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Optical anisotropy study in coupled quantum wells, a novel source of undisturbed systems

Doctoral Thesis in Applied Sciences
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ABBREVIATIONS

BZ	<i>Brillouin zone</i>
QS	Quantum Structures
QW	Quantum Well
CQWs	Coupled Quantum Wells
VB	Valence Band
CB	Conduction Band
SCQWs	Symmetric coupled quantum wells
ACQWs	Asymmetric coupled quantum wells
RAS	Reflectance Anisotropy Spectroscopy
PL	Photoluminiscense spectroscopy
PR	Photoreflectance spectroscopy
R	Reflectance spectroscopy
PRD	Photo-Reflectance Differential Spectroscopy
FDM	Finite differnce method
CCD	Charge coupled device
0D	Zero-dimensional
1D	One-dimensional
2D	Two-dimensional
3D	Three-dimensional
fcc	Face-centered cubic
<i>hh</i>	Heavy hole
<i>lh</i>	Light Hole
<i>e</i>	electron
2DEG	Two-dimensional electron gas
BL	Beer-Lambert-Law
TB	Tight-Binding method
PD	Photo-Detector
QM	Quantum Mechanics
$k \cdot p$	Semiempirical theoretical tool to calculate band-structure
TB	Semiempirical Thight-Binding Method
SOC	Spin-Orbit Coupling, also called Spin-Orbit interaction
LFLM	Dr. Luis Felipe Lastras Martinez group.

LIST OF CODES AND PACKAGES

This list denote the *Open-Source* packages, codes, tools, and repositories to develop this work. All inside of this work as images or numerical calculations are subject to the *Open-Source* ideology. Our codes are it housed in own GitHub repository, both personal as the laboratory repository. It's importantly to say that without develop of Open-Source codes like contents in this list, our codes they couldn't been enhanced.

ASE The Atomic Simulation Environment (ASE) is a set of tools and Python modules for setting up, manipulating, running, visualizing and analyzing atomistic simulations. [2]

Spglib Software library for crystal symmetry search [3]

SOLCORE A multi-scale, Python-based library for modelling solar cells and semiconductor materials [4]

Aestimo One-dimensional (1D) self-consistent Schrödinger-Poisson solver for semiconductor heterostructures [5]

VESTA 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies. [6]

PGF/TikZ PGF is a macro package for creating graphics. It is platform- and format-independent and works together with the most important TeXbackend drivers, including pdfTeX and dvips. It comes with a user-friendly syntax layer called TikZ. [7]

SYMBOLS

X⁻ Negative Trion

X⁺ Positive Trion

Al_xGa_{1-x}As AlGaAs semiconductor as a function of Al concentration x

\hbar Planck's constant (eV)

m_0 electron effective mass

(hkl) Family of lattice planes with Miller indices h , k and l

1

PHYSICAL BACKGROUND

In this chapter raise and explains the basis of fundamental physics in semiconductor and quantum structures, implemented to understand the results in this work.

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QUANTUM MECHANICS is basically electron behavior that exhibits many phenomena non explained by classical regime. Quantum structures (QS) are artificially systems conformed by semiconductors where electrons exhibit their quantum nature, this is a great platform to study and create quantum devices. Nowadays, the progress in creation of QS consist in precisely deposition of thin films, in which electrons show fundamentally new electrical and optical properties [8]. Most of these properties consist in quantum behavior as the energy confinement, which is the principal interest to study the electron and their consequent interactions which generates analogous hydrogen atom in semiconductors. Therefore, the interest to studying QS was increasing for many years ago and nowadays, those continue considering an excellent research area.

In this chapter, it presents the fundamental concepts to describe the physical phenomena resultant in this work, without intention to replicate concepts and models already explained in publications with major impact. Therefore, the purpose is to present an own interpretation to highlight the great obtained results.

1.1 Semiconductor Bandstructure

To starting with physical background to understand the QS, it has to start with understand the band structure of semiconductors. The band structure describes the electron behavior in a solid, therefore, we will need to invoke the Schrödinger equation to describe it behavior. But, due inside a solid around 10^{23} valence electrons contribute to the bonding in each cubic centimeter, this results in a many-body complex problem [9], then the general hamiltonian for a solid has the form [10, 11]:

$$H = \frac{1}{2M} \sum_{i=1}^{N_n} \mathbf{P}_j^2 + \frac{1}{2m_0} \sum_{j=1}^{N_e} \mathbf{p}_j^2 + \frac{Z^2}{2} \sum_{i,j=1, i \neq j}^{N_n} V_c(\mathbf{R}_i - \mathbf{R}_j) - Z \sum_{i=1}^{N_n} \sum_{j=1}^{N_e} V_c(\mathbf{r}_j - \mathbf{R}_i) + \frac{1}{2} \sum_{i,j=1, i \neq j}^{N_e} V_c(\mathbf{r}_i - \mathbf{r}_j). \quad (1.1)$$

