz' \qquad (4.2.15)$$

with *p(y,z)* being the uncorrelated probability of finding an electron and hole separated by a distance $|r|=\sqrt{y^{2}+z^{2}}$ (in the confinement plane), then it can be shown that

$$D=\int\limits_{0}^{n-m}\int\limits_{0}^{t-r}F(y,z)\,p(y,z)\,dy\,dz \qquad (4.2.16)$$

Consider now the term, A:

$$A=<j^{*}|\,H_{e}\,\lfloor j> \;=\;\int\limits_{All\,Space} j^{*}H_{j}\quad dz_{e}dz_{h}dy_{e}dy_{h}dx \qquad (4.2.17)$$

Now if $\nabla^{2}_{z_{e},y_{e}}$ as in (4.2.2) is given by $\nabla^{2}_{z_{e},y_{e}}=\left(\dfrac{\partial^{2}}{\partial z_{e}^{2}}+\dfrac{\partial^{2}}{\partial y_{e}^{2}}\right)$ it can be shown that

$$A=DE_{e}-\frac{\hbar^{2}}{2m_{e}^{*}}\int p(y,z)\,G(y,z)\,dy\,dz \qquad (4.2.18)$$

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where

$$G(y,z) = \int j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r \ dx \qquad (4.2.19)$$

In a similar way it can be shown that

$$\boldsymbol{B} = \boldsymbol{DE}_h - \frac{\mathbf{h}^2}{2m_h^*} \int p(y,z) \ G(y,z) \ dy \ dz \qquad (4.2.20)$$

Turning attention to $\boldsymbol{C}$:

$$\boldsymbol{C} = <j_r^* | H_r | j_r > \ = \int\limits_{All \ Space} j_r^* H_r j_r \ dx \ dy_e dy_h dz_e dz_h \qquad (4.2.21)$$

After a detailed calculation it is easily shown that:

$$\boldsymbol{C} = -\frac{\mathbf{h}^2}{2m} \int p(y,z) \ J(y,z) \ dy \ dz - \frac{e^2}{4pe} \int p(y,z) \ K(y,z) \ dy \ dz \qquad (4.2.22)$$

with

$$J(y,z) = \int j_r \left(\frac{\partial^2}{\partial x^2} \right) j_r \ dx \qquad (4.2.23)$$

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and

$$K(y, z) = \int j_r^2 \frac{1}{r} \, dx \qquad (4.2.24)$$

with

$$|r| = \sqrt{x^2 + y^2 + z^2} \qquad (4.2.25)$$

Further simplification requires a specific choice of the envelope function φ_r. However, the next two sections will show the validity of these equations, before a specific choice for the envelope function is made.

4.3 Solution to Expectation Value

Here the derivations of equations (4.2.17) through (4.2.24) are shown. Each individual term (**A, B, C** and **D**), from equation (4.2.11) is now considered:

First consider the term **A**:

$$A = \left\langle f^* \, | \, H_e \, | \, f \right\rangle \qquad (4.3.1)$$

$$A = \int_{AllSpace} f^* H_e f \quad dz_e dz_h dy_e dy_h dx \qquad (4.3.2)$$

This can be written as:

$$A = \int_{AllSpace} j_e^*(z_e, y_e) j_h^*(z_h, y_h) j_r^*(z_e, z_h, y_e, y_h, x) \times$$

$$\left[\frac{-\mathbf{h}^2}{2m_e^*} \nabla_{ze,ye}^2 + V_{Ce} \right] j_e(z_e, y_e) j_h(z_h, y_h) j_r(z_e, z_h, y_e, y_h, x) dz_{e,h} dy_{e,h} dx \qquad (4.3.3)$$

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$$A = \int\limits_{AllSpace} j_e^* j_h^* j_r^* \times$$

$$\left[\frac{-\mathbf{h}^2}{2m_e^*} \left(\left(\nabla_{ze,y}^2 j_e\right) j_h j_r + \left(\nabla_{ze,y}^2 j_h\right) j_e j_r + \left(\nabla_{ze,y}^2 j_r\right) j_e j_h \right) + V_C j_e j_h j_r \right] dz_{e,h} dy_{e,h} dx$$

(4.3.4)

(The operator V_{Ce} is simply multiplicative.)

Equation (4.3.4) can therefore be written as:

$$A = \int\limits_{AllSpace} j_e^* j_h^* j_r^* \times$$

$$\left[\frac{-\mathbf{h}^2}{2m_e^*} \left(j_h j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_e + j_e j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_h + j_e j_h \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r \right) + V_C j_e j_h j_r \right] dz_{e,h} dy_{e,h} dx$$

(4.3.5)

Now it can be written:

$$j_e^* = j_e$$
$$j_h^* = j_h$$
$$j_r^* = j_r$$

(4.3.6)

since none of the functions are imaginary.

Therefore:

$$\overbrace{H_e j_e = E_e j_e}^{}$$

$$A = \int\limits_{AllSpace} j_h^2 j_r^2 j_e \left(\frac{-\mathbf{h}^2}{2m_e^*} \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_e(z_e, y_e) + (V_C j_e) \right) dz_{e,h} dy_{e,h} dx \quad +$$

$$\int\limits_{AllSpace} j_e j_h j_r \left(\frac{-\mathbf{h}^2}{2m_e^*} j_e j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_h(z_h, y_h) \right) dz_{e,h} dy_{e,h} dx \quad + \quad (4.3.7)$$

$$\int\limits_{AllSpace} j_e j_h j_r \left(\frac{-\mathbf{h}^2}{2m_e^*} j_e j_h \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r(z_h, z_h, y_e, y_h, x) \right) dz_{e,h} dy_{e,h} dx$$

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$$A = \int\limits_{AllSpace} j_h^2 j_r^2 j_e (\boldsymbol{H} \boldsymbol{j}_e) dz_{e,h} dy_{e,h} dx \quad +$$

$$\int\limits_{AllSpace} j_e^2 j_r^2 j_h(z_h, y_h)\left(\frac{-\mathbf{h}^2}{2m_e^*}\left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) \right) j_h(z_h, y_h) dz_{e,h} dy_{e,h} dx \quad + \qquad (4.3.8)$$

$$\int\limits_{AllSpace} j_e^2 j_h^2 \left(\frac{-\mathbf{h}^2}{2m_e^*} j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r(z_{e,h} y_{e,h} x) \right) dz_{e,h} dy_{e,h} dx$$

If the second term of equation (4.3.8) is considered, it is clear that, since $\varphi_{\underline{h}}$ is not a function of the coordinates z_e and y_e, i.e.:

$$j_h \neq j_h(z_e, y_h) \text{ but } j_h = j_h(z_h, y_h) \qquad (4.3.9)$$

this function (φ_h) should be treated as a constant with respect to the differential operators. It is known however that the result of differentiation on a constant is zero. Thus the second term is reduced to zero, leaving:

$$A = \int\limits_{AllSpace} j_r^2 j_h^2 j_e (\boldsymbol{H} \boldsymbol{j}_e) dz_{e,h} dy_{e,h} dx \quad +$$

$$\int\limits_{AllSpace} 0 \quad dz_{e,h} dy_{e,h} dx \quad + \qquad (4.3.10)$$

$$\int\limits_{AllSpace} j_e^2 j_h^2 \left(\frac{-\mathbf{h}^2}{2m_e^*} j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r(z_{e,h} y_{e,h} x) \right) dz_{e,h} dy_{e,h} dx$$

$$A = \int\limits_{AllSpace} j_h^2 j_r^2 j_e^2 E_e dz_{e,h} dy_{e,h} dx \quad +$$

$$\int\limits_{AllSpace} j_e^2 j_h^2 \left(\frac{-\mathbf{h}^2}{2m_e^*} j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r(z_{e,h}, y_{e,h}, x) \right) dz_{e,h} dy_{e,h} dx \qquad (4.3.11)$$

$$A = E_e \int_{AllSpace} j_h^2 j_r^2 j_e^2 \, dz_{e,h} dy_{e,h} dx \quad +$$

$$\int_{AllSpace} j_e^2 j_h^2 \left(\frac{-\mathbf{h}^2}{2m_e^*} j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r (z_{e,h} y_{e,h} x) \right) dz_{e,h} dy_{e,h} dx \qquad (4.3.12)$$

Now, from equation (4.2.12) it is clear that, in the first term, the integral part of equation (4.3.12) is equal to **D**. Hence:

$$A = \mathbf{D}E_e - \frac{\mathbf{h}^2}{2m_e^*} \int_{AllSpace} j_e^2 j_h^2 \left(j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r \right) dz_{e,h} dy_{e,h} dx \qquad (4.3.13)$$

Now, to avoid confusion in the rest of this and following sections, call *z* = *a* and *y* = *b*. Then equation (4.3.13) can be written as:

$$A = \mathbf{D}E_e - \frac{\mathbf{h}^2}{2m_e^*} \int_{AllSpace} p(a,b)G(a,b) \, da db \qquad (4.3.14)$$

exactly as equation (4.2.18), with

$$G(a,b) = \int j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r \ dx \qquad (4.3.15)$$

as equation (4.2.19). The justification for introducing the terms *a* and *b* shall be shown later in this section.

In a similar way *B* can be found:

$$B = DE_h - \frac{\mathbf{h}^2}{2m_h^*} \int\limits_{AllSpace} p(a,b)G(a,b)dadb \qquad (4.3.16)$$

Consider now the term **C**:

$$C = \left\langle f^* \mid H_r \mid f \right\rangle \qquad (4.3.17)$$

$$= \int\limits_{AllSpace} (f^* H_r f) \; dz_e dz_h dy_e dy_h dx \qquad (4.3.18)$$

$$= \int f^* \left(-\frac{\mathbf{h}^2}{2m} \nabla_x^2 + V_{Coulomb} \right) f \; dz_{e,h} d_{ye,h} dx \qquad (4.3.19)$$

$$= \int f^* \left(-\frac{\mathbf{h}^2}{2m} \nabla_x^2 \right) f \; dz_{e,h} d_{ye,h} dx + \int f^* \left(V_{Coulomb} \right) f \; dz_{e,h} d_{ye,h} dx \qquad (4.3.20)$$

$$= -\frac{\mathbf{h}^2}{2m} \int j_e^*(z_e,y_e) j_h^*(z_h,y_h) j_r^*(z_{e,h},y_{e,h},x) \left(\frac{\partial^2}{\partial x^2} \right) j_e(z_e,y_e) j_h(z_h,y_h) j_r(z_{e,h},y_{e,h},x) \; dz_{e,h} d_{ye,h} dx \quad +$$

$$\int j^* j^* j_r^* \left(\frac{-e^2}{4per} \right) j j j_r \; dz_{e,h} dy_{e,h} dx$$

$$(4.3.21)$$

The terms in equation (4.3.21) can be grouped as shown by the curly brackets:

$$= -\frac{\mathbf{h}^2}{2\mathbf{m}} \int j_{e}^{2} j_{h}^{2} J_{r} \left(\frac{\partial^2}{\partial x^2} \right) j_{r} \underbrace{dz\, dy}_{} dx - \frac{e^2}{4pe} \int j_{e}^{2} j_{h}^{2} J_{r} \left(\frac{1}{r(x)} \right) j_{r} \underbrace{dz\, dy}_{} dx$$

(4.3.22)

This gives **C** as was shown in equation (4.2.22):

$$C = -\frac{\mathbf{h}^2}{2\mathbf{m}} \int p(a,b) J(a,b)\; dadb - \frac{e^2}{4pe} \int p(a,b) K(a,b)\; dadb \qquad (4.3.23)$$

with:

$$J(a,b) = \int j_{r} \left(\frac{\partial^2}{\partial x^2} \right) j_{r}\; dx \qquad (4.3.24)$$

and:

$$K(a,b) = \int j_{r}^{2} \frac{1}{r(x)}\, dx \qquad (4.3.25)$$

4.4 Vectors for 6D-space

In this section it will be shown how the terms a and b was introduced in the previous section (remember however that in section 4.3 it was stated that $z = a$ and $y = b$):

First, define:

$$a = |z_e - z_h| \qquad (4.4.1)$$

$$b = |y_e - y_h| \qquad (4.4.2)$$

$$x = |x_e - x_h| \qquad (4.4.3)$$
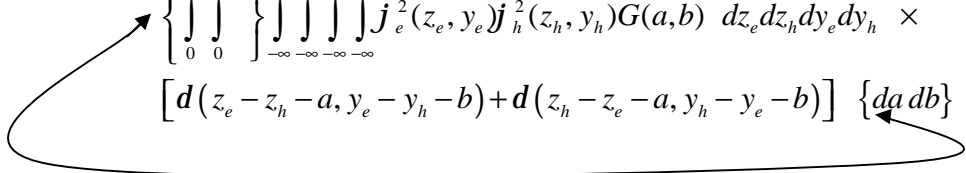
where these are the electron-hole separations in the x-, y- and z- directions respectively. Thus, consider:

$$A = DE_e - \frac{\mathbf{h}^2}{2m_e^*} \int\limits_{AllSpace} j_e^2 j_h^2 \left(j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r \right) dz_e dz_h dy_e dy_h dx \qquad (4.4.4)$$

Since φ_r is the only function of x, definite integration over x leaves only a function of a and b (bearing in mind that a is itself a function of z_e and b, in turn, is a function of y_e according to definitions (4.4.1) and (4.4.2)). Therefore it can be stated that the function G (as given by equations (4.2.19) and (4.3.15)) will be a function of a and b, i.e.

$$G = G(a, b) = G(z, y) \qquad (4.4.5)$$

Consider now the remainder of the definite integral over the coordinates z_e, z_h, y_e and y_h between "effective infinites":

$$\left\{ \int\limits_0^{2\infty} \int\limits_0^{2\infty} \right\} \int\limits_{-\infty}^{+\infty} \int\limits_{-\infty}^{+\infty} \int\limits_{-\infty}^{+\infty} \int\limits_{-\infty}^{+\infty} j_e^2(z_e, y_e) j_h^2(z_h, y_h) G(a,b) \ dz_e dz_h dy_e dy_h \ \times$$

$$\left[d(z_e - z_h - a, y_e - y_h - b) + d(z_h - z_e - a, y_h - y_e - b) \right] \ \{da \, db\} \qquad (4.4.6)$$

Note that the a and b values must be between 0 and ∞, i.e. negative values are not considered. This is so because, since a and b are representative of the *distance* between the electron and the hole (i.e. the *absolute* distance) it *cannot* be negative.

What does this mean? It is known that the square of a wave function gives the probability of the particle being at those specific coordinates. Therefore, if the electron has a good probability to be at the coordinate (z_e, y_e) and if the hole has a good probability to be at the coordinate (z_h, y_h) (bearing in mind that the coordinate axis $z, y \rightarrow 0$ in a Quantum Wire), it is required (by equation (4.4.6)) that the separation between the electron and hole is equal to a and b in the z- and y- directions respectively. But now, it can be written:

$$\int_0^{2\infty}\int_0^{2\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} j_e^2(z_e, y_e) j_h^2(z_h, y_h) G(a,b) dz_e dz_h dy_e dy_h \left[d\left(z_e - z_h - a, y_e - y_h - b \right) \right] da\, db$$

$$+\int_0^{2\infty}\int_0^{2\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} j_e^2(z_e, y_e) j_h^2(z_h, y_h) G(a,b) dz_e dz_h dy_e dy_h \left[d\left(z_h - z_e - a, y_h - y_e - b \right) \right] da\, db$$

$$(4.4.7)$$

Thus: the first term will only have a finite, non-zero value if:

$$a = z_e - z_h \qquad (4.4.8)$$

And at the same time: $\qquad b = y_e - y_h \qquad (4.4.9)$

(It is very important to note that these two conditions both have to hold *at the same time*!)

The second term only has a finite, non-zero value if:

$$a = z_h - z_e \qquad (4.4.10)$$

And at the same time: $\qquad b = y_h - y_e \qquad (4.4.11)$

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It is now guaranteed that, if there is a non-zero probability of existence at specific coordinates, the difference between these coordinates will be *a* and *b*. But what is the physical interpretation of this? Consider the following:

The amplitude of the wave function of the electron (hole) has a certain finite, non-zero value at various places inside the quantum box. This means the electron (hole) has a better probability to "exist" at some coordinates than at others. Therefore electron (hole) has a probability to "exist" at various places (albeit discrete places) inside the quantum box (if it is trapped inside!). But now, because a Coulomb force is also working in on the electron (hole) the "amount" of allowed existing points are altered, i.e. different from the situation if the electron was only in the box by itself. (This is like a particle trapped in a box, which is trapped in another box, since there are 2 confining potentials: the quantum confinement potential and the Coulomb potential!) Thus, since the electron and hole are only allowed to exist at places where the distance between them is given by *a* and *b* (inside an already discrete system due to the quantum confinement!), these are the positions/points of interest! Those "other" existing points will not be allowed since then the electron and hole won't be separated by (*a, b*). Thus, for such a situation, the Coulomb force would not be "turned on". Now since the Coulomb force is a continuous force, all values for *a* and *b* from 0 to ∞ are expected! So these values must conform to the quantum confinement, and not the other way around.

Of course this depends on the specific choice of the quantum confining potential. If $V_{Conf.}$ is infinite, *a* and *b* can be equal to L_y and L_z at maximum. If however a finite confining potential is used, and tunnelling is possible, then *a* and *b* can reach up to ∞. The upper integration parameters (for the appropriate integrals) will be adjusted for this condition.