Where N_n is the number of atomic nuclei, N_e is the number of electrons with mass m_0 , asumming that the nuclei are the same mass it's consider M and charge Z_e . As is obviously, this Hamiltonian is so complicated, the sum of five terms which consists in : kinetic energies to electrons and nuclei, the nucleus-nucleus, nucleus-electron and electron-electron Coulomb interactions, also \mathbf{R}_i are the positions of the nuclei and \mathbf{r}_j are the position of the electrons, the operators \mathbf{P} and \mathbf{p} are momentum operators to nuclei and electrons respectively. Finally, the consider of Coulomb potential V_c [10].

Fortunately, the QS are formed by crystalline materials, the Bloch theorem provide the most important tool to develop required equations. The Bloch theorem establish a periodic potential $U(\mathbf{r})$ for electrons, this due the material is periodic (definition of crystal structure) and the Schrödinger equation it can describe in terms of single electron as:

$$\left[-\frac{\hbar^2}{2m_0} \nabla^2 + U(\mathbf{r}) \right] \psi(r) = E\psi(\mathbf{r}) \quad (1.2)$$

The principal reason that the periodic potential in a crystal structure is highly important is their translational invariance concept and the consequent symmetry operations that are possible in a crystalline solid. The symmetry concept, as a tool to understand solids, is discussed with major detail in the next chapter. In according to Bloch's theorem we can associate a wave vector \mathbf{k} with each energy state, $E_n(\mathbf{k})$. Thus, it is useful to display the energies $E_n(\mathbf{k})$ as a function of the wave vector \mathbf{k} . This result also knowing as dispersion relation, but in general terms is the electron band structure of the given solid [9].

Even if, the calculation of electron band structure in solids are very complex by the distance between atoms that composes it's, and the Bloch's theorem provide the most important tool to reduce the problem to crystalline structures, exists several methods to calculate the realistic bandstructure for semiconductors that are categorized in two groups: Atomistic methods* (Tight-binding, orthogonalized plane wave methods) and Perturbative methods $(\mathbf{k} \cdot \mathbf{p})^\dagger$. These two main categories with theirs respective methods have special characteristics which becomes in the reasons to choose them. The reasons have to do with to the described bandstructure, this mean, in case of Atomistic methods the entire bands (valence and conduction) can describe, but in case of perturbative methods are reserve to near bandedge bandstructures. So, each of these methods can be chosen and enhanced as the system to study requires. We won't enter in discussion about of which of these methods are the best, the reasons are simple, each method is powerful, and we must be remembered that the complexity of solutions requires that these are solved by numerical techniques therefore this convert it to good approximations. Then, basically the electron behavior inside a semiconductor consist in solutions of the appropriate Schrödinger equation [12].

1.1.1 Valence and Conduction Bands

The most important characteristic of semiconductors even we can call as the fingerprint of these, is their bands structure, this characteristic sort out the solids as insulators, metals, and semiconductors. These are the reason of many mechanisms and phenomena

*In this category can include the ab initio methods, these are the most complex methods due to propose solutions of the many-body problem

[†]In fact, both TB and $\mathbf{k} \cdot \mathbf{p}$ also consider in same kind, because both are *semi-empirical* methods due to they consider experimental parameters.

by which study this structures. In general, the bands of semiconductors composed by valence and conduction bands separated by a region known as bandgap. The bandgap, which is proportional to separation energy of valence and conduction bands also is called as forbidden region, this is because doesn't exist electron states, therefore this gap energy determine the electron conduction in a semiconductor and the difference they have with the insulators and metals as shows Figure 1.1.



Figure 1.1: Band energy diagram for insulators (left), semiconductors (center) and metals (right). The principal difference is the gap energy, for insulators this is longer than semiconductors, although in semiconductors gap energy depends on materials, finally in metals doesn't exist gap energy instead exist an overlap bands characterize these. Dashed line determine Fermi's level.

So, the bandgap determines many characterizes and functionalities in semiconductors. The bandgap energy classifies semiconductors in direct and indirect semiconductors, but doesn't only depend on this energy, in reality the band structure is the liable for this. As before mentioned, it is so difficult to describe electrons behaviors over the solids due to the many body interactions that exists in its, and therefore the Schrödinger equation that's describe electrons behaviors is complicatedly to solve. Fortunately, the semiconductor structures have one of the most important characterize and his has to do with their atomic structure, that's periodically arrangement of atoms. This periodicity is the key to propose solutions and describe the semiconductor band structure. Starting with describe bulk semiconductors, for example GaAs which consists in with the family III-V cube semiconductor so that their lattice structure consist in a two sublattices correspond to each atom which it conform as shows in Figure 1.2. For this case, when the atoms in two sublattice are different, the crystal structure is then called *zinc-blende* [13].