Now consider:

$$\int\limits_{0}^{2\infty}\int\limits_{0}^{2\infty} \int\limits_{-\infty}^{+\infty}\int\limits_{-\infty}^{+\infty}\int\limits_{-\infty}^{+\infty}\int\limits_{-\infty}^{+\infty} j_e^2(z_e, y_e) j_h^2(z_h, y_h) G(a,b)\ dz_e dz_h dy_e dy_h \ \times$$

$$\left[d\left(z_{\underset{z}{\mathbf{123}}} - a, y_{\underset{y}{\mathbf{123}}} - b \right) + d\left(z_h - z_e - a, y_h - y_e - b \right) \right] dadb \tag{4.4.12}$$
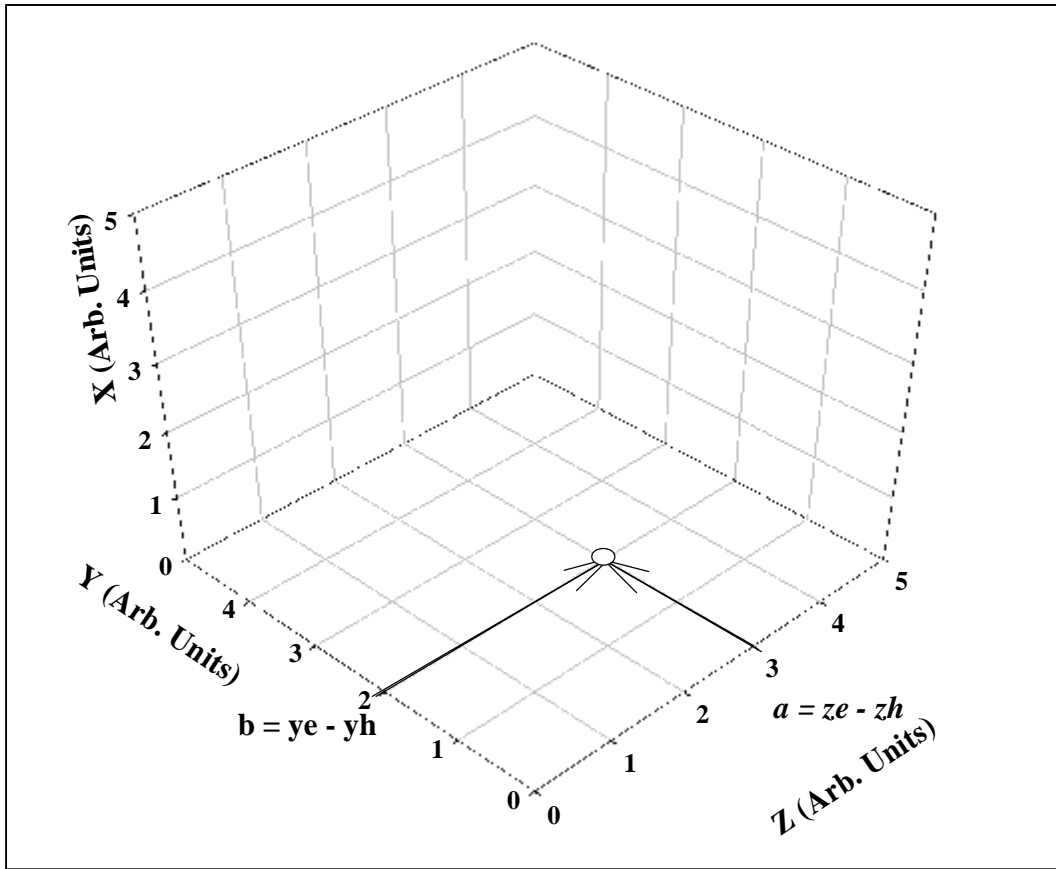
Figure 4.4.1: An example of a point where the amplitude of the wave squared might have a finite, non-zero probability.

The wave functions exist at points in a plane. In order for the δ-distribution to have a non-zero value somewhere, one must integrate over *dy* and *dz **at the same time.*** But since this is impossible, this δ-distribution must be redefined! Let:

$$\overset{\text{uu}}{\boldsymbol{p}_e} = (z_e, y_e) = \text{Position Vector of electron} \qquad (4.4.13)$$

and

$$\overset{\text{uu}}{\boldsymbol{p}_h} = (z_h, y_h) = \text{Position Vector of hole} \qquad (4.4.14)$$

Also, let:

$$\overset{\text{\tiny{I}}}{\boldsymbol{s}} = \overset{\text{uu}}{\boldsymbol{p}_e} - \overset{\text{uu}}{\boldsymbol{p}_h} = (z_e - z_h, y_e - y_h) = (a, b) \qquad (4.4.15)$$
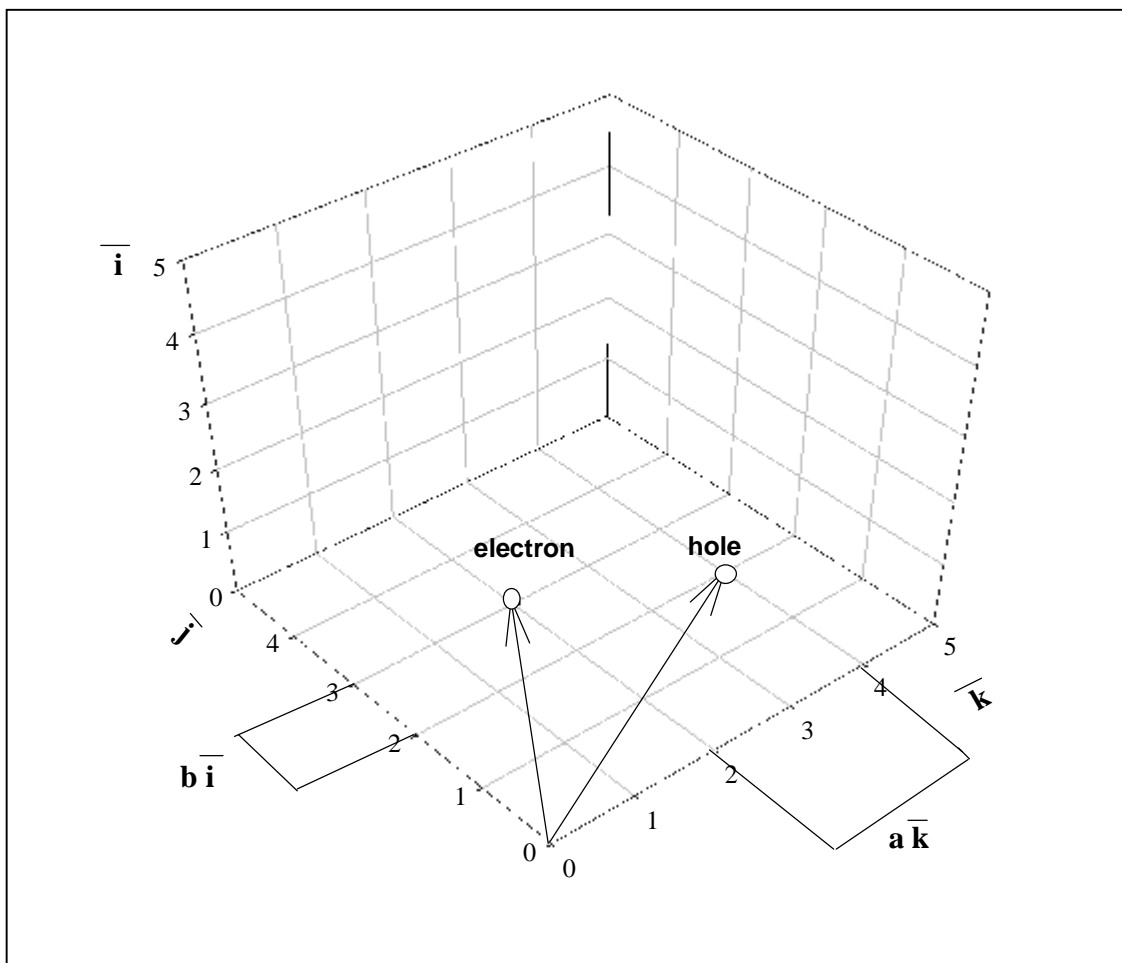
Figure 4.4.2.: Representation of the different vector components.

Now the integral (4.4.12) can be written as:

$$\int\limits_{0}^{2\infty} \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} j_e^{\,2}(\vec{p}_e)\, j_h^{\,2}(\vec{p}_h)\, G(\vec{s}) \times \left[d\left(\vec{p}_e - \vec{p}_h - \vec{s}\right) + d(\vec{p}_h - \vec{p}_e - \vec{s}) \right] d\vec{s} \qquad (4.4.16)$$

$$\int\limits_{0}^{2\infty} \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} j_e^{\,2}(\vec{p}_e)\, j_h^{\,2}(\vec{p}_h)\, G(\vec{s})\, d\vec{p}_e\, d\vec{p}_h \times \left[d\left(\vec{p}_e - \vec{p}_h - \vec{s}\right) \right] +$$

$$\int\limits_{0}^{2\infty} \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} j_e^{\,2}(\vec{p}_e)\, j_h^{\,2}(\vec{p}_h)\, G(\vec{s})\, d\vec{p}_e\, d\vec{p}_h \times \left[d\left(\vec{p}_h - \vec{p}_e - \vec{s}\right) \right] d\vec{s} \qquad (4.4.17)$$

Performing the integration over $\vec{p}_h$ first leaves:

1st Term: Finite value when:

$$\vec{p}_h = \vec{p}_e - \vec{s} \qquad (4.4.18)$$

2nd Term: Finite value when:

$$\vec{p}_h = \vec{p}_e + \vec{s} \qquad (4.4.19)$$

Hence:

$$\int\limits_{0}^{2\infty} \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} \left| j_e^{\,2}(\vec{p}_e) \right| \left| j_h^{\,2}(\vec{p}_e - \vec{s}) \right| G(\vec{s})\, d\vec{p}_e\, d\vec{s} + \int\limits_{0}^{2\infty} \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} \left| j_e^{\,2}(\vec{p}_e) \right| \left| j_h^{\,2}(\vec{p}_e + \vec{s}) \right| G(\vec{s})\, d\vec{p}_e\, d\vec{s} \qquad (4.4.20)$$

Let $\vec{p} = \vec{p}_e - \vec{s} = (z, y) = (z_e, y_e) - (a, b) = (z_e - a,\, y_e - b)$ in the first term. Then:

$$\vec{p}_e = \vec{p} + \vec{s} \qquad (4.4.21)$$

Therefore $d\overset{\rightharpoonup}{p} = d\overset{\rightharpoonup}{p_e}$; since $\vec{s}$ is a constant.

Now, remember that the infinite integration parameters as given in the equations in this section are actually "effective infinities":

$$m = -\infty, n = +\infty, r = -\infty, t = +\infty \tag{4.4.22}$$

(as given in section 4.2.) The integration parameters for equation (4.4.20) will now change according to this new definition with $\overset{\rightharpoonup}{p}$. First consider the lower integration parameters, i.e. μ ($= -\infty$) and $\rho($ $= -\infty):$

$$\overset{\rightharpoonup}{p_e} = \overset{\rightharpoonup}{p} + \vec{s}$$
$$\overset{\rightharpoonup}{p_e} = (z + a, y + b) \tag{4.4.23}$$

Replace the variables over which will be integrated with the lower integration parameters:

$$\overset{\rightharpoonup}{p_e} = (m + a, r + b) = (z_e, y_e) \tag{4.4.24}$$

Now it can be written (since $\overset{\rightharpoonup}{p} = \overset{\rightharpoonup}{p_e} - \vec{s} = (z_e - a, y_e - b)$) :

$$
\begin{aligned}
z &= (z_e) - a \\
&= (m + a) - a \\
&= m
\end{aligned}
$$

$$
\begin{aligned}
y &= (y_e) - b \\
&= (r + b) - b \\
&= r
\end{aligned}
\tag{4.4.25}
$$

And thus the new lower integration parameter will be:

$$\vec{p}_{lower} = (m, r) \qquad (4.4.26)$$

The same procedure applies for the upper integration parameters, $v(=+\infty)$ and $\tau(=+\infty)$:

Since:

$$z_e = n \qquad (4.4.27)$$

and

$$y_e = t \qquad (4.4.28)$$

It can be written:

$$
\begin{aligned}
z_e &= (z_e) - a \\
&= n - a \\
y_e &= (y_e) - b \\
&= t - b
\end{aligned} \qquad (4.4.29)
$$

And thus:

$$\vec{p}_{upper} = (u - a, t - b) \qquad (4.4.30)$$

Subsequently, by making all the appropriate substitutions in the first term, equation (4.4.20) can be written as:

$$\int_{0}^{s=(n-m)} G(s) \int_{\vec{p}=(m,r)}^{\vec{p}=(u-a,t-b)} |j_e^2(\vec{p}+\vec{s})||j_h^2(\vec{p})| \, d\vec{p} d\vec{s} + \int_{0}^{s=(u-m)} G(s) \int_{\vec{p}=(m,r)}^{\vec{p}=(n-a,t-b)} |j_e^2(\vec{p}_e)||j_h^2(\vec{p}_e+\vec{s})| \, d\vec{p}_e d\vec{s}$$

$$(4.4.31)$$

Now, rename $\overset{\rightharpoonup}{p_e}$ to $\overset{\rightharpoonup}{p}$ in the 2nd term. Then:

$$\overset{\overset{\mathbf{r}}{s=(n-m)}}{\underset{0}{\int}} G(s) \left[\overset{\overset{\mathbf{r}}{p=(u-a,t-b)}}{\underset{p=(m,r)}{\int}} |j_e^2(\mathbf{p}+s)||j_h^2(\mathbf{p})|\,d\mathbf{p} + \overset{\overset{\mathbf{r}}{p=(n-a,t-b)}}{\underset{p=(m,r)}{\int}} |j_e^2(\mathbf{p})||j_h^2(\mathbf{p}+s)|\,d\mathbf{p} \right] \quad (4.4.32)$$

And then:

$$A = DE_e - \frac{\mathbf{h}^2}{2m_e^*} \overset{\overset{\mathbf{r}}{s=(u-m)}}{\underset{0}{\int}} G(s)\,p(s)\,ds \quad (4.4.33)$$

$$A = DE_e - \frac{\mathbf{h}^2}{2m_e^*} \overset{u-m}{\underset{0}{\int}} G(a,b)\,p(a,b)\,dadb \quad (4.4.34)$$

A similar procedure can be applied to the terms **B** and **C** to show the validity of the introduced *a* and *b* parameters.

4.5   Specific choice for the Envelope Function φ_r

With these equations now in hand, this section shows the solution to the probability term p(y,z) and discusses the difference between an infinite and finite confining potentials to the model at hand.

Further simplification of equations (4.2.13) through to (4.2.24) requires a specific choice of the envelope function φ_r. The function (a similar form is often used in literature) [13,**Error! Reference source not found.**,**Error! Reference source not found.** among others]

$$y_r = e^{-\left(\frac{\sqrt{x^2 + \Omega^2(y_e - y_h)^2 + z^2(z_e - z_h)^2}}{l} \right)} \quad (4.5.1)$$

is chosen as the trial wave function describing the relative motion of the electron hole pair. Here Ω, ζ and λ are chosen as variational parameters with the first two being dimensionless and λ having units of Å, representing the distance between the electron and the hole.

Once the choice for this function has been made with the appropriate variational parameters it is a simple matter of minimizing the total energy E (4.2.11) via a variational calculation:

$$E = E_g + E_e + E_h + \left[\frac{-\dfrac{\mathbf{h}^2}{2m}\left[\int p(y,z)G(y,z)dydz + \int p(y,z)J(y,z)dydz\right] - \dfrac{e^2}{4pe}\int p(y,z)K(y,z)dydz}{\displaystyle\int\limits_{0}^{n\text{-}m}\int\limits_{0}^{t-r} F(y,z)p(y,z)dydz} \right] \quad (4.5.2)$$

$$E = E_g + E_e + E_h + E_b \quad (4.5.3)$$

$$E_b = \left[\frac{-\dfrac{\mathbf{h}^2}{2m}\left[\int p(y,z)G(y,z)dydz + \int p(y,z)J(y,z)dydz\right] - \dfrac{e^2}{4pe}\int p(y,z)K(y,z)dydz}{\displaystyle\int\limits_{0}^{n\text{-}m}\int\limits_{0}^{t-r} F(y,z)p(y,z)dydz} \right] \quad (4.5.4)$$

where E_b is the binding energy of the exciton. An important point to note is that in the current formalism of solving (4.5.2) the binding energy can be calculated *independent* of the single particle eigenvalues. Thus the binding energy of the exciton can be found by simply minimizing E_b (i.e. maximizing $|E_b|$, since E_b will be negative as long as the electron is bound to the hole).

Another important point to note is the presence of the single particle wave functions (the eigenfunctions φ_e and φ_h) in the binding energy term E_b via the probability equation $p(y,z)$ (4.2.15). This will allow the binding energy to have a finite confining potential character even if an infinite confining potential is used. Also, different confining potential shapes can easily be incorporated into the binding energy term, by simply adjusting the single particle eigenfunctions in $p(y,z)$ appropriately to the chosen confining potential shape.

In order to show the effectiveness of the current formalism, an infinite rectangular confining potential is used, i.e.

$$V_e = V_h = \theta(|z_e|-L)V_\infty \tag{4.5.5}$$

where $\theta(z)$ is the Heaviside unit step function.