To calculate bandstructures of bulk semiconductors it's important to define specific symmetry direction, this mean that it's not possible to plot dispersion relation. For each three-dimensional wave vector \mathbf{k} , then the plot energy as a function of \mathbf{k} is along of different

high-symmetry directions [9]. In this work the structures to study are composed of semiconductors III-V, being GaAs the bulk in each structure. GaAs is a direct semiconductor so that the [001] direction is the high-symmetry direction then is denoted by Γ point (at $\mathbf{k} = 0$)

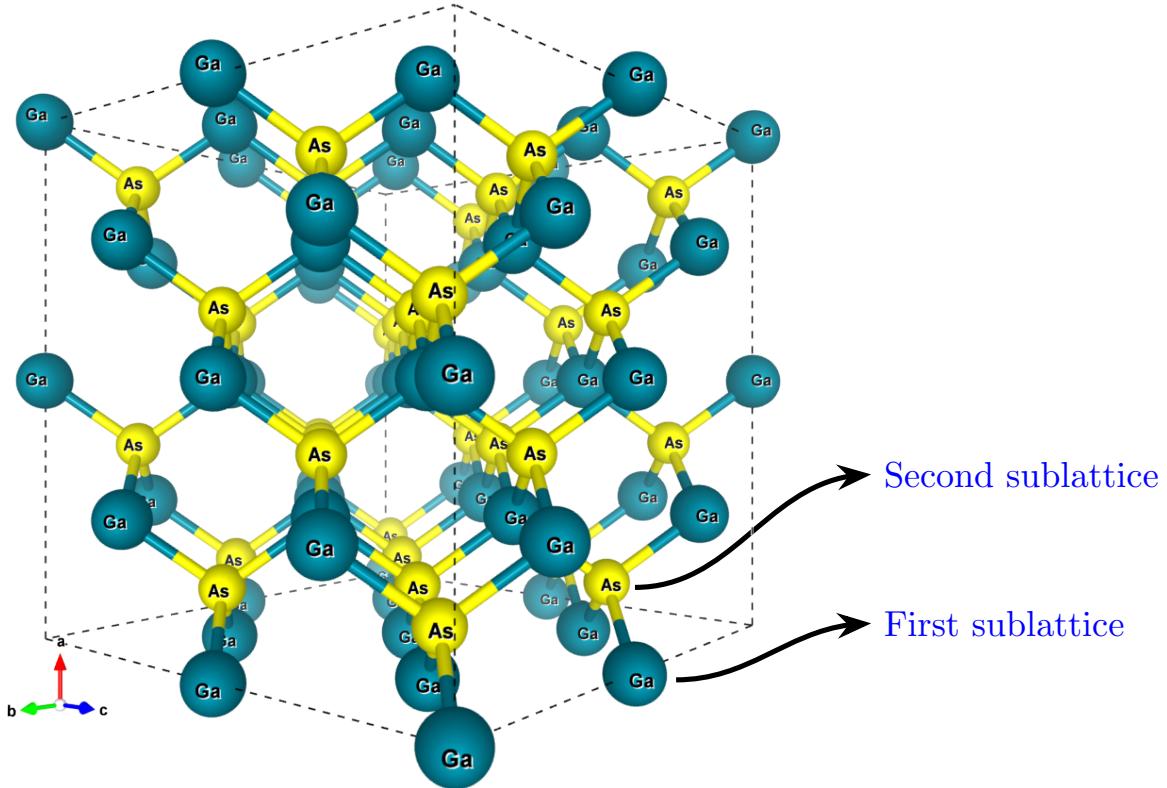


Figure 1.2: GaAs crystal lattice, where the each sublattice correspond of each atom species Ga and As.

As before mentioned several times, it's very complex to compute the Schrödinger equation in the solids. The most “exact” compute is employed by DFT theory, these calculations commonly are called atomistic even some semiempirical models can consider as atomistic, but the semiempirical models are good approximations in comparison with the DFT theory. So, which is the reason to call “exact” solutions to the DFT results? The answer leads us to great discussion and it's not intended to get into controversy, but in general the DFT calculations have the capacity to calculate in terms of electrons interaction and the empirical methods are based in potential choice.

We will, don't into details about band calculations theories and models, but we will make a general reference to the importance in this work. The models more performed in semiconductor heterostructures as GaAs/AlGaAs are semiempirical, this is because DFT theory and their derived models are very limited to carried out in large structures,

their electron interaction nature need high computational perform. So that in comparison with empirical models where the main role is the potential of semiconductor structures, this reduces computational reduce. So, the most models used in semiconductor band calculations are empirical models, these models are distinguished by low computational requires for this reason are considered like approximations. The importance to discuss these concepts will take relevance when we discuss the physics model proposed in this work.

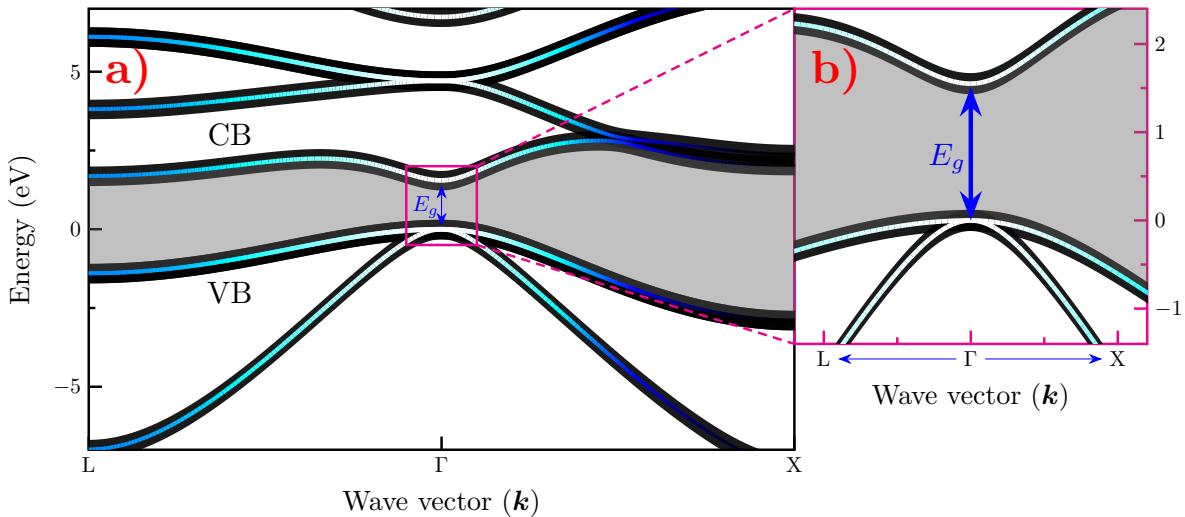


Figure 1.3: Band structure of GaAs, (a) shows the zoom around of Γ to denote the direct band gap and the electrons energy needed to jump from valence to conduction band. (b) denotes the two directions to dispersion of the bands corresponds to Brillouin zone: $\Gamma \rightarrow X$ and $\Gamma \rightarrow L$. [1]

The Section 1.1.1 shows the results of calculations of TB model as discuss it in [14] and the code was implemented by R. Muller [15]. The model purposes by Vogl et al. take into account small number of localized pseudo-orbitals and based the empirical parameters to substitute on TB Hamiltonian. The importance to get bandstructure it's based importance to study optical properties of solid structures, if it doesn't exist band electrons it's like look a place without map, so, the band structure far from being a complex tool it's the key to get the information to investigate the optical properties.

As shown in Figure 1.3(a) the GaAs bandstructure shows that it's a direct semiconductor as a previously mentioned, this gives way to get electron transitions from VB to CB and the energy to success this it. In Figure 1.3(b) it's plotted, the band dispersion around Γ point, it's the most symmetry point. It is well-known that the band dispersion increasing \mathbf{k} along two different directions of the Brillouin zone, from $\mathbf{k} = (0, 0, 0)$ to X point $\mathbf{k} = (2\pi a_L)(1, 0, 0)$ and L point $\mathbf{k} = (2\pi a_L)(1, 1, 1)$. So, these figures, are the typical representation of direct gap to III-V semiconductors around of $\mathbf{k} = 0$, then, is obviously that the shape of dispersion is parabolic. For the GaAs bandstructure calculations shown

in Section 1.1.1 doesn't take into account the contribution of spin*, therefore it's focus on three bands dispersion correspond to a single *s*-like conduction band and two *p*-like valence bands. Is important to say that the characteristic curvature $E-\mathbf{k}$ of dispersion bands corresponds to an electron (*e*) in case of positive curvature while the negative curvature correspond to holes states; heavy (*hh*) and light hole (*lh*) bands, so, this denotes that the transitions, are of dipole nature [1, 11]. All the above disputed is significant to refers of one