Note now that choosing the confining potential as above will have no effect on the binding energy term whatsoever. The only effect it will have will be on the range of the integration parameters and on the choice of the single particle eigenfunctions, φ_e and φ_h, in the probability term $p(y,z)$ as these eigenfunctions will now be similar to that of the particle confined in a 2D box:

$$\varphi_e(y_e,z_e)=\varphi_h(y_h,z_h)=\sqrt{\frac{4}{L_y L_z}}\sin\left(\frac{\pi y}{L_y}\right)\sin\left(\frac{\pi z}{L_z}\right) \tag{4.5.6}$$

where only the ground-state is being considered ($n = 1$).
This will lead to $p(y,z)$ having the form:

$$p(y,z) = \frac{1}{4L_y{}^2 L_z{}^2 p} \left(\left[4p(L_y - y) - 2p(y - L_y)\cos\left[\frac{2py}{L_y}\right] + 3L_y\sin\left[\frac{2py}{L_y}\right] \right] \times \right.$$
$$\left. \left[4p(L_z - z) - 2p(z - L_z)\cos\left[\frac{2pz}{L_z}\right] + 3L_z\sin\left[\frac{2pz}{L_z}\right] \right] \right) \tag{4.5.7}$$

Now, for a finite confining potential it is usually the convention to use:

$$V_{confining} = 0 \text{ for } 0 \leq y,\ z \leq L_{y,z}$$
$$V_{confining} = V_0 \text{ for } y,z > L_{y,z}$$

and hence:

$$j(y,z) = \begin{bmatrix} Ae^{-K|y|}e^{-K|z|} & \text{for } |y,z| \geq L_{y,z} \\ B\sin ky \sin kz & \text{for } 0 \leq |y,z| \leq L_{y,z} \end{bmatrix} \tag{4.5.8}$$

Thus, the single particle eigenfunctions has the same form inside the confined region, whether a finite or infinite potential model is used, and in the finite potential model only an exponential decay term is "added" during the integration. Thus as the integration range is only over the confined region in the infinite potential model, and the integration range is over the entire space, the only difference between these two integrand solutions should be the effect of this decaying ("tunnelling") exponential part. The effect of this will be to *lower* the calculated energy values as will be seen in Chapter 5: Results and Discussion. Figure 4.5.1 and Figure 4.5.2 show a comparison between the single particle probability densities for an infinite and finite potential well. Both particles are trapped in a Quantum Well-Wire of dimensions 10 Å.
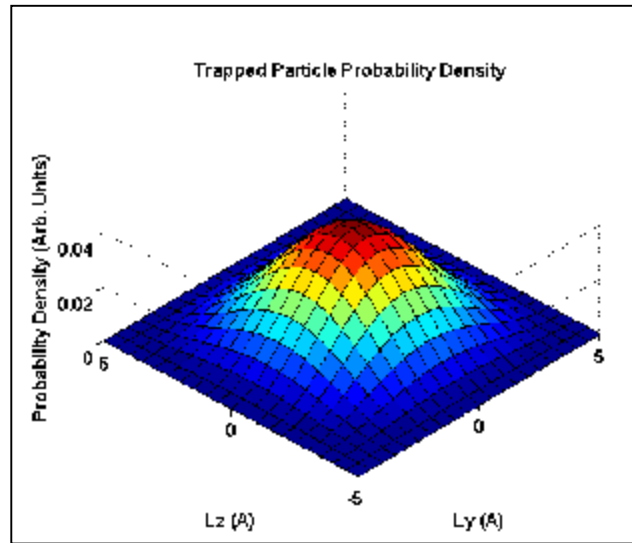
Figure 4.5.1: The probability density for a single particle trapped in a
infinite potential well with Quantum Well – Wire dimensions
$L_y = L_z = 10 \, Å$
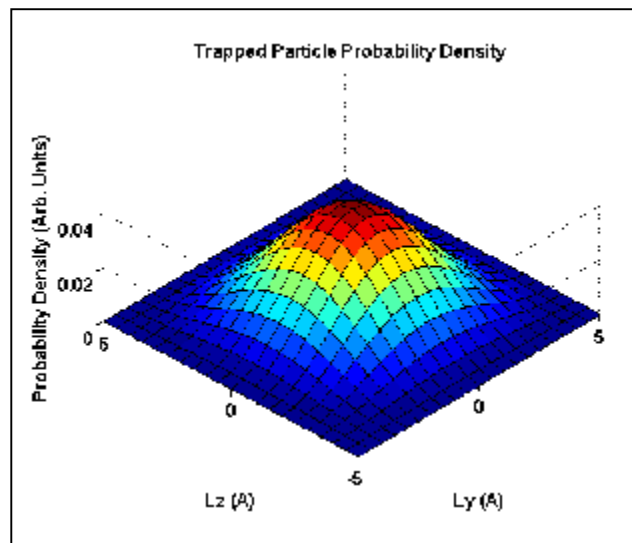
Figure 4.5.2 The probability density for a single particle trapped in a finite
potential well with Quantum Well – Wire dimensions
$L_y = L_z = 10 \, Å$

From figures 4.5.1 and 4.5.2, it is clear that the *shape* of the two probability densities (from the middle of the box outward) is more or less the same within the box parameters.

Hence, the presence of the single particle eigenfunctions in the binding energy term via $p(y,z)$ gives the binding energy a finite confining potential character regardless of whether an infinite confining potential is used for V_e and V_h.

It is also useful to see that the unitarily principle (conservation of probability) is not violated:

$$\int_0^{L_y} \int_0^{L_z} \frac{1}{4L_y{}^2 L_z{}^2 \boldsymbol{p}^2} \left(\begin{array}{l} \left(4(-y+L_y)\boldsymbol{p} - 2(y-L_y)\boldsymbol{p}\ cos\left[\dfrac{2yp}{L_y}\right] + 3L_y\ sin\left[\dfrac{2yp}{L_y}\right] \right) \times \\ \left(4(-z+L_z)\boldsymbol{p} - 2(z-L_z)\boldsymbol{p}\ cos\left[\dfrac{2zp}{L_z}\right] \right) \end{array} \right) dzdy = 1$$

(4.5.9)

as it should be for a infinite confining potential .

4.6   Simplification via substitution and differentiation

The functions $F(y,z)$, $G(y,z)$, $J(y,z)$ and $K(y,z)$ are simplified in ***Appendix A: Mathematical Solutions***. The main idea there is to simplify the integration parameters which are from *0* to ∞, to between *0* and *1*. This is done in order to increase the accuracy and calculation time of the final numerical solution to these equations. The solution to the probability equation, $p(y,z)$, is also shown in the same appendix. These functions are then solved numerically and minimized with a software program custom developed (in a Windows environment with a Visual Basic 6.0 platform) specifically for these functions and the solutions are incorporated in the binding energy equation, equation (4.5.4), to minimize this binding energy and hence to find the ground state solution to the binding energy.

4.7   Summary of final equations

In this section a summary of the equations that are simplified, and then solved numerically to minimize the exciton binding energy, E_b, as given by equation (4.5.4) is presented.

The binding energy term is as follows:

$$E_b = \left[\frac{-\dfrac{\mathbf{h}^2}{2m}\left[\int p(y,z)G(y,z)dydz + \int p(y,z)J(y,z)dydz \right] - \dfrac{e^2}{4pe}\int p(y,z)K(y,z)dydz}{\displaystyle\int_0^{n\text{-}m}\int_0^{t-r} F(y,z)p(y,z)dydz} \right] \qquad (4.7.1)$$

The terms $F(y,z)$, $G(y,z)$, $J(y,z)$ and $K(y,z)$ are then substituted into equation (4.7.1):

$$F(y,z) = \sqrt{R}\int_0^1 \left[\frac{(1-x^2)}{x^2} \right]\left| \exp\left(-\frac{2\sqrt{R\left(\left[1/2\left(1/x+x\right)-1\right]^2+1\right)}}{1} \right) \right| dx \qquad (4.7.2)$$

$$G(y,z)=\sqrt{R}\int_0^1\left[\frac{1-x^2}{x^2}\right]\left[\frac{e^{\frac{2\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right)^2\right]}}{1}}}{1^2\left(R\left(1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right)^2\right)\right)^{3/2}}\right]\left[\left(-1R\left(1-\frac{1}{2}\left(\frac{1}{x}+x\right)\right)^2\left(z^2+\Omega^2\right)+z^2\left[\Omega^2b^2+\Omega^2a^2+\left(\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right)^2\right]}\right)(R)\right]\right]\right]dx$$

$$(4.7.3)$$

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$$J(y,z) = \sqrt{R} \int_0^1 \left[\frac{(1-x^2)}{x^2} \right] \left[\frac{e^{-\frac{R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)}{l^2}}}{l^2\left(R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)\right)^{3/2}} \right] \left[\left(\frac{R\left(-1+\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2\times\right.}{\sqrt{R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)}} \right) \right] dx$$

(4.7.4)

$$K(y,z) = \sqrt{R} \int_0^1 \left[\frac{1-x^2}{x^2} \right] \frac{\left(e^{-\frac{\sqrt{R\left(1+\left[\frac{1}{2}\left(\frac{1}{x}+x\right)\right]\right)^2+1}}{l}} \right)^2}{\left(R\left(\left[\frac{1}{2}\left(\frac{1}{x}+x\right)\right]-1\right)^2+b^2+a^2 \right)^{1/2}} dx \qquad (4.7.5)$$

And finally the probability equation is as follows (remember that $a = z$ and $y = b$):

$$p(y,z) = \frac{1}{4L_y^2 L_z^2 p} \left[\begin{array}{l} \left(4(L_y - b)p - 2(b - L_y)p \cos\left[\frac{2bp}{L_y}\right] + 3L_y \sin\left[\frac{2bp}{L_y}\right] \right) \times \\ \left(4(L_z - a)p - 2(a - L_z)p \cos\left[\frac{2ap}{L_z}\right] + 3L_z \sin\left[\frac{2ap}{L_z}\right] \right) \end{array} \right] \quad (4.7.6)$$

Equation (4.7.6) is also substituted into equation (4.7.1).

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'*The secret to creativity is knowing how to hide your sources. '*

- Albert Einstein

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Chapter 5
Results and Discussion

'The great tragedy of science - the slaying of a beautiful hypothesis by an ugly fact.'

- Thomas Huxley

R*esults of the numerical calculations (as discussed in Chapter 4) are presented in this chapter. Quantitative comparisons with previous calculations for Quantum Wells are made (in the wire limit where $L_z \rightarrow \infty$) to find a good agreement between finite and infinite potential models up to a point of 100 Å.*

Using the appropriate parameters for the GaAs well in the GaAs/AlGaAs system ($m_e* = 0.067$, $m_h* = 0.45$, $\varepsilon = 12.53$) a variational calculation for Quantum Well Wire sizes ranging from $L_y = L_z = 3000$ Å ('effective infinity") to 0 Å has been done.

Note that atomic units where used throughout this chapter (where $\hbar = e^2/2 = 2m = 1$) unless stated otherwise [1].

Figure 5.1 is presented as the result of such a calculation.
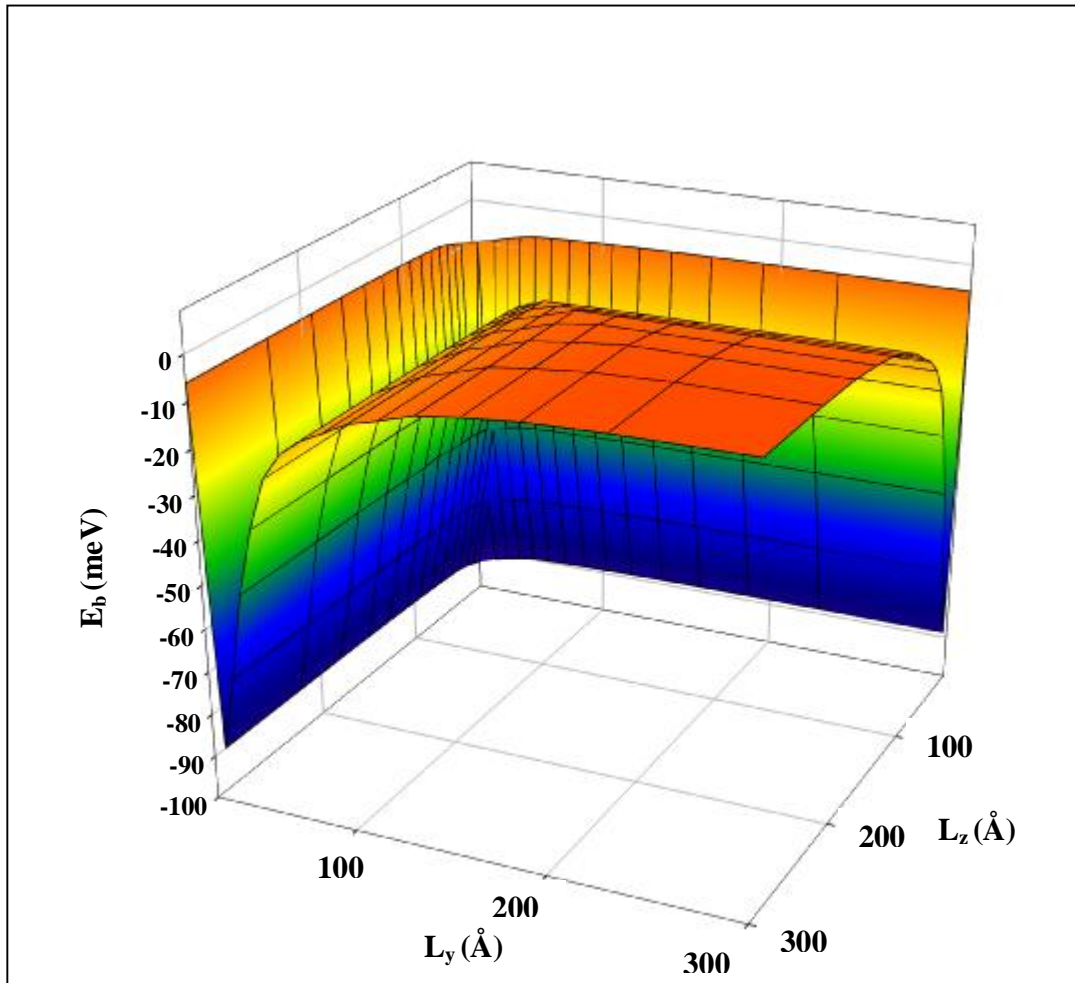
Figure 5.1 Exciton binding energy as a function of Quantum Well-Wire parameters L_y and L_z

Notice that the binding energy of the exciton is negative, as it should be for any bound system. For clarity figure 5.1 is presented in an inverted fashion in figure 5.2
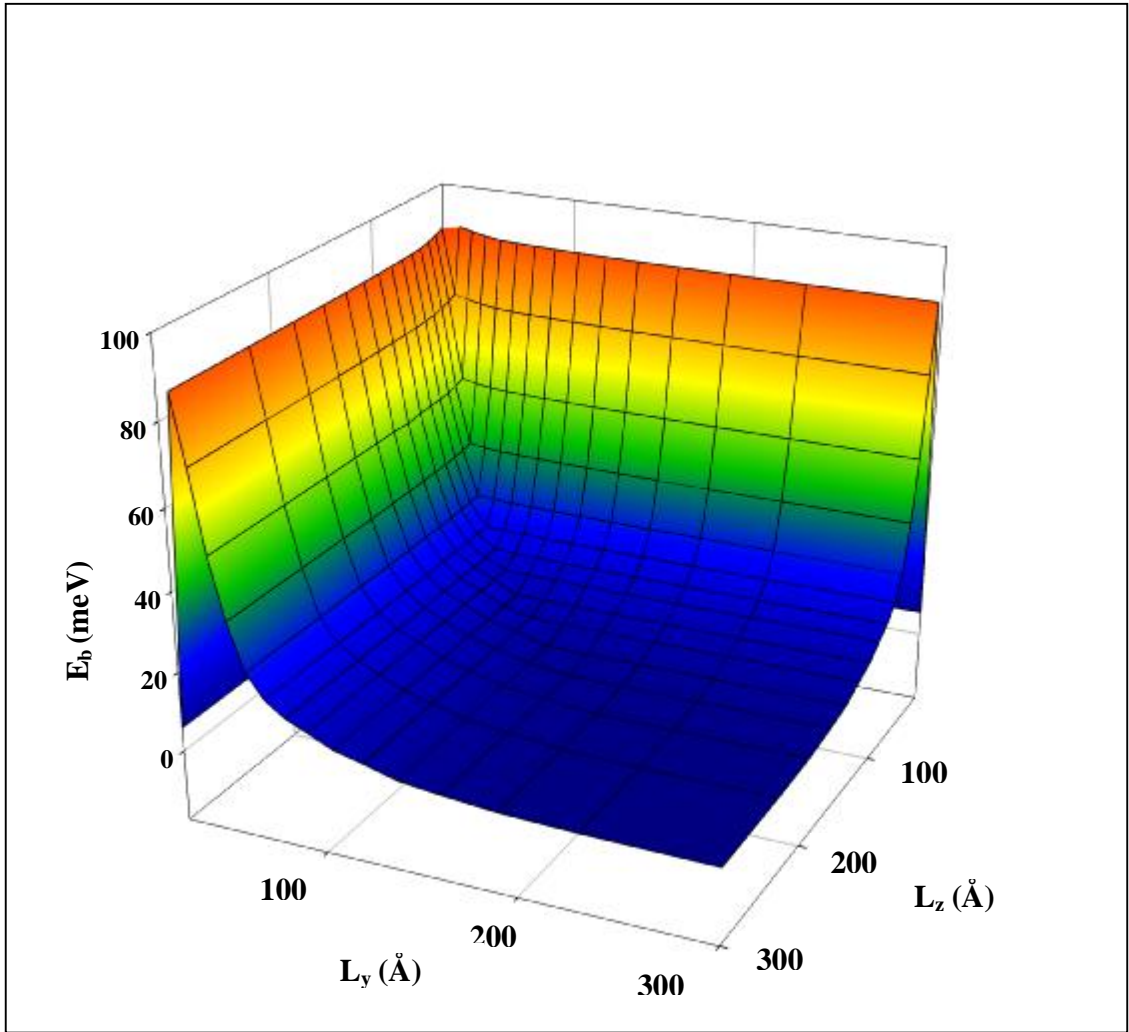
Figure 5.2 Inverted exciton binding energy as a function of Quantum Well - Wire parameters L_y and L_z

A few things are noteworthy on this figure. Firstly it is clear that for large parameters L_y and L_z, the exciton binding energy approaches that of the bulk material namely *5.048 meV* [2]. It is known that when the well becomes infinitely wide the confined exciton should behave like a free exciton, i.e. the one-particle wave functions become more widespread and begin to resemble free Bloch states which constitute free excitons found in bulk crystals, [3 - 4] i.e.

$$\lim_{Lw \to \infty} E_b = E_b^{free} \tag{5.1}$$
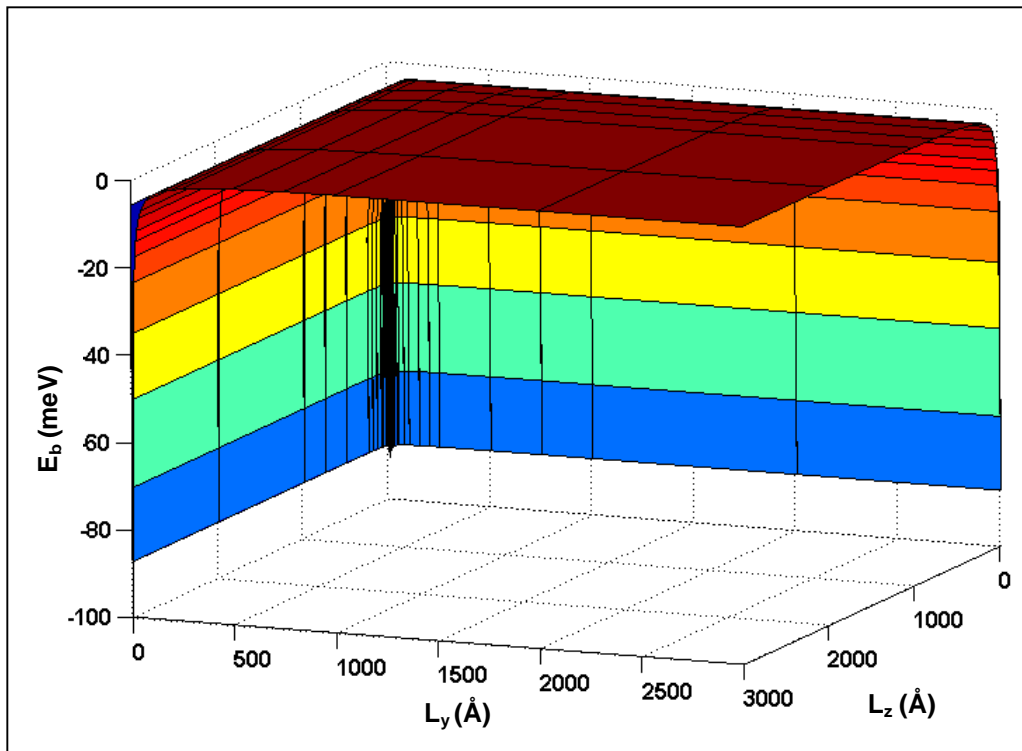
***Figure 5.3: Binding energy versus L_y and L_z for extended Quantum Well Wire
parameters***