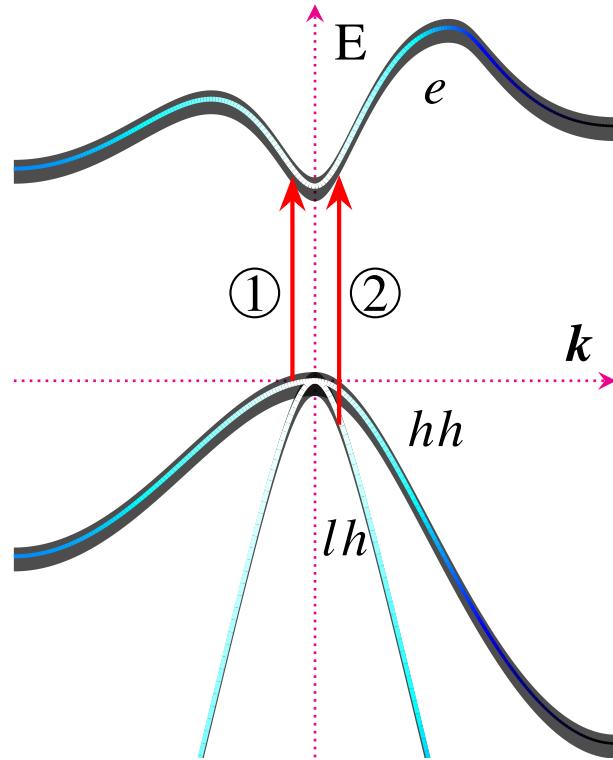


Figure 1.4: Two typical transitions for GaAs near $\mathbf{k} = 0$. The first one correspond to the heavy-hole and second one to the light-hole.

of the most indispensable quantum mechanisms in solids, this is absorption. The electron absorption, specifically interband absorption, give way to a fundamental physical process that involves the principle of many basic studies of semiconductors, applications, and the importance to understand the electron behavior in a semiconductor structures disputed in this work. Then the Figure 1.4 schematizes the two typical transitions in GaAs bulk, this transitions are near to $k=0$, so that is called interband absorption. Is important to remark that the interband transitions are observed in all solids, but the mechanisms are different dependently of their bandstructure, for what, being repetitive when mentioning that the bandstructure is the key to study solids.

In case of GaAs the interband tranisitions are called as direct transitions, this is because their bandstructure proofs GaAs is a direct Gap semiconductor. This process is determined by quantum mechanical rate $W_{i \rightarrow f}$ for exciting an electron in a initial quantum state

*This spin contribution as called as split-off (so) hole band.

ψ_i to final state ψ_f by absorption of a photon of angular frequency ω [1]. As is very known, this is given by Fermi's golden rule. Later this is disputed according to highlight the model and results obtained. It has been mentioned that the direct transitions are of dipole nature, as before mentioned the CB is type *s*-like while the VB is *p*-like, then it's electric-dipole allowed transitions $p \rightarrow s$. The excitation of electron in CB carries to leave an initial state unoccupied, this is called as a hole creation, then the electron in the final state and the hole is considered as **electron-hole pair**. The next part subject this theme with major focus.

1.1.2 Excitons

The importance to study bandstructure of semiconductors is very clear so far, so that could be said that absorption process is the source of optical properties of solids. It's due to this that the importance to study of semiconductors in the optoelectronics applications. But, this process give rise to formation of one of the most important excitations in the crystal structures. The photon absorption process carries to an electron is excited from CB to VB, this generates an empty location in VB which has positive charge. This positive empty location called as hole, therefore the electron and hole have opposite charge then it's to be expected that they are attracted, so, this creates a bound state called an exciton [16].

From Figure 1.4 and Figure 1.5 is clearly that excitons are commonly presented in direct band gap semiconductors as GaAs, this was denoted by absorption experiments, after mentioned in ?? this is the cause in photoluminescence mechanism.



Figure 1.5: Qualitative scheme of exciton creation in GaAs as direct gap.

1.2 Semiconductor Low-Dimensional Structures

The previous section engaged to explain the principles of semiconductors, this is the bandstructure, the importance of these is practically the fingerprint of all semiconductor, without bandstructure the understanding of these would be improbable. The first approximations were based in GaAs bulk, their cubic symmetry practically defines their nature and consequently the physical effects as excitons existence. But, what happens if joined several semiconductors with same symmetry and structural parameters? The bulk properties and physical properties are the same?. The answers they are well-known, when two materials with relatively same structural parameters, as lattice constant can create a heterojunction, the union of several heterojunction make up a heterostructure.*

The Figure 1.6 is a general scheme of a heterostructure, in this case is presents three

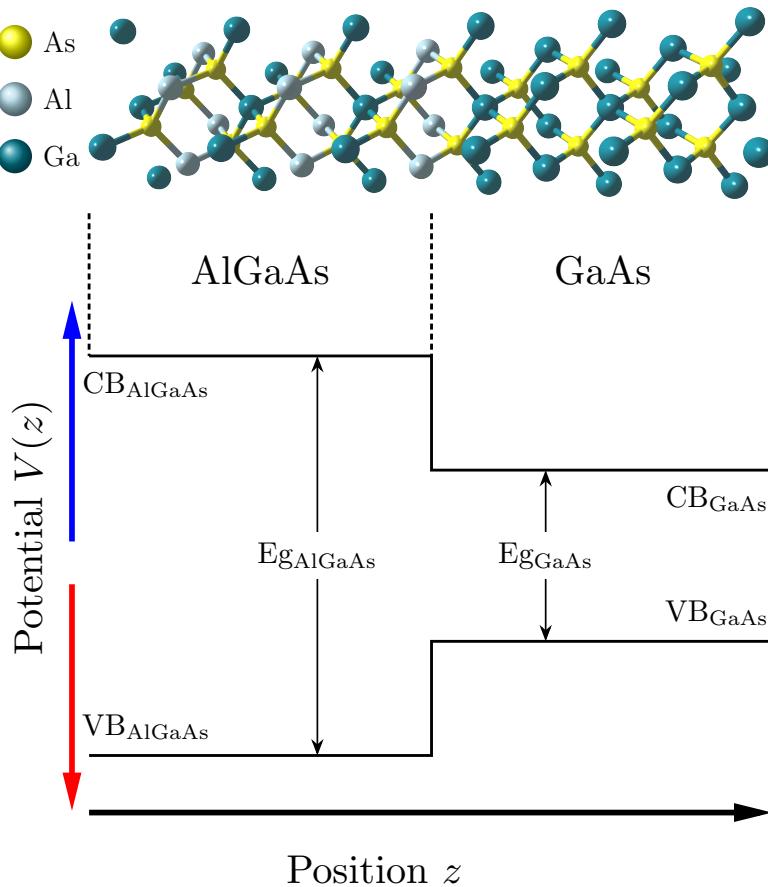


Figure 1.6: General scheme of $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ heterostructure, at top show the scheme of atomic arranged of this heterjunction, the dashed lines are the matched between two dissimilar materials. In bottom shows the band-edge profile.

*The samples studied in this work are heterostructures, for this reason, and by nomenclature it's we refer to that way.

species of atoms Al, As, Ga. These atoms can locate in columns III-V of the periodic table, hence its name of III-V semiconductors. The principal characteristic of these atoms is that it can create matched structures as GaAs, AlAs and ternary alloys as $\text{Al}_x\text{Ga}_{1-x}\text{As}$ with specific Al concentration. The matched semiconductors produce a material with new properties based principally in the difference of bandgap which involves the alloys.

As can see in Figure 1.6 it's consisting a GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$ heterostructure, these interface is well-matched due to the lattice parameters is relatively equals, therefore and thanks to powerful growth technics as MBE it's possible to get high-quality quantum structures.

Also, the heterostructure composed by two semiconductors with different band gaps generate a discontinuity in either the conduction or the valence band can be represented by a constant potential term [17]. The theory to treatment the electron behavior in these structures, is relatively simple if we consider the above. Although, in this chapter doesn't have intention to explore the theory of electron behavior in that, worth noting that it get one-dimensional potential $V(z)$ to both bands, so the Schrödinger equation can solve simple.

1.2.1 Quantum wells

Doubtless the creation or growth of heterostructures increased the interest in the study of quantum structures, the interactions, and physical behavior of light-matter they would not have been possible without these. The major relevance is due the quantum confinement, the junction of semiconductors results in an interest quantum structures with specific dimensions. From 3D bulk the dimensions reduce to 2D, 1D and 0D dimensional structures. Therefore each of that has interest properties and their correspond applications. The Figure 1.7 schematics the low dimensional heterostructures from 3D bulk, the first low dimensional from 3D to 2D is the Quantum Wells, then from 2D to 1D it have the Quantum Wires finally with 0D have the Quantum Dots. The quantum confinement so is the principal reason to study that structures, the electron behavior which exhibits in it should can to help understand a great variety of quantum mechanical phenomena as electron interaction on a crystal. Suppose a heterostructure composed with a two semiconductor alloys as sandwich, this 2D quantum structure is called a Single Quantum Well (SQW).

This dissimilar semiconductors in terms of their potential energy ($V(z)$) can be schematized as Figure 1.8. The Gap difference of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and GaAs is due to x Al concentration in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ therefore it obtains a one dimensional potential profile, with that can confinement electrons in a 2D plane along z direction. All of these carries to quantum mechanics formalism, the electron behavior should be obeyed these rules. If we have an electron closed in two potential barriers an L distance, the wave which describe it will be spatially confined. So if we confined many electrons in these potential, we have two important physical aspects: the first one is knowing as Pauli's exclusion principle,



Figure 1.7: Heterostructures from bulk (3D), to Quantum Wells (2D), Quantum Wires (1D) and Quantum Dots (0D).

which as of its Fermion nature prevents carriers with the same spin occupying the same region in of space [17, 18], the second one and one of the most relevant in the birth of the quantum mechanics; the Heisenberg's uncertainty principle. That last, it can say that is the consequence of quantum confinement due to the space reduction of the electrons is expected that momentum increases by an amount of the order \hbar/L . Therefore, the energy of that confined particles increases, and it's referred to as confinement energy [11].