Figure 5.3 shows the exciton binding energy as a function of the Quantum Well-Wire parameters for L_y and L_z extended to the "effective infinity" of *3000 Å*. Detailed analysis of the calculation results show that the onset of significant change in the binding energy of the exciton as it moves away from the bulk value of *5.048 meV*, is at about *100 Å*. This size range corresponds to the regime of quantum confinement: in this regime the spatial extent of the single particle wave functions are comparable with the Quantum Well-Wire size (in at least one dimension). As a result of these "geometrical" constraints, the electron – hole pair is very responsive to the presence of the well-wire borders and react to changes in well-wire size by adjusting their energy. (This phenomenon is known as the quantum – size effect) [5]
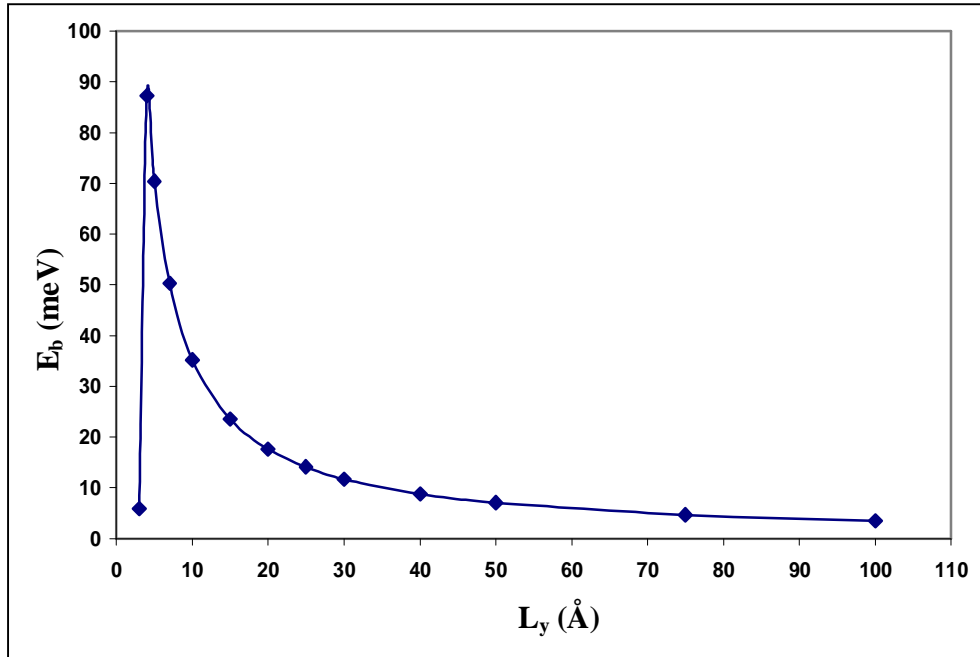
Figure 5.4: Binding energy versus L_y. The z - dimension is extended to infinity to approach the quantum well limit.

Figure 5.4 shows the binding energy of the Quantum Well–Wire when the L_z parameter is taken to be infinitely wide and the quantum well limit is approached, i.e. two spatial dimensions (*z* and *x*) are of infinite extent and one dimension (*y*) is in the same size order as the electron and hole wave functions.

Two limiting situations can be observed: an infinitely wide well, $L_z \rightarrow \infty$, and an infinitely narrow well, $L_z \rightarrow 0$. For the first situation, the exciton takes the bulk-barrier character. For the latter case, the carrier wave function spreads and penetrates into the barriers, making the binding energy decrease towards the value appropriate to the bulk material. For intermediary well width values, when increasing confinement, the binding energy is enhanced and then displays a maximum for a critical width value. This line shape of E_b (L_y) seems then to be characteristic of *2D* quantum well systems independent of the profile of the confining potential [4].

Figure 5.5 shows a comparison between the results of the present dissertation and previous research. The different calculations with different potentials give similar results for well dimensions up to about *100 Å*. Important to notice is that, an increase in the confining potential, leads to an increase in the value of the maximum as well as a shift to smaller spacing of this maximum peak. Hence, since in the current research an "effective infinity" was used, it is expected that the maximum/peak should also rise to "effective infinity" and be shifted towards smaller spacing to be equal to infinity at $L_y \approx 0$. From figure 5.4 it can be seen that this peak lies at $L_y = 4 \, Å$.
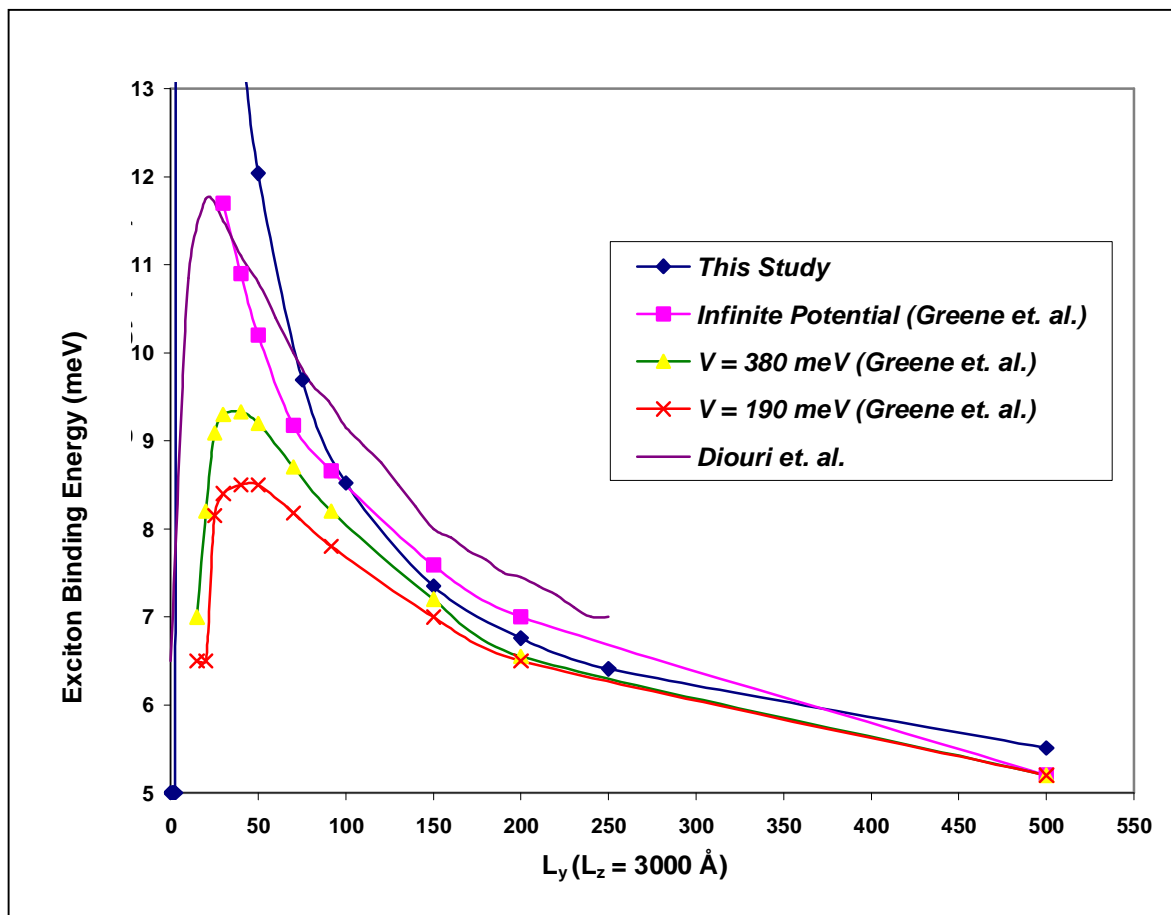
Figure 5.5: ***Results for different quantum well potentials [Greene et. al. [6], Diouri et al [4]]***
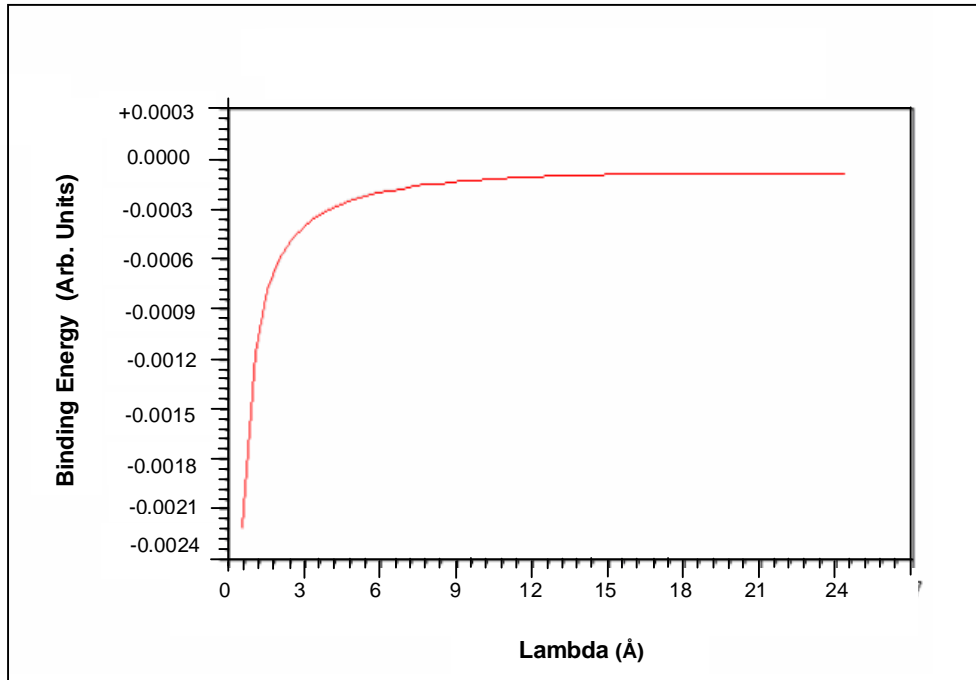
Figure 5.6: Plot of binding energy vs. the variational parameter λ for
$$L_z \rightarrow \infty \text{ and } L_y \rightarrow \infty$$

A plot of the binding energy versus the variational parameter λ (representing the distance between the electron and the hole) for Quantum Well-Wire parameters approaching infinity ($L_z \rightarrow \infty$, $L_y \rightarrow \infty$), gives the expected binding energy curve similar to that of an electron inside a Hydrogen atom. When the electron is close to the hole, the binding energy value is very large and negative, but as the electron is moved further away from the hole, the binding energy approaches zero to be essentially free at infinity.

However when the Quantum Well –Wire parameters approaches zero ($L_y \rightarrow 0$, $L_z \rightarrow 0$) something quite different is observed. Figure 5.7 shows a plot of the binding energy vs. the variational parameter λ for the above described situation. (This graph has not yet been scaled, since the axis values of this graph are not of importance now, but only the graph trend).
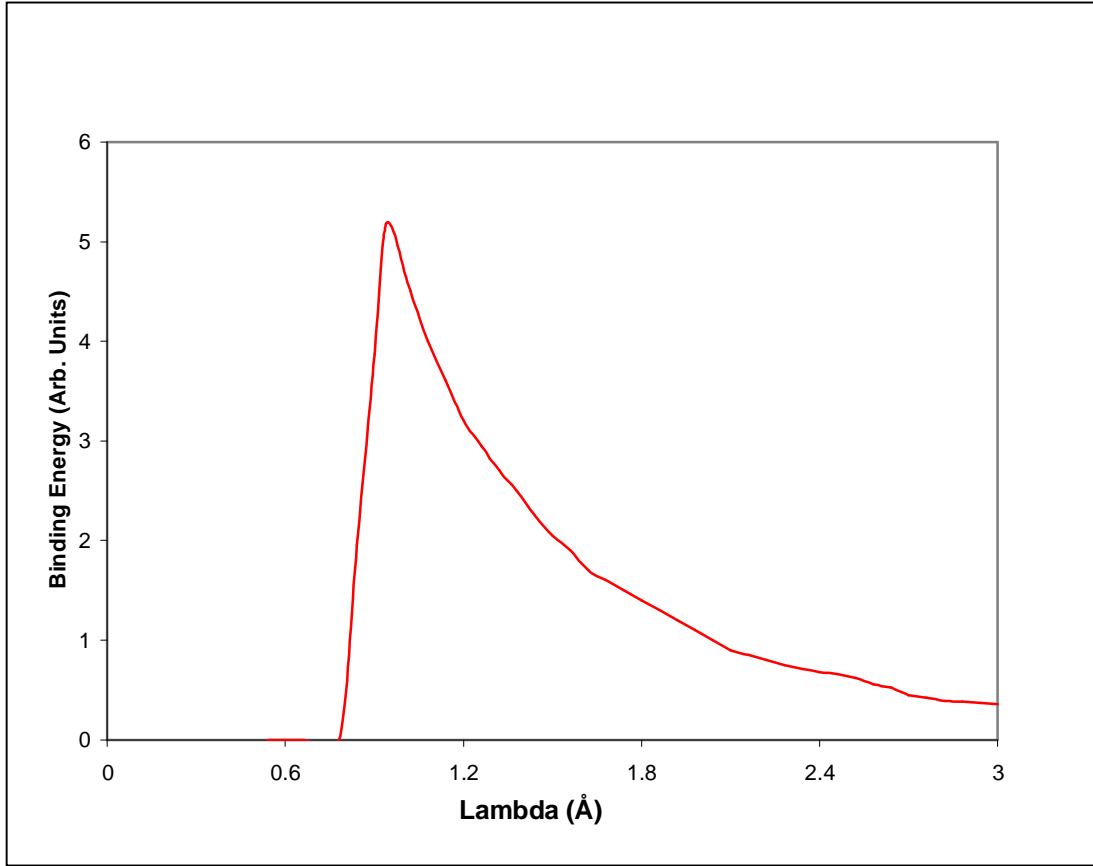
Figure 5.7: Plot of binding energy vs. variational parameter λ for zero
$L_y \rightarrow 0$ and $L_z \rightarrow 0$ (Note that this graph has not yet been scaled)

It is clear from the figure that the binding energy *increases* positively as the electron approaches the hole. It appears that the hole is now repelling the electron! This can be best explained by looking at what happens inside the valence band as the Quantum Well-Wire is reduced in size. For L_y and $L_z \rightarrow \infty$, the electrons in the valence band, fills up a relatively large region of real space (the entire crystal with bulk parameters) compared to the region of real space it fills up when the crystal is reduced in size, i.e. when L_y and $L_z \rightarrow 0$. Now, taking into account that the number of electrons in the valence band have not been reduced (the dielectric constant of the medium has not changed, i.e. $\varepsilon \neq \varepsilon(L_y, L_z)$) the electron density has increased since the size of the Quantum Well-Wire has been reduced. Hence the density of the electrons now screening the hole in the valence band from the other excitonic component (the electron part of the exciton, i.e. the electron in

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the conduction band, bound to the hole in the valence band) has increased. Consequently it becomes increasingly more difficult for the electron and hole to recombine due to the repulsion/screening of the other electrons in the valence band as the size of the Quantum Well-Wire is reduced. In fact, an amount of energy will have to be added to the electron in order for the electron to penetrate this repulsive screening "layer" of electrons in order for the electron and hole to recombine.

Now the above would obviously not hold for Quantum Well-Wires grown via some or other chemical process, i.e. the above is not true for a Quantum Well-Wire with a fixed size, since the amount of electrons in the VB acting as screening electrons remain constant and the size of the Quantum Well-Wire does not change. Thus the above does not mean that Quantum Well-Wires with dimensional parameters → *0* will all exhibit this property. For theoretically predicting the behaviour of systems like these it is important to include in such a model not only the different dielectric constants for the barrier and the well-wire materials (as has been done often in literature [3,7]), but also to include *the change in dielectric constant due to a change in size*, *i.e. $\varepsilon = \varepsilon$ (L),* i.e. to take into account the decrease in the amount of electrons in the VB due to a decrease in size of the Quantum Well-Wire.

However for Quantum Well-Wire systems where the amount of electrons in the VB remains constant, even as the size of the Quantum Well-Wire is reduced, the above would hold. This might be achieved by applying a confining potential in the form of an electric field and then systematically changing the position of that electric field as to confine an ever smaller and smaller region of space while at the same time (via this confining electric field) forcing all the electrons in the VB into this smaller region of space.

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Chapter 6

Conclusion and Future Work

'Where were you, when I set the foundations of the earth? Tell me, if you have understanding. Who set its measurements, if you know, or who stretched a line over it? Upon what have its bases been grounded, and who set forth its cornerstone...'

- Job 38: 4-6

$\mathbf{A}$ theoretical method presented by Harrison *et. al.* was expanded to do a variational calculation within the envelope function and effective mass approximations on the binding energy of an electron hole pair trapped in an infinite confining potential in a quantum well-wire. A three parameter trial wave function, in which the symmetry of the component of the wave function representing the relative motion is allowed to vary from the one- to the two- and three-dimensional limits was used, however the technique can be used for any choice of trial wave function.

Results of these numerical calculations were presented. Quantitative comparisons with previous calculations for quantum wells were made (in the wire limit where $L_z \rightarrow \infty$) and it was found that there exists a good agreement between this infinite- and other finite- as well as infinite - potential models up to a point of *100 Å*.

A plot of the binding energy versus the variational parameter λ revealed that the electron in the exciton has a very similar behaviour to the electron in the hydrogen atom (or for that matter any particle trapped inside a radial decreasing (i.e. *V~1/r*) potential field). However on reducing the size and dimensions of the quantum structure, it seems that the screening of the other electrons surrounding the hole start to play a very important role and the shape of a plot of binding energy versus λ is very similar to that of an alpha particle trapped in an atomic nucleus. Further study on this is required.

It is concluded from this that for accurately predicting the behaviour of systems like these it is important to include in such a model not only the different dielectric constants for the barrier and the well-wire materials, but also to include *the change in dielectric constant due to a change in size*, *i.e. $\varepsilon = \varepsilon$ (L),* i.e. to take into account the decrease in the amount of electrons in the VB due to a decrease in size of the Quantum Well-Wire.

Future work could include adapting the model for finite potentials as well as adjusting the confining potentials appropriate to calculate exciton binding energies for cylindrical, T-shaped and all sorts of different shaped Quantum Wires.