Then the quantum confinement is our started point to understand the optical properties in QWs. As is referred in the figure, the uni-dimensional potential profile can well describe by top conduction- and bottom valence-bands, the band offset in these two of correspond gap energy between that, while Al concentration increases their bandgap and the band offset (Q_c to CB and Q_v to VB) also to.

It's so clearly that the QWs have the potential to presents amazing quantum properties, even if all of these are very important we focus on the optical properties, basically our interest is the light-matter interaction through its result mechanisms.

1.2.2 Preliminary approach of Quantum Confinement effect in QWs

As the title describes, here it will try to explain as the first approach the quantum confinement effect in QWs. If it starts with the scoop, which it can be reduced the



Figure 1.8: GaAs/Al_xGa_{1-x}As Single Quantum Well

electrons space, then this mean that in reciprocal space it has two components k_x and k_y . Then say in crystal symmetry properties to the case of GaAs/Al_xGa_{1-x}As QWs it's Γ the central point, as long as $x < 0.4^*$ the bandstructure depends on confinement energ, so say which the bandstructure depends on confinement energy. In this case, the electronic properties in comparison with a bulk semiconductor properties can solve trough particle-in-a-box as textbook problem as first approach. Nevertheless, even if usually can solver without much mathematical formalism is very essential that it dedicates a chapter with their solution, this is because will employ a physical formalism exclusively to QWs structures. In general way, as it before mentioned the Schrödinger equation solution is the fundamental pillar to understand, where it's taken into account which in a crystal the periodic potential is the key. Here are important remarks before to continue, when it has a heterostructure starting with the bulk model it's clearly that the system doesn't same, the Quantum Mechanics which is behind take into account the symmetry properties, then it can be developed a Hamiltonian to understand that system. In the next chapter will be explained details and the formalism both physical and mathematical to solve and discuss it's. The model which give the tools to get the solutions is called as Effective Mass

*It will be explained in the next section, although it's due to the Gap go from direct to indirect, shortly the symmetry $\Gamma \rightarrow X$.



Figure 1.9: General scheme of typical Schrödinger's equation solutions to one-dimensional potential as (a) where the Eigenenergies of both electron and holes are denoted with same color depending on n value.(b) It's plot, of the subbands in the same case of (a) to both particles.

Approximation, thus their correspond Schrödinger equation is [1, 17, 19–22]:

$$-\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial z^2} \psi(z) + V(z)\psi(z) = E\psi(z), \quad (1.3)$$

where the m^* is the effective mass in each material, and $V(z)$ is the potential profile got by heterostructure materials properties. Therefore, that differential equation can solve as in textbooks explained [1, 17, 19, 21, 23–26]. The idea is thinking as a one particle in a finite potential well, where is well important established the boundary conditions and solve the Schrödinger equation in each part of single QW, this means that need to create a potential function. Then it's can obtain the Eigenfunctions and their correspond Eigenenergies.

The principal idea doesn't is reproducing something which is very well known, the objective of this part is established the scoop of the next chapter. Therefore, before to continue, we will finish with to explain the dispersion in-plane of single QW. As in the QW the one-dimensional potential set up the 1D confinement, is important doesn't confuse which the QW is a 2D structure, but their confinement is along of z direction this mean 1D. Then, the particle can motion in the $x - y$ plane. By this reason, even if consider 3D Schrödinger equation and the above is considered it obtain Equation (1.3) therefore, the solutions in the one-dimensional potential produce discrete states of energy $E_z = E_n$ [17],

where n is the energy level it which produce subbands as shows in Figure 1.9. In contrast, before it called as “energy bands” in the bulk case, now due to the quantum confinement gets subbands to both conduction- and valence bands.

These subbands are the result of the sum of E_z and $E_{x,y}$, which are the 1D confinement energy and the in-plane momentum $k_{x,y}$ then [17]:

$$E = E_n + \frac{\hbar^2 |\mathbf{k}_{x,y}|^2}{2m^*}. \quad (1.4)$$

From equation the effective mass m^* depends on particle, i.e the effective mass to electrons in CB and the holes in VB. So, the most relevant in the solutions is the energy E_n (Figure 1.9(a)) is discrete, this is the quantum confinement in the low-dimensional heterostructures.