Appendix A

Mathematical Solutions

'Don't worry about your problems with mathematics, I assure you: mine are much greater'

- Albert Einstein, in a letter to a high school student Barbara Wilson, 7 January 1943

$\textbf{T}$his section proceeds to prove the validity of the equations used as well as present the solutions to these equations

First note that, for this section the following holds:

$$r'^2 = (x_e - x_h)^2 + (y_e - y_h)^2 + (z_e - z_h)^2$$

$$r'^2 = x_\perp{}^2 + \Omega^2 b^2 + z^2 a^2$$

$$r' = \sqrt{x_\perp{}^2 + \Omega^2 b^2 + z^2 a^2}$$

_F(a,b)_

Consider the term _F(a, b)_, from equation (4.2.13), where _x_ has been called $x_\perp$:

$$F(a,b) = \int_{-\infty}^{+\infty} |j_r|^2 dx_\perp$$

$$= 2\int_{0}^{+\infty} |j_r|^2 dx_\perp$$

$$= 2\int_{0}^{+\infty} \left| \exp\left(-\frac{r'}{l}\right) \right|^2 dx_\perp$$

$$= 2\int_{0}^{+\infty} \left| \exp\left(-\frac{\sqrt{\left(x_\perp^2 + \Omega^2 b^2 + z^2 a^2\right)}}{l}\right) \right|^2 dx_\perp$$

$$= 2\int_{0}^{+\infty} \left| \exp\left(-\frac{2\sqrt{\left(x_\perp^2 + \Omega^2 b^2 + z^2 a^2\right)}}{l}\right) \right| dx_\perp$$

Now:

Let $\underline{x_\perp = -\sqrt{R} + x}$ where $\underline{R = \Omega^2 b^2 + z^2 a^2}$

$x_\perp^2 = (-\sqrt{R} + x)^2$

Then $x = x_\perp + \sqrt{R}$

And $\dfrac{dx}{dx_\perp} = 1$ since $\sqrt{R} = \text{constant}$

$dx = dx_\perp$

So the influence of this substitution on the integration parameters will be as follows:

If $x_\perp = \infty$ *then* $x = \infty + \sqrt{R}$

$$x = \infty$$

If $x_\perp = 0$ *then* $x = 0 + \sqrt{R}$

$$x = \sqrt{R}$$

So:

$$F(a,b) = 2 \int\limits_{x=\sqrt{R}}^{x=+\infty} \left| \exp\left(-\frac{2\sqrt{\left(\left(-\sqrt{R}+x\right)^2 + \Omega^2 b^2 + z^2 a^2\right)}}{1} \right) \right| \, dx$$

$$= 2 \int\limits_{\sqrt{R}}^{+\infty} \left| \exp\left(-\frac{2\sqrt{\left(\left(-\sqrt{R}+x\right)^2 + R\right)}}{1} \right) \right| \, dx$$

Now:

Substitute: $x = \sqrt{R}\cosh q \quad \rightarrow \quad \dfrac{dx}{dq} = \sqrt{R}\sinh q$

$$dx = \sqrt{R}\sinh q \, dq$$

So, consider the influence of this substitution on the integration parameters:

If: $x = \infty$ then $q = \cosh^{-1}\left(\dfrac{x}{\sqrt{R}}\right)$

$$= \cosh^{-1}\left(\dfrac{\infty}{\sqrt{R}}\right)$$

$$= \cosh^{-1}(\infty)$$

$$q_{\max} = \infty$$

If: $x = \sqrt{R}$ then $q = \cosh^{-1}\left(\dfrac{x}{\sqrt{R}}\right)$

$$= \cosh^{-1}\left(\dfrac{\sqrt{R}}{\sqrt{R}}\right)$$

$$= \cosh^{-1}(1)$$

$$q_{\min} = 1$$

Thus:

$$F(a,b) = 2\int_0^\infty \left| \exp\left(-\frac{2\sqrt{\left(\left(-\sqrt{R}+\sqrt{R}\cosh q\right)^2 + R\right)}}{l} \right) \right| \sqrt{R}\sinh q \; dq$$

$$= 2\sqrt{R}\int_0^\infty \left| \exp\left(-\frac{2\sqrt{\left(\left(-\sqrt{R}\left(-1+\cosh q\right)\right)^2 + R\right)}}{l} \right) \right| \sinh q \; dq$$

$$= 2\sqrt{R}\int_0^\infty \left| \exp\left(-\frac{2\sqrt{R\left(\left(\left(-1+\cosh q\right)\right)^2 + 1\right)}}{l} \right) \right| \sinh q \; dq$$

Now:

Substitute : $q = -\ln x$ or $-q = \ln x$

$$\textbf{x}\textbf{и}\textbf{и}\textbf{а}\textbf{и}^{-q}$$

And $dq = \dfrac{-dx}{\textbf{uuuuuuйи}}$

So the influence on the integration parameters will be:

If $\underline{q = \infty}$ then $x = e^{-q}$

$$= e^{-\infty}$$

$$\text{and} = 0$$

If $q = 0$ then $x = e^{-q}$

$$= e^{-0}$$

$$\text{and} = 1$$

Also, since:

$$\cosh q = \frac{1}{2}\left(e^q + e^{-q}\right) = \frac{1}{2}(\frac{1}{x} + x)$$

$$\sinh q = \frac{1}{2}\left(e^q - e^{-q}\right) = \frac{1}{2}(\frac{1}{x} - x)$$

it can be written:

$$F(a,b) = 2\sqrt{R} \int\limits_{x=1}^{x=0} \left| \exp\left(-\frac{2\sqrt{R\left(\left[\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right]^2+1\right)}}{l} \right) \left[\frac{1}{2}\left(\frac{1}{x}-x\right)\right]\left[\frac{-dx}{x}\right] \right|$$

$$= -2\sqrt{R}\int\limits_{1}^{0} \frac{1}{2}\left|\left[\frac{1/x-x}{x}\right]\right| \exp\left(-\frac{2\sqrt{R\left(\left[1/2(1/x+x)-1\right]^2+1\right)}}{l} \right) dx$$

$$= -(-1)\sqrt{R}\int\limits_{0}^{1} \left|\left[\frac{(1-x^2)/x}{x}\right]\right| \exp\left(-\frac{2\sqrt{R\left(\left[1/2(1/x+x)-1\right]^2+1\right)}}{l} \right) dx$$

$$F(a,b) = \sqrt{R}\int\limits_{0}^{1} \left|\left[\frac{(1-x^2)}{x^2}\right]\right| \exp\left(-\frac{2\sqrt{R\left(\left[1/2(1/x+x)-1\right]^2+1\right)}}{l} \right) dx$$

This final equation will be the one that is solved numerically as a function of variational parameters and of Quantum Well-Wire size parameters.

G(a,b)

Now, consider the term $G(a, b)$, from equation (4.2.19):

$$G(a,b) = \int j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r \, dx$$

$$= 2 \int_0^{+\infty} j_r \left(\frac{\partial^2}{\partial z_e^2} + \frac{\partial^2}{\partial y_e^2} \right) j_r \, dx$$

$$= 2 \int_0^{+\infty} j_r \left(\frac{\partial^2 j_r}{\partial z_e^2} + \frac{\partial^2 j_r}{\partial y_e^2} \right) dx$$

$$= 2 \int_0^{+\infty} j_r \left(\frac{\partial^2}{\partial z_e^2} \left(\exp\left(-r'/l\right) \right) + \frac{\partial^2}{\partial y_e^2} \left(\exp\left(-r'/l\right) \right) \right) dx$$

$$= 2 \int_0^{+\infty} j_r \left(\frac{\partial^2}{\partial z_e^2} \left(\exp\left(-\frac{\sqrt{x^2 + \Omega^2 b^2 + z'^2 a^2}}{l} \right) \right) + \frac{\partial^2}{\partial y_e^2} \left(\exp\left(-\frac{\sqrt{x^2 + \Omega^2 b^2 + z'^2 a^2}}{l} \right) \right) \right) dx$$

$$= 2 \int_0^{+\infty} j_r \left(\frac{\partial^2}{\partial z_e^2} \left(\exp\left(-\frac{\sqrt{x^2 + \Omega^2 b^2 + z'^2 \left(z_e - z_h \right)^2}}{l} \right) \right) + \frac{\partial^2}{\partial y_e^2} \left(\exp\left(-\frac{\sqrt{x^2 + \Omega^2 \left(y_e - y_h \right)^2 + z'^2 a^2}}{l} \right) \right) \right) dx$$

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Now the solution to the **general** derivative $\dfrac{d^2}{dx^2}$ have to be found. So let the terms that will be constants with regard to the derivative variable be k, l, m, b and r. Then:

$$\frac{d}{dx}\left(e^{-\left(\frac{\sqrt{r(x-b)^2+k+l}}{m}\right)}\right)$$

Use the chain rule

$$\frac{de^u}{dx}=e^u\frac{du}{dx}\quad\text{where}\quad u=-\frac{\sqrt{r(x-b)^2+k+l}}{m}$$

Then:

$$=e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}}\frac{d}{dx}\left(-\frac{\sqrt{r(x-b)^2+k+l}}{m}\right)$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$= -\frac{e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}}}{m} \frac{d}{dx}\left(\sqrt{r(x-b)^2+k+l}\right)$$

Use the chain rule:

$$\frac{du^n}{dx} = nu^{n-1}\frac{du}{dx} \text{ where } u = r(x-b)^2+k+l \text{ and } n = 1/2$$

$$= -\frac{e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}}}{2m\sqrt{r(x-b)^2+k+l}} \frac{d}{dx}\left(r(x-b)^2+k+l\right)$$

The derivative of a sum is the sum of the derivatives:

$$= -\frac{e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}}\left(\frac{d}{dx}(k)+\frac{d}{dx}(l)+\frac{d}{dx}(r(x-b)^2)\right)}{2m\sqrt{r(x-b)^2+k+l}}$$

The derivative of the constants k and l is 0:

$$= -\frac{e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}}\left(\frac{d}{dx}(r(x-b)^2)\right)}{2m\sqrt{r(x-b)^2+k+l}}$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$= -\frac{e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}}r}{2m\sqrt{r(x-b)^2+k+l}}\left(\frac{d}{dx}(x-b)^2\right)$$

Use the chain rule:

$$\frac{du^n}{dx} = nu^{n-1}\frac{du}{dx} \text{ where } u = x-b \text{ and } n = 2$$

$$= -\frac{e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}}r(x-b)}{m\sqrt{r(x-b)^2+k+l}}\frac{d}{dx}(x-b)$$

The derivative of a sum is the sum of the derivatives:

$$= -\frac{e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}} r(x-b)\left(\frac{d}{dx}(-b)+\frac{d}{dx}(x)\right)}{m\sqrt{r(x-b)^2+k+l}}$$

The derivative of the constant $-b$ is 0:

$$= -\frac{e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}} r(x-b)}{m\sqrt{r(x-b)^2+k+l}} \quad \frac{d}{dx}(x)$$

The derivative of x^n is nx^{n-1}:

$$= -\frac{e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}} r(x-b)}{m\sqrt{r(x-b)^2+k+l}}$$

Simplify, assuming x is positive:

$$= \frac{e^{-\frac{\sqrt{r(b-x)^2+k+l}}{m}} r(b-x)}{m\sqrt{r(b-x)^2+k+l}}$$

Now do the second derivative:

$$\frac{d^2}{dx^2}\left(e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}}\right)$$

The second derivative is the derivative of the derivative

$$= \frac{d}{dx}\left(\frac{d}{dx}\left(e^{-\frac{\sqrt{r(x-b)^2+k+l}}{m}}\right)\right)$$

Copy the first derivative from above:

$$= \frac{d}{dx}\left(\frac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} r(b-x)}{m\sqrt{r(b-x)^2+k+l}} \right)$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$= \frac{r}{m}\frac{d}{dx}\left(\frac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} (b-x)}{\sqrt{r(b-x)^2+k+l}} \right)$$

Use the product rule

$$\frac{d(uv)}{dx} = \frac{du}{dx}v + u\frac{dv}{dx}$$

where $u = e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}$ and $v = \frac{x-b}{\sqrt{r(b-x)^2+k+l}}$

$$= \frac{r\left(\frac{x-b}{\sqrt{r(b-x)^2+k+l}}\frac{d}{dx}\left(e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} \right) + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\frac{d}{dx}\left(\frac{x-b}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

Use the chain rule

$$\frac{de^u}{dx} = e^u \frac{du}{dx}$$

where $u = \dfrac{\sqrt{r(b-x)^2 + k + l}}{m}$

$$= \frac{r\left(\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}(x-b)}{\sqrt{r(b-x)^2+k+l}} \dfrac{d}{dx}\left(\dfrac{\sqrt{r(b-x)^2+k+l}}{m} \right) + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} \dfrac{d}{dx}\left(\dfrac{x-b}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$= \frac{r\left(\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}(x-b)}{m\sqrt{r(b-x)^2+k+l}} \dfrac{d}{dx}\left(\sqrt{r(b-x)^2+k+l} \right) + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} \dfrac{d}{dx}\left(\dfrac{x-b}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

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Use the chain rule:

$$\frac{du^n}{dx} = nu^{n-1u}\frac{du}{dx}$$

where $u = r(b-x)^2 + k + l$ and $n = 1/2$

$$= \frac{r\left(\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}(x-b)}{2m(r(b-x)^2+k+l)}\dfrac{d}{dx}\left(\sqrt{r(b-x)^2+k+l}\right) + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\dfrac{d}{dx}\left(\dfrac{x-b}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

The derivative of a sum is the sum of the derivatives:

$$= \frac{r\left(\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}(x-b)\left(\dfrac{d}{dx}(k)+\dfrac{d}{dx}(l)+\dfrac{d}{dx}(r(b-x)^2)\right)}{2m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\dfrac{d}{dx}\left(\dfrac{x-b}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

The derivative of the constants k and l is 0:

$$= \frac{r\left(\frac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}(x-b)\left(\frac{d}{dx}(r(b-x)^2)\right)}{2m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\frac{d}{dx}\left(\frac{x-b}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

The derivative of a constant times a function is the constant time the derivative of the function:

$$= \frac{r\left(\frac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}r(x-b)\left(\frac{d}{dx}((b-x)^2)\right)}{2m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\frac{d}{dx}\left(\frac{x-b}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

Use the chain rule:

$$\frac{du^n}{dx} = nu^{n-1u}\frac{du}{dx}$$

where $u = b - x$ and $n = 2$

$$= \frac{r\left(\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} r(b-x)(x-b)\left(\dfrac{d}{dx}(b-x) \right)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} \dfrac{d}{dx}\left(\dfrac{x-b}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

The derivative of a sum is the sum of the derivatives:

$$= \frac{r\left(\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} r(b-x)(x-b)\left(\dfrac{d}{dx}(b) + \dfrac{d}{dx}(-x) \right)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} \dfrac{d}{dx}\left(\dfrac{x-b}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

The derivative of the constant b is 0:

$$= \frac{r\left(\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} r(b-x)(x-b)}{m(r(b-x)^2+k+l)} \dfrac{d}{dx}(-x) + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} \dfrac{d}{dx}\left(\dfrac{x-b}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$= \frac{r\left(-\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} r(b-x)(x-b)}{m(r(b-x)^2+k+l)} \dfrac{d}{dx}(x) + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} \dfrac{d}{dx}\left(\dfrac{x-b}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

The derivative of x^n is nx^{n-1}:

$$= \frac{r\left(-\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} r(b-x)(x-b)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}} \dfrac{d}{dx}\left(\dfrac{x-b}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

Use the product rule:

$$\frac{d(uv)}{dx} = \frac{du}{dx}v + u\frac{dv}{dx}$$

where $u = \dfrac{1}{\sqrt{r(b-x)^2+k+l}}$ and $v = x-b$

$$= \frac{r\left(-\dfrac{e^{\frac{\sqrt{r(b-x)^2+k}+l}{m}} r(b-x)(x-b)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k}+l}{m}}\left((x-b)\dfrac{d}{dx}\left(\dfrac{1}{\sqrt{r(b-x)^2+k+l}} \right) + \dfrac{1}{\sqrt{r(b-x)^2+k+l}}\dfrac{d}{dx}(x-b) \right) \right)}{m}$$

The derivative of a sum is the sum of the derivatives:

$$= \frac{r\left(-\dfrac{e^{\frac{\sqrt{r(b-x)^2+k}+l}{m}} r(b-x)(x-b)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k}+l}{m}}\left((x-b)\dfrac{d}{dx}\left(\dfrac{1}{\sqrt{r(b-x)^2+k+l}} \right) + \dfrac{d/dx(-b)+d/dx(x)}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$= \frac{r\left(-\dfrac{e^{\frac{\sqrt{r(b-x)^2+k}+l}{m}} r(b-x)(x-b)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k}+l}{m}}\left((x-b)\dfrac{d}{dx}\left(\dfrac{1}{\sqrt{r(b-x)^2+k+l}} \right) + \dfrac{d/dx(x)-d/dx(b)}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

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The derivative of x^n is nx^{n-1}

$$= \frac{r\left(-\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}r(b-x)(x-b)}{m(r(b-x)^2+k+l)}+e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left((x-b)\dfrac{d}{dx}\left(\dfrac{1}{\sqrt{r(b-x)^2+k+l}}\right)+\dfrac{1-d/dx\,(b)}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

The derivative of the constant b is 0:

$$= \frac{r\left(-\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}r(b-x)(x-b)}{m(r(b-x)^2+k+l)}+e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left((x-b)\dfrac{d}{dx}\left(\dfrac{1}{\sqrt{r(b-x)^2+k+l}}\right)+\dfrac{1}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

Use the chain rule:

$$\frac{du^n}{dx}=nu^{n-1}\frac{du}{dx}$$

where $u=r(b-x)^2+k+l$ and $n=-1/2$

$$= \frac{r\left(-\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\,r(b-x)(x-b)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left(-\dfrac{(x-b)}{2(r(b-x)^2+k+l)^{3/2}} + \dfrac{1}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

The derivative of a sum is the sum of the derivatives:

$$= \frac{r\left(-\dfrac{e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\,r(b-x)(x-b)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left(-\dfrac{(x-b)\left(\frac{d}{dx}(k) + \frac{d}{dx}(l) + \frac{d}{dx}(r(b-x)^2) \right)}{2(r(b-x)^2+k+l)^{3/2}} + \dfrac{1}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

The derivative of the constant k and l is 0:

$$= \frac{r\left(-\dfrac{e^{\frac{-\sqrt{r(b-x)^2+k+l}}{m}}\,r(b-x)(x-b)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left(-\dfrac{(x-b)\left(\frac{d}{dx}(r(b-x)^2) \right)}{2(r(b-x)^2+k+l)^{3/2}} - \dfrac{1}{\sqrt{r(b-x)^2+k+l}} \right) \right)}{m}$$

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The derivative of a constant times a function is the constant times the derivative of the function:

$$= \frac{r\left(-\dfrac{e^{\frac{-\sqrt{r(b-x)^2+k+l}}{m}} r(b-x)(x-b)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left(-\dfrac{r(x-b)\left(\dfrac{d}{dx}((b-x)^2)\right)}{2(r(b-x)^2+k+l)^{3/2}} - \dfrac{1}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

Use the chain rule:

$$\frac{du^n}{dx} = nu^{n-1}\frac{du}{dx}$$

where $u = b - x$ n $= 2$

$$= \frac{r\left(-\dfrac{e^{\frac{-\sqrt{r(b-x)^2+k+l}}{m}} r(b-x)(x-b)}{m(r(b-x)^2+k+l)} + e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left(-\dfrac{r(b-x)(x-b)\left(\dfrac{d}{dx}(b-x)\right)}{(r(b-x)^2+k+l)^{3/2}} - \dfrac{1}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

The derivative of a sum is the sum of the derivatives:

$$= \frac{r\left(-\dfrac{e^{\frac{-\sqrt{r(b-x)^2+k+l}}{m}}r(b-x)(x-b)}{m(r(b-x)^2+k+l)}+e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left(-\dfrac{r(b-x)(x-b)\left(\dfrac{d}{dx}(b)+\dfrac{d}{dx}(-x)\right)}{(r(b-x)^2+k+l)^{3/2}}-\dfrac{1}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

The derivative of the constant b is 0:

$$= \frac{r\left(-\dfrac{e^{\frac{-\sqrt{r(b-x)^2+k+l}}{m}}r(b-x)(x-b)}{m(r(b-x)^2+k+l)}+e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left(-\dfrac{r(b-x)(x-b)\left(\dfrac{d}{dx}(-x)\right)}{(r(b-x)^2+k+l)^{3/2}}-\dfrac{1}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$= \frac{r\left(-\dfrac{e^{\frac{-\sqrt{r(b-x)^2+k+l}}{m}}r(b-x)(x-b)}{m(r(b-x)^2+k+l)}+e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left(+\dfrac{r(b-x)(x-b)\left(\dfrac{d}{dx}(x)\right)}{(r(b-x)^2+k+l)^{3/2}}-\dfrac{1}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

The derivative of x^n is nx^{n-1}

$$= \dfrac{r\left(-\dfrac{e^{\frac{-\sqrt{r(b-x)^2+k+l}}{m}}\, r(b-x)(x-b)}{m(r(b-x)^2+k+l)}+e^{\frac{\sqrt{r(b-x)^2+k+l}}{m}}\left(\dfrac{r(b-x)(x-b)}{(r(b-x)^2+k+l)^{3/2}}-\dfrac{1}{\sqrt{r(b-x)^2+k+l}}\right)\right)}{m}$$

Simplify assuming variable x is positive:

$$= \dfrac{e^{-\frac{\sqrt{r(b-x)^2+k+l}}{m}}\, r\left(r\sqrt{r(b-x)^2+k+l}\,(b-x)^2-km-lm\right)}{m^2(r(b-x)^2+k+l)^{3/2}}$$

Hence with this general solution in hand, $G(a,b)$ can now be written as:

$$G(a,b)=2\int_0^{+\infty} j_r \left[\left(\dfrac{e^{\frac{-\sqrt{x^2+\Omega^2 b^2+z^2(z_h-z_e)^2}}{l}}\, z^2(-\Omega^2 b^2 l - x^2 l + z^2(z_h-z_e)^2\sqrt{\Omega^2 b^2 + z_h^2 z^2 + x^2 + z^2 z_e^2 - 2z_h z^2 z_e})}{l^2\left(\Omega^2 b^2 + x^2 + z^2(z_h-z_e)^2\right)^{3/2}}\right)+\left(\dfrac{e^{\frac{-\sqrt{x^2+z^2 a^2+\Omega^2(y_h-y_e)^2}}{l}}\,\Omega^2\left(-z^2 a^2 l - x^2 l + \Omega^2(y_h-y_e)^2\sqrt{z^2 a^2 + y_h^2\Omega^2 + x^2 + \Omega^2 y_e^2 - 2y_h\Omega^2 y_e}\right)}{l^2\left(z^2 a^2 + x^2 + \Omega^2(y_h-y_e)^2\right)^{3/2}}\right)\right]\,dx$$

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Now: Let $x = -\sqrt{R} + x'$ where $R = \Omega^2 b^2 + z^2 a^2$ so that: $x^2 = (-\sqrt{R} + x')^2$.

Then: $x' = x + \sqrt{R}$

And: $\dfrac{dx'}{dx} = 1$ since $\sqrt{R} = $ Constant

$\qquad$ dx'=dx

Then:

If $x = \infty$ then $x' = \infty + \sqrt{R}$

$\qquad\qquad$ x'=∞

If $x = 0$ then $x' = 0 + \sqrt{R}$

$\qquad\qquad$ x'=√R

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So:

$$G(a,b) = 2\int_{\sqrt{R}}^{\infty} \left(\left(e^{-\frac{\sqrt{R+\left(-\sqrt{R}+x'\right)^2}}{l}} \right) \left(\frac{e^{-\frac{\sqrt{R+\left(-\sqrt{R}+x'\right)^2}}{l}} z^2 \left(-l\left(x^2+\Omega^2 b^2\right)+z^2 a^2\left(\sqrt{x^2+\Omega^2 b^2+z^2 a^2}\right)\right)}{l^2\left(R+\left(-\sqrt{R}+x'\right)^2\right)^{3/2}} \right) + \left(\frac{e^{-\frac{\sqrt{R+\left(-\sqrt{R}+x'\right)^2}}{l}} \Omega^2\left(-l\left(x^2+z^2 a^2\right)+\Omega^2 b^2\left(\sqrt{x^2+\Omega^2 b^2+z^2 a^2}\right)\right)}{l^2\left(R+\left(-\sqrt{R}+x'\right)^2\right)^{3/2}} \right) \right) dx'$$

$$= 2\int_{\sqrt{R}}^{\infty} \left(\left(e^{-\frac{\sqrt{R+\left(-\sqrt{R}+x'\right)^2}}{l}} \right) \left(\frac{e^{-\frac{\sqrt{R+\left(-\sqrt{R}+x'\right)^2}}{l}} z^2 \left(-l\left(\left(-\sqrt{R}+x'\right)^2+\Omega^2 b^2\right)+z^2 a^2\left(\sqrt{R+\left(-\sqrt{R}+x'\right)^2}\right)\right)}{l^2\left(R+\left(-\sqrt{R}+x'\right)^2\right)^{3/2}} \right) + \left(\frac{e^{-\frac{\sqrt{R+\left(-\sqrt{R}+x'\right)^2}}{l}} \Omega^2\left(-l\left(\left(-\sqrt{R}+x'\right)^2+z^2 a^2\right)+\Omega^2 b^2\left(\sqrt{R+\left(-\sqrt{R}+x'\right)^2}\right)\right)}{l^2\left(R+\left(-\sqrt{R}+x'\right)^2\right)^{3/2}} \right) \right) dx'$$

$$= 2\int_{\sqrt{R}}^{\infty}\left(\left(\frac{e^{-\frac{\sqrt{R+(-\sqrt{R}+x')^2}}{l}}}{l^2\left(R+\left(-\sqrt{R}+x'\right)^2\right)^{3/2}}\right)\left(e^{-\frac{\sqrt{R+\left(-\sqrt{R}+x'\right)^2}}{l}}z^2\left(-l\left(\left(-\sqrt{R}+x'\right)^2+\Omega^2b^2\right)+z^2a^2(P)\right)+\Omega^2\left(-l\left(\left(-\sqrt{R}+x'\right)^2+z^2a^2\right)+\Omega^2b^2(P)\right)\right)\right)dx'$$

With:

$$P=\sqrt{R+\left(-\sqrt{R}+x'\right)^2}$$

$$= 2\int_{\sqrt{R}}^{\infty}\frac{e^{-\frac{\sqrt{R+(-\sqrt{R}+x')^2}}{l}}}{l^2\left(R+\left(-\sqrt{R}+x'\right)^2\right)^{3/2}}\left[e^{-\frac{\sqrt{R+\left(-\sqrt{R}+x'\right)^2}}{l}}\left(-l\left(\left(-\sqrt{R}+x'\right)^2\left[z^2+\Omega^2\right]+z^2\Omega^2b^2+z^2\Omega^2a^2+z^4a^2P+\Omega^2b^2P\right)\right)\right]dx'$$

$$= 2\int_{\sqrt{R}}^{\infty}\frac{e^{-\frac{2\sqrt{R+(-\sqrt{R}+x')^2}}{l}}}{l^2\left(R+\left(-\sqrt{R}+x'\right)^2\right)^{3/2}}\left[\left(-l\left(\left(-\sqrt{R}+x'\right)^2\left[z^2+\Omega^2\right]+z^2\left(\Omega^2b^2+\Omega^2a^2+z^2a^2\left(\sqrt{R+\left(-\sqrt{R}+x'\right)^2}\right)+\Omega^2b^2\left(\sqrt{R+\left(-\sqrt{R}+x'\right)^2}\right)\right)\right)\right)\right]dx'$$

Now:

Let $x=\sqrt{R}\cosh q$

Then: $\dfrac{dx'}{dq}-\sqrt{R}\sinh q$

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$$\text{If } x' = \infty \text{ then } q = \cosh^{-1}\left(\frac{x'}{\sqrt{R}}\right)$$

$$= \cosh^{-1}\left(\frac{\infty}{\sqrt{R}}\right)$$

$$= \cosh^{-1}\left(\infty\right)$$

$$q = \infty$$

$$\text{If } x' = \sqrt{R} \text{ then } q = \cosh^{-1}\left(\frac{x'}{\sqrt{R}}\right)$$

$$= \cosh^{-1}\left(\frac{\sqrt{R}}{\sqrt{R}}\right)$$

$$= \cosh^{-1}\left(1\right)$$

$$q = 0$$

So:

$$G(a,b) = 2\int\limits_{q=0}^{q=\infty}\left[\frac{e^{-\frac{2\sqrt{R+\left(-\sqrt{R}+\sqrt{R}\cosh q\right)^2}}{I}}}{I^2\left(R+\left(-\sqrt{R}+\sqrt{R}\cosh q\right)^2\right)^{3/2}}\right]\left[\left(-I\left(-\sqrt{R}+\left(\sqrt{R}\cosh q\right)\right)^2\left[z^2+\Omega^2\right]+z^2\left[\begin{array}{l}\Omega^2 b^2+\Omega^2 a^2+z^2 a^2\left(\sqrt{R+\left(-\sqrt{R}+\sqrt{R}\cosh q\right)^2}\right)+\\ \Omega^2 b^2\left(\sqrt{R+\left(-\sqrt{R}+\sqrt{R}\cosh q\right)^2}\right)\end{array}\right]\right)\right]\sqrt{R}\sinh q\,dq$$

$$= 2\int\limits_{q=0}^{q=\infty}\left[\frac{e^{-\frac{2\sqrt{R+\left(-\sqrt{R}\left(1-\cosh q\right)\right)^2}}{I}}}{I^2\left(R+\left(-\sqrt{R}\left(1-\cosh q\right)\right)^2\right)^{3/2}}\right]\left[\left(-I\left(-\sqrt{R}+\left(\sqrt{R}\cosh q\right)\right)^2\left[z^2+\Omega^2\right]+z^2\left[\begin{array}{l}\Omega^2 b^2+\Omega^2 a^2+z^2 a^2\left(\sqrt{R+\left(-\sqrt{R}\left(1-\cosh q\right)\right)^2}\right)+\\ \Omega^2 b^2\left(\sqrt{R+\left(-\sqrt{R}\left(1-\cosh q\right)\right)^2}\right)\end{array}\right]\right)\right]\sqrt{R}\sinh q\,dq$$

$$= 2\int\limits_{q=0}^{q=\infty}\left[\frac{e^{-\frac{2\sqrt{R+R(1-\cosh q)^2}}{I}}}{I^2\left(R+R(1-\cosh q)^2\right)^{3/2}}\right]\left[\left(-I\,R\left(1-\cosh q\right)^2\left(z^2+\Omega^2\right)+z^2\left[\begin{array}{l}\Omega^2 b^2+\Omega^2 a^2+z^2 a^2\left(\sqrt{R+R(1-\cosh q)^2}\right)+\\ \Omega^2 b^2\left(\sqrt{R+R(1-\cosh q)^2}\right)\end{array}\right]\right)\right]\sqrt{R}\sinh q\,dq$$

$$= 2\int\limits_{q=0}^{q=\infty}\left[\frac{e^{-\frac{2\sqrt{R\left[1+(1-\cosh q)^2\right]}}{I}}}{I^2\left(R\left(1+(1-\cosh q)^2\right)\right)^{3/2}}\right]\left[\left(-I\,R\left(1-\cosh q\right)^2\left(z^2+\Omega^2\right)+z^2\left[\begin{array}{l}\Omega^2 b^2+\Omega^2 a^2+z^2 a^2\left(\sqrt{R\left[1+(1-\cosh q)^2\right]}\right)+\\ \Omega^2 b^2\left(\sqrt{R\left[1+(1-\cosh q)^2\right]}\right)\end{array}\right]\right)\right]\sqrt{R}\sinh q\,dq$$

$$= 2 \int_{q=0}^{q=\infty} \left[\frac{e^{-\frac{2\sqrt{R\left[1+(1-\cosh q)^2\right]}}{l}}}{l^2 \left(R\left(1+(1-\cosh q)^2\right)\right)^{3/2}} \right] \left[\left(-l\, R(1-\cosh q)^2 \left(z^2 + \Omega^2\right) + z^2 \left[\frac{\Omega^2 b^2 + \Omega^2 a^2 + z^2 a^2 \left(\sqrt{R\left[1+(1-\cosh q)^2\right]} \right) +}{\Omega^2 b^2 (\sqrt{R\left[1+(1-\cosh q)^2\right]})} \right] \right) \right] \sqrt{R}\, \sinh q\, dq$$

Now:

Substitute $q = -\ln x$ or $-q = \ln x$

$$x = e^{-q}$$

Then : $dq = \dfrac{-dx}{x}$

If $q = \infty$ then $x = e^{-\infty}$

$$\textbf{\textit{und}}$$

If $q = 0$ then $x = e^{-0}$

$$\textbf{\textit{und}}$$

The following identities also hold:

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$$\cosh q = \frac{1}{2}\left(e^q + e^{-q}\right) = \frac{1}{2}\left(\frac{1}{x} + x\right)$$

$$\sinh q = \frac{1}{2}\left(e^q - e^{-q}\right) = \frac{1}{2}\left(\frac{1}{x} - x\right)$$

Thus:

$$G(a,b) = 2\int_{x=1}^{x=0}\left[\frac{e^{-\frac{2\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}}{I}}}{I^2\left(R\left(1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right)\right)^{3/2}}\right]\left[\left(-IR\left(1-\frac{1}{2}\left(\frac{1}{x}+x\right)\right)^2\left(z^2+\Omega^2\right)+z^2\left[\begin{array}{c}\Omega^2b^2+\Omega^2a^2+z^2a^2\left(\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}\right)+\\\Omega^2b^2\left(\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}\right)\end{array}\right]\right)\right]\sqrt{R}\left(\frac{1}{2}\left(\frac{1}{x}-x\right)\right)\left(\frac{-dx}{x}\right)$$

$$= \frac{(-1)(-2)}{2}\int_0^1\left[\frac{e^{-\frac{2\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}}{I}}}{I^2\left(R\left(1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right)\right)^{3/2}}\right]\left[\left(-IR\left(1-\frac{1}{2}\left(\frac{1}{x}+x\right)\right)^2\left(z^2+\Omega^2\right)+z^2\left[\begin{array}{c}\Omega^2b^2+\Omega^2a^2+z^2a^2\left(\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}\right)+\\\Omega^2b^2\left(\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}\right)\end{array}\right]\right)\right]\sqrt{R}\frac{1}{x}\left(\frac{1}{x}-x\right)dx$$

$$= \sqrt{R}\int_0^1\left[\frac{1-x^2}{x^2}\right]\left[\frac{e^{-\frac{2\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}}{I}}}{I^2\left(R\left(1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right)\right)^{3/2}}\right]\left[\left(-IR\left(1-\frac{1}{2}\left(\frac{1}{x}+x\right)\right)^2\left(z^2+\Omega^2\right)+z^2\left[\begin{array}{c}\Omega^2b^2+\Omega^2a^2+z^2a^2\left(\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}\right)+\\\Omega^2b^2\left(\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}\right)\end{array}\right]\right)\right]dx$$

$$= \sqrt{R}\int_0^1\left[\frac{1-x^2}{x^2}\right]\left[\frac{e^{-\frac{2\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}}{I}}}{I^2\left(R\left(1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right)\right)^{3/2}}\right]\left[\left(-I\,R\left(1-\frac{1}{2}\left(\frac{1}{x}+x\right)\right)^2(z^2+\Omega^2)+z^2\left[\Omega^2 b^2+\Omega^2 a^2+\left(\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}\right)\underbrace{(z^2 a^2+\Omega^2 b^2)}_{R}\right]\right)\right]dx$$

$$G(a,b)=\sqrt{R}\int_0^1\left[\frac{1-x^2}{x^2}\right]\left[\frac{e^{-\frac{2\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}}{I}}}{I^2\left(R\left(1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right)\right)^{3/2}}\right]\left[\left(-I\,R\left(1-\frac{1}{2}\left(\frac{1}{x}+x\right)\right)^2(z^2+\Omega^2)+z^2\left[\Omega^2 b^2+\Omega^2 a^2+\left(\sqrt{R\left[1+(1-\frac{1}{2}\left(\frac{1}{x}+x\right))^2\right]}\right)(R)\right]\right)\right]dx$$

This final equation will be the one that is solved numerically as a function of variational parameters and of Quantum Well-Wire size parameters.

J(a,b)

Consider the term $J(a, b)$, from equation (4.2.23), where x has been called $x_\perp$:

$$J(a,b) = \int j_r \left(\frac{\partial^2}{\partial x^2} \right) j_r \, dx$$

$$J(a,b) = \int j_r \left(\frac{\partial^2}{\partial x_\perp^{\,2}} \right) j_r \, dx_\perp$$

$$J(a,b) = 2 \int_0^\infty e^{\left(-\frac{r'}{l} \right)} \left[\frac{\partial^2 j_r}{\partial x_\perp^{\,2}} \right] dx_\perp$$

$$J(a,b) = 2 \int_0^\infty e^{\left(-\frac{r'}{l} \right)} \left[\frac{\partial^2}{\partial x_\perp^{\,2}} \left(e^{-\frac{r'}{l}} \right) \right] dx_\perp$$

$$J(a,b) = 2 \int_0^\infty e^{\left(-\frac{r'}{l} \right)} \left[\frac{\partial^2}{\partial x_\perp^{\,2}} \left(e^{-\frac{\sqrt{x_\perp^{\,2} + \Omega^2 b^2 + z^2 a^2}}{l}} \right) \right] dx_\perp$$

Thus the solution to the general derivative $\dfrac{\partial^2}{\partial x^2} \left(e^{\frac{-\sqrt{k^2 + p^2 + x^2}}{l}} \right)$ must now be found. This is done as follows:

$$\frac{d}{dx}\left(e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\right)$$

Use the chain rule:

$$\frac{de^u}{dx}=e^u\frac{du}{dx}$$

Where:

$$u=-\frac{\sqrt{k^2+p^2+x^2}}{l}$$

$$=e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\frac{d}{dx}\left(-\frac{\sqrt{k^2+p^2+x^2}}{l}\right)$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$=-\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}}{l}\frac{d}{dx}\left(\sqrt{k^2+p^2+x^2}\right)$$

Use the chain rule:

$$\frac{du^n}{dx}=nu^{n-1}\frac{du}{dx}$$

Where:

$$u = k^2 + p^2 + x^2 \text{ and } n = \frac{1}{2}$$

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}}{2l\sqrt{k^2 + p^2 + x^2}} \frac{d}{dx}\left(k^2 + p^2 + x^2\right)$$

The derivative of a sum is the sum of the derivatives:

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(\frac{d}{dx}\left(k^2\right)+\frac{d}{dx}\left(p^2\right)+\frac{d}{dx}\left(x^2\right)\right)}{2l\sqrt{k^2 + p^2 + x^2}}$$

The derivative of the constants k^2 and p^2 are 0:

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}}{2l\sqrt{k^2 + p^2 + x^2}} \frac{d}{dx}\left(x^2\right)$$

The derivative of x^n is nx^{n-1}:

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}} x}{l\sqrt{k^2+p^2+x^2}}$$

Now do the second derivative:

$$\frac{d^2}{dx^2}\left(e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\right)$$

The second derivative is the derivative of the derivative:

$$\frac{d}{dx}\left(\frac{d}{dx}\left(e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\right)\right)$$

Copy the first derivative from three lines above:

$$\frac{d}{dx}\left(-\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}} x}{l\sqrt{k^2+p^2+x^2}}\right)$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$= -\frac{1}{l}\frac{d}{dx}\left(\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x}{\sqrt{k^2+p^2+x^2}}\right)$$

Use the product rule:

$$\frac{d(uv)}{dx} = \frac{du}{dx}v + u\frac{dv}{dx}$$

Where:

$$u = e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}} \quad \text{and} \quad v = \frac{x}{\sqrt{k^2+p^2+x^2}}$$

$$= -\left(\frac{\dfrac{x}{\sqrt{k^2+p^2+x^2}}\dfrac{d}{dx}\left(e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\right) + e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\dfrac{d}{dx}\left(\dfrac{x}{\sqrt{k^2+p^2+x^2}}\right)}{l}\right)$$

Use the chain rule:

$$\frac{de^u}{dx} = e^u \frac{du}{dx}$$

Where:

$$u = -\frac{\sqrt{k^2 + p^2 + x^2}}{l}$$

$$= -\left(\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}} \frac{d}{dx}\left(\frac{x}{\sqrt{k^2 + p^2 + x^2}} \right) + \frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}} x}{\sqrt{k^2 + p^2 + x^2}} \frac{d}{dx}\left(-\frac{\sqrt{k^2 + p^2 + x^2}}{l} \right)}{l} \right)$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$= -\left(\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}} \frac{d}{dx}\left(\frac{x}{\sqrt{k^2 + p^2 + x^2}} \right) - \frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}} x}{l\sqrt{k^2 + p^2 + x^2}} \frac{d}{dx}\left(\sqrt{k^2 + p^2 + x^2} \right)}{l} \right)$$

Use the product rule:

$$\frac{d(uv)}{dx} = \frac{du}{dx}v + u\frac{dv}{dx}$$

Where:

$$u = x \text{ and } v = \frac{1}{\sqrt{k^2 + p^2 + x^2}}$$

$$= -\left(\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(\frac{1}{\sqrt{k^2+p^2+x^2}}\frac{d}{dx}(x) + x\frac{d}{dx}\left(\frac{1}{\sqrt{k^2+p^2+x^2}}\right)\right) - \frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x}{l\sqrt{k^2+p^2+x^2}}\frac{d}{dx}\left(\sqrt{k^2+p^2+x^2}\right)}{l}\right)$$

The derivative of x^n is nx^{n-1}:

$$= -\left(\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(x\frac{d}{dx}\left(\frac{1}{\sqrt{k^2+p^2+x^2}}\right) + \frac{1}{\sqrt{k^2+p^2+x^2}}\right) - \frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x}{l\sqrt{k^2+p^2+x^2}}\frac{d}{dx}\left(\sqrt{k^2+p^2+x^2}\right)}{l}\right)$$

Use the chain rule:

$$\frac{du^n}{dx} = nu^{n-1}\frac{du}{dx}$$

Where:

$$u = k^2 + p^2 + x^2 \text{ and } n = -\frac{1}{2}$$

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(\frac{1}{\sqrt{k^2+p^2+x^2}} - \frac{x}{2\left(k^2+p^2+x^2\right)^{3/2}}\frac{d}{dx}\left(k^2+p^2+x^2\right)\right) - \frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x}{l\sqrt{k^2+p^2+x^2}}\frac{d}{dx}\left(\sqrt{k^2+p^2+x^2}\right)}{l}$$

The derivative of a sum is the sum of the derivatives:

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(\frac{1}{\sqrt{k^2+p^2+x^2}} - \frac{x\left(\frac{d}{dx}(k^2)+\frac{d}{dx}(p^2)+\frac{d}{dx}(x^2)\right)}{2\left(k^2+p^2+x^2\right)^{3/2}}\right) - \frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x}{l\sqrt{k^2+p^2+x^2}}\frac{d}{dx}\left(\sqrt{k^2+p^2+x^2}\right)}{l}$$

The derivative of the constants k^2 and p^2 is 0:

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(\dfrac{1}{\sqrt{k^2+p^2+x^2}} - \dfrac{x}{2\left(k^2+p^2+x^2\right)^{3/2}}\dfrac{d}{dx}\left(x^2\right)\right) - \dfrac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x}{l\sqrt{k^2+p^2+x^2}}\dfrac{d}{dx}\left(\sqrt{k^2+p^2+x^2}\right)}{l}$$

The derivative of x^n is nx^{n-1}:

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(\dfrac{1}{\sqrt{k^2+p^2+x^2}} - \dfrac{x^2}{\left(k^2+p^2+x^2\right)^{3/2}}\right) - \dfrac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x}{l\sqrt{k^2+p^2+x^2}}\dfrac{d}{dx}\left(\sqrt{k^2+p^2+x^2}\right)}{l}$$

Use the chain rule:

$$\frac{du^n}{dx} = nu^{n-1}\frac{du}{dx}$$

Where:

$$u = k^2 + p^2 + x^2 \text{ and } n = \frac{1}{2}$$

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$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(\dfrac{1}{\sqrt{k^2+p^2+x^2}}-\dfrac{x^2}{\left(k^2+p^2+x^2\right)^{3/2}}\right)-\dfrac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x}{2l\left(k^2+p^2+x^2\right)}\dfrac{d}{dx}\left(k^2+p^2+x^2\right)}{l}$$

The derivative of a sum is the sum of the derivatives:

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(\dfrac{1}{\sqrt{k^2+p^2+x^2}}-\dfrac{x^2}{\left(k^2+p^2+x^2\right)^{3/2}}\right)-\dfrac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x\left(\dfrac{d}{dx}(k^2)+\dfrac{d}{dx}(p^2)+\dfrac{d}{dx}(x^2)\right)}{2l\left(k^2+p^2+x^2\right)}}{l}$$

The derivative of the constants k^2 and p^2 is 0:

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(\dfrac{1}{\sqrt{k^2+p^2+x^2}}-\dfrac{x^2}{\left(k^2+p^2+x^2\right)^{3/2}}\right)-\dfrac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x}{2l\left(k^2+p^2+x^2\right)}\dfrac{d}{dx}(x^2)}{l}$$

The derivative of x^n is nx^{n-1}:

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(\dfrac{1}{\sqrt{k^2+p^2+x^2}} - \dfrac{x^2}{\left(k^2+p^2+x^2\right)^{3/2}}\right) - \dfrac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}x^2}{l\left(k^2+p^2+x^2\right)}}{l}$$

Simplify, assuming the variable x is positive:

$$= -\frac{e^{-\frac{\sqrt{k^2+p^2+x^2}}{l}}\left(-lk^2 - lp^2 + x^2\sqrt{k^2+p^2+x^2}\right)}{l^2\left(k^2+p^2+x^2\right)^{3/2}}$$

Thus, with this solution now in hand, $J(a,b)$ can now be written as:

$$J(a,b) = 2\int_0^\infty e^{\left(-\frac{\sqrt{x_\perp^2+\Omega^2b^2+z^2a^2}}{l}\right)}\left[\frac{e^{-\frac{\sqrt{x_\perp^2+\Omega^2b^2+z^2a^2}}{l}}\left(-l\Omega^2b^2 - lz^2a^2 + x_\perp^2\sqrt{x_\perp^2+\Omega^2b^2+z^2a^2}\right)}{l^2\left(x_\perp^2+\Omega^2b^2+z^2a^2\right)^{3/2}}\right]dx_\perp$$

$$J(a,b) = 2\int_0^\infty\left[\frac{e^{-\frac{\left(x_\perp^2+\Omega^2b^2+z^2a^2\right)}{l^2}}}{l^2\left(x_\perp^2+\Omega^2b^2+z^2a^2\right)^{3/2}}\right]\left[\left(-l\left(\Omega^2b^2+z^2a^2\right)+x_\perp^2\sqrt{x_\perp^2+\Omega^2b^2+z^2a^2}\right)\right]dx_\perp$$

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Now:

Let $x_\perp = x - \sqrt{R} \longrightarrow x_\perp^2 = (x - \sqrt{R})^2$ where $R = \Omega^2 b^2 + z^2 a^2$

Then $x = x_\perp + \sqrt{R}$

And $\dfrac{dx}{dx_\perp} = 1$ *since* $\sqrt{R} = $ constant

$\qquad dx = dx_\perp$

Then:

If $x_\perp = \infty$ *then* $x = \infty + \sqrt{R}$

$\qquad\qquad x = \infty$

If $x_\perp = 0$ *then* $x = 0 + \sqrt{R}$

$\qquad\qquad x = \sqrt{R}$

So:

$$J(a,b) = 2\int\limits_{x=\sqrt{R}}^{x=\infty} \left[\frac{e^{-\frac{\left(\left(x-\sqrt{R}\right)^2 + R\right)}{l^2}}}{l^2\left(\left(x-\sqrt{R}\right)^2 + R\right)^{3/2}} \right] \left[\left(-l(R) + \left(x-\sqrt{R}\right)^2 \sqrt{\left(x-\sqrt{R}\right)^2 + R} \right) \right] dx$$

Let:

$$x = \sqrt{R}\cosh q \quad \text{Then:} \quad \frac{dx}{dq} = \sqrt{R}\sinh q$$

$$dx = \sqrt{R}\sinh q\,dq$$

So:

$$\textit{If } x = \infty \text{ then } q = \cosh^{-1}\left(\frac{x}{\sqrt{R}}\right)$$

$$= \cosh^{-1}\left(\frac{\infty}{\sqrt{R}}\right)$$

$$= \cosh^{-1}(\infty)$$

$$q = \infty$$

$$\textit{If } x = \sqrt{R} \text{ then } q = \cosh^{-1}\left(\frac{x}{\sqrt{R}}\right)$$

$$= \cosh^{-1}\left(\frac{\sqrt{R}}{\sqrt{R}}\right)$$

$$= \cosh^{-1}(1)$$

$$q = 0$$

Hence:

$$J(a,b) = 2\int_{q=0}^{q=\infty}\left[\frac{e^{-\frac{\left(\left(\sqrt{R}\cosh q-\sqrt{R}\right)^2+R\right)}{I^2}}}{I^2\left(\left(\sqrt{R}\cosh q-\sqrt{R}\right)^2+R\right)^{3/2}}\right]\left[\left(-I(R)+\left(\sqrt{R}\cosh q-\sqrt{R}\right)^2\times\sqrt{\left(\sqrt{R}\cosh q-\sqrt{R}\right)^2+R}\right)\right]\left[\sqrt{R}\sinh q\,dq\right]$$

$$J(a,b) = 2\sqrt{R}\int_0^{\infty}\left[\frac{e^{-\frac{\left(\left(\sqrt{R}(\cosh q-1)\right)^2+R\right)}{I^2}}}{I^2\left(\left(\sqrt{R}(\cosh q-1)\right)^2+R\right)^{3/2}}\right]\left[\left(-I(R)+\left(\sqrt{R}(\cosh q-1)\right)^2\times\sqrt{\left(\sqrt{R}(\cosh q-1)\right)^2+R}\right)\right]\left[\sinh q\,dq\right]$$

$$J(a,b) = 2\sqrt{R}\int_0^{\infty}\left[\frac{e^{-\frac{\left(\left(R(\cosh q-1)^2\right)+R\right)}{I^2}}}{I^2\left(\left(R(\cosh q-1)^2\right)+R\right)^{3/2}}\right]\left[\left(-I\,R+\left(R(\cosh q-1)^2\right)\times\sqrt{\left(R(\cosh q-1)^2\right)+R}\right)\right]\left[\sinh q\,dq\right]$$

$$J(a,b) = 2\sqrt{R}\int_0^{\infty}\left[\frac{e^{-\frac{R((\cosh q-1)^2+1)}{I^2}}}{I^2\left(R((\cosh q-1)^2+1)\right)^{3/2}}\right]\left[\left(R(-I+(\cosh q-1)^2\times\sqrt{R((\cosh q-1)^2+1)})\right)\right]\left[\sinh q\,dq\right]$$

Now, substitute:

$$q = -\ln x \quad \text{or} \quad -q = \ln x$$

$$x = e^{-q}$$

Then:

$$dq = \frac{-dx}{x}$$

If $q = \infty$ then $x = 0$

If $q = 0$ then $x = 1$

The following identities also hold:

$$\cosh q = \frac{1}{2}\left(e^{q} + e^{-q}\right) = \frac{1}{2}\left(\frac{1}{x} + x\right) \longrightarrow \cosh^{2} q = \frac{1}{4}\left(\frac{1}{x} + x\right)^{2}$$

$$\sinh q = \frac{1}{2}\left(e^{q} - e^{-q}\right) = \frac{1}{2}\left(\frac{1}{x} - x\right)$$

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So:

$$J(a,b) = 2\sqrt{R}\int_1^0 \left[\frac{e^{-\frac{R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)}{l^2}}}{l^2\left(R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)\right)^{3/2}}\right]\left[\left(R\left(-1+\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2\times\sqrt{R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)}\right)\right]\left[\frac{1}{2}\left(\frac{1}{x}-x\right)\left(\frac{-dx}{x}\right)\right]\right]$$

$$J(a,b) = -2\sqrt{R}\int_1^0 \frac{1}{2}\left[\frac{\left(\frac{1}{x}-x\right)}{x}\right]\left[\frac{e^{-\frac{R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)}{l^2}}}{l^2\left(R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)\right)^{3/2}}\right]\left[\left(R\left(-1+\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2\times\sqrt{R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)}\right)\right]\left[dx\right]$$

$$J(a,b) = -(-1)\sqrt{R}\int_0^1 \left[\frac{(1-x^2)}{x^2}\right]\left[\frac{e^{-\frac{R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)}{l^2}}}{l^2\left(R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)\right)^{3/2}}\right]\left[\left(R\left(-1+\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2\times\sqrt{R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)}\right)\right]dx$$

$$J(a,b) = \sqrt{R}\int_0^1 \left[\frac{(1-x^2)}{x^2}\right]\left[\frac{e^{-\frac{R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)}{l^2}}}{l^2\left(R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)\right)^{3/2}}\right]\left[\left(R\left(-1+\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2\times\sqrt{R\left(\left(\frac{1}{2}\left(\frac{1}{x}+x\right)-1\right)^2+1\right)}\right)\right]dx$$

This final equation will be the one that is solved numerically as a function of variational parameters and of Quantum Well-Wire size parameters.

K(a,b)

Now, consider the term $K(a, b)$, from equation (4.2.24), where x has been called $x_\perp$:

$$K(a,b) = \int j_r^2 \frac{1}{r} \, dx_\perp$$

$$K(a,b) = 2\int_0^\infty \left(\frac{1}{(\sqrt{x_\perp^2 + b^2 + a^2})} \right) \left(e^{-\frac{\sqrt{x_\perp^2 + b^2 + a^2}}{l}} \right)^2 dx_\perp$$

$$K(a,b) = 2\int_0^\infty \left(x_\perp^2 + b^2 + a^2 \right)^{-1/2} \left(e^{-\frac{\sqrt{x_\perp^2 + b^2 + a^2}}{l}} \right)^2 dx_\perp$$

Now:

Let $x^\perp = -\sqrt{R} + x$ where $R = \Omega^2 b^2 + z^2 a^2 \longrightarrow x_\perp^2 = (-\sqrt{R} + x)^2$

Then: $x = x_\perp + \sqrt{R}$

And: $\dfrac{dx}{dx_\perp} = 1$ since $\sqrt{R} = \text{Constant}$

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Then:

If $x_\perp = \infty$ then $x = \infty + \sqrt{R}$

$$x = \infty$$

If $x_\perp = 0$ then $x = 0 + \sqrt{R}$

$$x = \sqrt{R}$$

So:

$$K(a,b) = 2 \int_{x=\sqrt{R}}^{x=\infty} \left((-\sqrt{R} + x)^2 + b^2 + a^2 \right)^{-1/2} \left(e^{-\frac{\sqrt{(-\sqrt{R}+x)^2 + R}}{l}} \right)^2 dx$$

Now, let:

$$x = \sqrt{R} \cosh q \longrightarrow \frac{dx}{dq} = \sqrt{R} \sinh q$$

$$dx = \sqrt{R} \sinh q \, dq$$

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Then:

$$\text{If } x = \infty \text{ then } q = \cosh^{-1}\left(\frac{x}{\sqrt{R}}\right)$$

$$= \cosh^{-1}\left(\frac{\infty}{\sqrt{R}}\right)$$

$$= \cosh^{-1}(\infty)$$

$$q = \infty$$

$$\text{If } x = \sqrt{R} \text{ then } q = \cosh^{-1}\left(\frac{x}{\sqrt{R}}\right)$$

$$= \cosh^{-1}\left(\frac{\sqrt{R}}{\sqrt{R}}\right)$$

$$= \cosh^{-1}(1)$$

$$q = 0$$

Thus:

$$K(a,b) = 2 \int_{q=0}^{q=\infty} \left((-\sqrt{R} + \sqrt{R}\cosh q)^2 + b^2 + a^2\right)^{-1/2} \left(e^{-\frac{\sqrt{(-\sqrt{R}+\sqrt{R}\cosh q)^2 + R}}{1}}\right)^2 \left[\sqrt{R}\sinh q\, dq\right]$$

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$$K(a,b) = 2 \int_{q=0}^{q=\infty} \left((\sqrt{R}(-1+\cosh q))^2 + b^2 + a^2 \right)^{-1/2} \left(e^{-\frac{\sqrt{(-\sqrt{R}(1+\cosh q))^2+R}}{1}} \right)^2 \left[\sqrt{R} \sinh q \, dq \right]$$

$$K(a,b) = 2\sqrt{R} \int_{q=0}^{q=\infty} \left(R(-1+\cosh q)^2 + b^2 + a^2 \right)^{-1/2} \left(e^{-\frac{\sqrt{R(1+\cosh q)^2+1}}{1}} \right)^2 \left[\sinh q \, dq \right]$$

Now, substitute:

$q = -\ln x$ or $-q = \ln x$

$$x = e^{-q}$$

Then:

$$dq = \frac{-dx}{\textbf{\rule{1cm}{1ex}}}$$

If $q = \infty$ then $x = e^{-\infty}$

$$\textbf{\rule{0.8cm}{1ex}}$$

If $q = 0$ then $x = e^{-0}$

$$\textbf{\rule{0.8cm}{1ex}}$$

The following identities also hold:

$$\cosh q = \frac{1}{2}\left(e^q + e^{-q}\right) = \frac{1}{2}\left(\frac{1}{x} + x\right) \longrightarrow \cosh^2 q = \frac{1}{4}\left(\frac{1}{x} + x\right)^2$$

$$\sinh q = \frac{1}{2}\left(e^q - e^{-q}\right) = \frac{1}{2}\left(\frac{1}{x} - x\right)$$

So:

$$K(a,b) = 2\sqrt{R}\int_{x=1}^{x=0}\left(R(-1+\left[\frac{1}{2}\left(\frac{1}{x}+x\right)\right])^2 + b^2 + a^2\right)^{-1/2}\left(e^{-\frac{\sqrt{R(1+\left[\frac{1}{2}\left(\frac{1}{x}+x\right)\right])^2+1}}}{1}}\right)^2\left[\left[\frac{1}{2}\left(\frac{1}{x}-x\right)\right]\left[\frac{-dx}{x}\right]\right]$$

$$K(a,b) = -2\sqrt{R}\int_{1}^{0}\frac{1}{2}\left[\frac{1/x - x}{x}\right]\left(R(\left[\frac{1}{2}\left(\frac{1}{x}+x\right)\right])-1)^2 + b^2 + a^2\right)^{-1/2}\left(e^{-\frac{\sqrt{R(1+\left[\frac{1}{2}\left(\frac{1}{x}+x\right)\right])^2+1}}}{1}}\right)^2 dx$$

$$K(a,b) = -(-1)\sqrt{R}\int_{0}^{1}\left[\frac{1-x^2}{x^2}\right]\frac{\left(e^{-\frac{\sqrt{R(1+\left[\frac{1}{2}\left(\frac{1}{x}+x\right)\right])^2+1}}}{1}}\right)^2}{\left(R(\left[\frac{1}{2}\left(\frac{1}{x}+x\right)\right])-1)^2 + b^2 + a^2\right)^{1/2}} dx$$

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$$K(a,b) = \sqrt{R}\int_0^1 \left[\frac{1-x^2}{x^2}\right]\frac{\left(e^{-\frac{\sqrt{R(1+\left[\frac{1}{2}\left(\frac{1}{x}+x\right)\right])^2+1}}{l}}\right)^2}{\left(R(\left[\frac{1}{2}\left(\frac{1}{x}+x\right)\right]-1)^2+b^2+a^2\right)^{1/2}}\,dx$$

This final equation will be the one that is solved numerically as a function of variational parameters and of Quantum Well-Wire size parameters.

_P(a,b)_

It is useful to see how the solution of the probability equation $p(a,b)$ was derived. First note the following:

For a particle in a box with infinite potential walls the wave function for a 2D box-model is:

$$y_{nm}(y,z) = \left[\sqrt{\frac{2}{L_y}} \sin\left(\frac{np\,y}{L_y}\right) \right]\left[\sqrt{\frac{2}{L_z}} \sin\left(\frac{mp\,z}{L_z}\right) \right]$$

So, for this infinite potential Quantum Well-Wire, let the single-particle functions be:

$$f_{\text{single particle}} = f_e = f_h = \sqrt{\frac{4}{L_y L_z}}\left[\sin\left(\frac{np\,y}{L_y}\right) \right]\left[\sin\left(\frac{mp\,z}{L_z}\right) \right]$$

with $n = m = 1$ for the ground state.

Hence:

$$p(a,b) = \int\limits_{m}^{n-a} \int\limits_{r}^{t-b} \left|f(z+a, y+b)\right|^2 \left|f(z, y)\right|^2 + \left|f(z, y)\right|^2 \left|f(z+a, y+b)\right|^2 dydz$$

$$= 2\int\limits_{0}^{L_z-a} 2\int\limits_{0}^{L_y-b} \left|f(z+a, y+b)\right|^2 \left|f(z, y)\right|^2 + \left|f(z, y)\right|^2 \left|f(z+a, y+b)\right|^2 dydz$$

This is so because:

1)   By changing integration parameters form -∞ to *0* requires a factor of *2*,

2)   Infinite potentials are considered at the boundaries. So there is no possibility of escape at all, i.e. no tunneling. Therefore the particle doesn't exist from *L* to ∞, but only between the boundaries of the box (i.e. the length and width of the box). Hence, the change from the effective infinities n and t to L_z and L_y.

Now, the above form of the equation *p(a,b)* is the more general symmetric form. However, since the single particle function i.e. for the hole and for the electron are exactly the same, the above form of the *p(a,b)* equation isn't exactly the right one to use, since it considers exactly the same function *twice*. This leads to the probability density to have a value of *200%*, not *100%* as required, i.e.

Probability Density $= \int\limits_{0}^{L_z} \int\limits_{0}^{L_y} p(a,b)da\ da = 2$

So, the form to use (to compensate for the similarity between f_e and f_h, is:

$$p(a,b) = 2 \int\limits_{0}^{L_z - a} 2 \int\limits_{0}^{L_y - b} |f(z, y)|^2 |f(z+a, y+b)|^2 dy\ dz$$

This equation has the property:

Probability Density $= \int\limits_{0}^{L_z} \int\limits_{0}^{L_y} p(a,b)da\ da = 1$

as it should be.

This leads to:

$$p(a,b) = 2 \int\limits_{0}^{L_z - a} 2 \int\limits_{0}^{L_y - b} \left| \sqrt{\frac{4}{LyLz}} \left[\sin\left(\frac{p(y+b)}{L_y}\right) \right] \left[\sin\left(\frac{p(z+a)}{L_z}\right) \right] \right|^2 \left| \sqrt{\frac{4}{LyLz}} \left[\sin\left(\frac{p\,y)}{L_y}\right) \right] \left[\sin\left(\frac{pz}{L_z}\right) \right] \right|^2 dydz$$

The software program Mathematica 4.1 was used to find the solution to this equation, leading to:

$$p(a,b) = \frac{1}{4 L_y^2 L_z^2 p} \left[\left(4(L_y - b)p - 2(b - L_y)p \cos\left[\frac{2bp}{L_y}\right] + 3L_y \sin\left[\frac{2bp}{L_y}\right] \right) \times \left(4(L_z - a)p - 2(a - L_z)p \cos\left[\frac{2ap}{L_z}\right] + 3L_z \sin\left[\frac{2ap}{L_z}\right] \right) \right]$$

This final equation is the one that was used.

Appendix B

Quantum Structure Glossary

Band gap (E_G)

Electron energy levels are not allowed to exist in any form inside the E_G. The band gap is a quantum mechanical phenomenon, and is the energy difference that is usually on the order of about one electron volt for most semiconductors. The valence band and the (more energetic) conduction band is separated by the band gap and it is therefore more difficult for electrons to be excited to the conduction band, since they have to absorb energy in some form or another in order to do that. In a regular semiconductor crystal, the band gap is fixed owing to continuous energy states. In a quantum dot crystal, the band gap is size dependent and can be altered to produce a range of energies between the valence and conduction band. Quantum mechanics dictates that the band gap of a quantum dot will always be larger in magnitude.

Conduction Band (CB)

The conduction band is the energy state that electrons occupy when they have been excited across the band gap. It thus contains the energy levels above the band gap and higher. Because the band gap is always much larger that the distance between energy levels, not many electrons can be excited across the band gap and cross into the conduction band from the valence band. However thermal collisions do allow a very small number of electrons to naturally occupy the conduction band.

When electrons absorb radiation with energy greater than or equal to the band gap energy, electrons can be stimulated across the band gap into the conduction band. This fact, and their subsequent emission of radiation as the electrons fall back down to the valence band, is the basis for the utility of quantum dots, wires and wells.

Continuous

When the separation between energy levels is so small that it may be treated as if it wasn't separated by any energy amount at all, the energy band is said to be continuous. This type of model works well for semiconductor crystals with large numbers of atoms and physical dimensions much greater than 10 nanometers. The most important consequence of approximating energy levels as continuous is that under those conditions, the band gap of a material may be treated as fixed and unchangeable.

Discrete

When the addition or subtraction of an atom or an electron to a crystal will measurably change the energy of the band gap, it is said that such a system has discrete energy levels.

It is when a semiconductor crystal has discrete states that it can be defined as a quantum dot, and this is when it takes on useful and interesting properties, because by adding or subtracting an atom (a relatively easy engineering process) the crystal emits at a different (and specifiable, to within limits) wavelength. This specification and tunability would be impossible with a traditional semiconductor with continuous energy levels, because one atom is insignificant given the size of such a bulk semiconductor, which are many orders of magnitude larger in number of atoms than a low-dimensional structure. So for large traditional semiconductors the adding/subtraction of an atom make the change in the band gap so small, that it is impossible to measure to measure or use lucratively. This results in a fixed band gap.

Energy Level

Quantum mechanics dictates that the electrons of all materials may only have certain allowable energies. Electrons can only exist at one energy level and not in between them. For example, a hypothetical electron may exist with 1 units of energy, or 2 units of energy, but not with 1.3547 units of energy.

Also, the Pauli Exclusion Principle says that only 2 electrons can exist at any one energy level. Thus, in any crystal, electrons will start filling the lowest energy levels first, and continue to fill levels with higher energies until no more electrons remain without energy levels.

For very small Exciton Bohr radii the distance between levels are appreciable larger than what it would for a bulk semiconductor crystal. It never becomes zero since there is always some finite distance between energy levels. However, if the dimensions of a semiconductor crystal become much larger than the Exciton Bohr Radius of the material, then the distance between energy levels in the crystal becomes very small, and it is then convenient to describe the energy levels as continuous.

Exciton

When an electron leaves the valence band and enters the conduction band and electron-hole pair is created bound by Coulomb forces. This electron-hole pair is treated as one single particle with zero net charge and is called an exciton. Excitons have a natural physical separation between the electron and the hole that varies from substance to substance; this average distance is called the ***Exciton Bohr Radius***. The exciton bohr Radius is small compared to the crystal in a large (bulk) semiconductor crystals. Thus the exciton is allowed to wander through the crystal relatively unrestricted. In a quantum dot, wire or well, however, the Exciton Bohr Radius is in the order of the physical dimension of the low dimensional structure or smaller, and the exciton is confined. This is known as quantum confinement, which means the exciton itself will have discrete, rather than continuous energy levels.

Exciton Bohr Radius

When an electron is excited from the valence band to the conduction band it leaves behind a hole and these two particles are separated by a distance that is known as the Exciton Bohr Radius. The size of this radius controls how large a crystal must be before its energy bands can be treated as continuous. Therefore, the Exciton Bohr

Radius can rightly be said to define whether a crystal can be called a semiconductor quantum dot, or simply a bulk semiconductor.

Hole

The absence of an electron in the valence band energy state is usually coined a hole. Holes can be treated as positively charged, and arise when a negatively charged electron jumps to the conduction band. The combination of the electron and the hole together is called an exciton.

Oscillator Strength

The oscillator strength is a measure of the probability that a transition represented by an electronic oscillator will occur. It is independent of the physical conditions under which the atom is radiating.

Quantum Confinement

When a crystal is in the order of or smaller than the Exciton Bohr Radius of its constituent compound, this system is quantum confined. Under quantum confinement, energy levels may be treated as discrete. By definition, quantum dots are in a state of quantum confinement.

Quantum Structure/Low Dimensional Structure

There are many acceptable definitions. For the purpose of this dissertation, a quantum structure is defined as:

1) a crystal of semiconductor compound (eg. CdSe, PbS, GaAs) with a diameter on the order of the compound's Exciton Bohr Radius. Quantum structures have a range of useful electrical and optical properties that diverge in character from those of bulk material. Quantum dots, for example, are between 2 and 10 nanometers wide (10 to 50 atoms).

2)   an electromagnetic radiation emitter with an easily tunable band gap.

Valence Band (VB)

The valence band contains all the electrons that are at the very outer edges of the atoms making up the crystal. This band contains all the electrons from the one with the lowest energy, to the one with energy just on the lower edge of the band gap. Since electrons tend to occupy energy states with the lowest energy possible, the valence band's energy levels are usually almost completely full.

Wannier Exciton

For a Wannier exciton the electron is bound very weakly to the hole with an average radius larger than the lattice spacing. These exciton are different to the Frenkel excitons where the electron is bound much stronger to the hole and therefore it is essentially confined to within a single lattice constant.

Conference contributions and publications

1. **Confinement of excitons in Quantum - Wires**
   Harris, R.A., Swart, H.C., Terblans, J.J.
   South African Institute of Physics Conference
   2005

2. **Exciton binding energy in an infinite potential Quantum Well – Wire**
   Harris, R.A., Swart, H.C., Terblans, J.J.
   Special Issue of Organic Electronics
   Submitted 31 January 2006

3. **The effect of the dielectric constant on the binding energy of an exciton**
   Harris, R.A., Swart, H.C., Terblans, J.J.
   South African Institute of Physics Conference
   2006

4. **Influence of size on an exciton's binding energy in a low-dimensional structure**
   Harris, R.A., Swart, H.C., Terblans, J.J.
   South African Institute of Physics Conference
   2006

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*B*ut the Lord, responding to Job from a whirlwind, said:

{38:2} Who is this that wraps sentences in unskilled words?

{38:3} Gird your waist like a man. I will question you, and you must answer me.

{38:4} Where were you, when I set the foundations of the earth? Tell me, if you have understanding.

{38:5} Who set its measurements, if you know, or who stretched a line over it?

{38:6} Upon what have its bases been grounded, and who set forth its cornerstone,

{38:7} when the morning stars praised me together, and all the sons of God made a joyful noise?

{38:8} Who enclosed the sea with doors, when it broke forth as if issuing from the womb,

{38:9} when I stationed a cloud as its garment and wrapped it in a mist as if swaddling an infant?

{38:10} I encircled it with my limits, and I positioned its bars and doors.

{38:11} And I said: "This far you will approach, and you will proceeded no further, and here you will break your swelling waves."

{38:12} Did you, after your birth, command the birth of the sun and show the sunrise its place?

{38:13} And did you hold the extremities of the earth, shaking them, and have you shaken the impious out of it?

{38:14} The seal will be restored like clay, and it will remain in place like a garment.

{38:15} From the impious, the light will be taken away, and the exalted arm will be broken.

{38:16} Have you entered the depths of the sea, and have you taken a walk in the uttermost parts of the abyss?

{38:17} Have the gates of death been opened to you, and have you seen the doors of darkness?

{38:18} Have you considered the breadth of the earth? If you know all things, reveal them to me.

{38:19} Which is the way that holds the light, and which is the place of darkness?

{38:20} In this way, you might lead each thing to its final place, and understand the paths of its house.

{38:21} So then, did you know when you were to be born? And did you know the number of your days?

{38:22} Have you been admitted into the storehouses of the snows, and have you gazed upon the stockpile of the brimstone,

{38:23} which I have prepared for the time of the enemy, for the day of the battle and the war?

{38:24} In what way is the light scattered, and the heat distributed, over the earth?

{38:25} Who gave a course to the rainstorms, and a path to the resounding thunder,

{38:26} so that it would rain on the earth far from man, in the wilderness where no mortal lingers,

{38:27} so that it would fill impassable and desolate places, and would bring forth green plants?

{38:28} Who is the father of rain, or who conceived the drops of dew?

{38:29} From whose womb did the ice proceed, and who created the frost from the air?

{38:30} The waters are hardened to become like stone, and the surface of the abyss freezes over.

{38:31} Will you have the strength to join together the sparkling stars of the Pleiades, or are you able to disperse the circling of Arcturus?

{38:32} Can you bring forth the morning star, in its time, and make the evening star rise over the sons of the earth?

{38:33} Do you know the order of heaven, and can you explain its rules here on the earth?

{38:34} Can you lift up your voice to the clouds, so that an onslaught of waters will cover you?

{38:35} Can you send forth lightning bolts, and will they go, and on returning, say to you: "Here we are?"

{38:36} Who placed discernment in the guts of man, or who gave the rooster intelligence?

{38:37} Who can describe the rules of the heavens, or who can put to rest the harmony of heaven?

{38:38} When was the dust cast to become the earth, and when were its clods fastened together?

{38:39} Will you seize prey for the lioness, and will you sustain the lives of her young,

{38:40} as they rest in their dens or lie in wait in pits?

{38:41} Who provides the raven with its meal, when her chicks cry out to God, as they wander around because they have no food?

Job 42:3-6

Who is this that hideth counsel without knowledge? Therefore have I uttered that which I understood not, things too wonderful for me, which I knew not. Hear, I beseech Thee, and I will speak; I will demand of Thee, and declare Thou unto me. I had heard of Thee by the hearing of the ear; but now mine eye seeth Thee; wherefore I abhor my words, and repent, seeing I am dust and ashes. . .