1.3 Summary

In this chapter, was exposed the generalities of semiconductor band structure and low-dimensional heterostructures, highlighting or taking in major GaAs/Al_xGa_{1-x}As that's the semiconductors of major importance in this work. The band structure interpretation usually be so hard, and their calculations even more, but the impact and relevance in optical properties of semiconductors starts from that interpretation, from here arises the mathematical arsenal to right physical interpretation. Another significant concept which was treatment as first approach is the effective mass concept, even if, when solved, the bulk Hamiltonian it considers the mass as constant parameter or depending on semiconductor material, contrary in low-dimensional structures have an important role.

In generally, the band structure of semiconductors is the key to understand quantum properties of solids, in this work the relevant is the light-matter. Remember that light-matter interaction in solids can be studied by process resulting in it, as absorption, reflection, transmission, diffraction, scattering, and others [27]. Although, the light-matter interactions are fundamentally quantum electrodynamical, also, can be studied in quantum way through before mentioned process. Firstly, is the photon absorption process can help to understand or calculate the fundamental parameter in semiconductors as is bandgap energy. This parameter is the started point in the study of semiconductors, this is the start point in the map called bandstructure, if it ignores the gap value in the semiconductor to study it couldn't possibly get the principal optical properties of that.

Then, the bandstructure of semiconductors is the map to understand them, without these routes or fundamental parameters couldn't have quantum devices.



PHYSICAL MODEL

In this chapter, it's exposing the fundamental physics to understand the experimental results' through physical model, both numerical and phenomenological. It is emphasis in symmetry properties of semiconductors, which is the base to get our model.

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SEMICONDUCTORS are alloy of materials with pure structural characteristics, it's the alloys which can generate an amazing quantum process that is quantum confinement. But, all of them couldn't possibly be achieved without understand of semiconductor bands, are bands the reason to get semiconductor heterostructures. Now, the objective is proposing the model to study Coupled Quantum Wells. The CQWs are heterostructures grown from a semiconductor substrate as GaAs as previously treated SQW (see Figure 1.8) but coupled by a thin barrier which have a very significant role. But before to mention the objective of study this structures and the physical model which explain their experimental results is important to call about of the symmetry and their relevance to understand the physics of these QS.

Previously, we were very repeating in the importance of semiconductor band structure, also to remark difficult of get them. It was saying the complexity of calculate semiconductor bands is high, by this reason it's developed models to approximate it. But, all of these couldn't be possible if it would not be taken into account the *symmetry* role in physics [28]. Thanks to symmetry, it's possible to understand from Quantum to Universe. It is clear that to talk the symmetry is inevitable to think in geometry or nature patterns inherently way, but in the next sections it's established the symmetry role from the band structure calculation to the importance in the electron behavior in CQWs structures.

2.1

The Symmetry Context

Talk about *symmetry* is talk of shapes or in a romanticism way as the natural harmony that makes something appear beautiful to us [29,30]. But, what is the reason the *symmetry* is very important in physics?. The reason the *symmetry* is very important has to do with a *transformation*, this mean that if a physical system is affected or perturbed by a thing and this appears to be exactly the same before and after that *transformation*, it is said to be *invariant* under that *transformation*. The symmetry of the system is made up of all the transformation operations that leave the system invariant [29].

In this section doesn't have the purpose to be a one more copy or re-interpreted version of a group theory book, yes, the group theory not symmetry theory, it's important to remember that to understand of symmetry physics of solids it's important to understand the group concept. In generally, a group is a set or collection of elements that obey certain criteria and are related to each other through a specific rule of interaction and obey four group axioms [29, 31, 32]. It is important to remark which the heterostructure to will study is composed by $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ semiconductors, then we started with the GaAs crystal to propound the symmetry role in the CQWs. Then, already raised the starting point, remember that the crystal solid can be defined as an arrangement of atoms in strictly periodic arrays [33,34], from here arises two concepts: basis and lattice, where that

last is the set of mathematical points to which the basis is attached [33]. These crystal concepts give place of crystal primitive cell in three dimensions also considered as the seed to reproduce a crystal. So, it gets fundamental types of lattices defined by a collection of *symmetry* operations (rotation, translation etc.), then it's compose a lattice point group. In the three-dimensional case, the point symmetry groups require the 14 different lattices types*, where are classified into seven systems. Into these systems it's found the *cubic* system, it which posses three number of lattices. Remember that the GaAs crystal is *cubic*, specifically, is the type FCC lattice. The FCC lattice is easy to imagine, if place an atom in each corner of a cube and in a center of each face of it. Therefore, it is easier to define the planes and crystal directions if we take the cube faces as a reference it gets (hkl) plane and the directions [hkl] which must be perpendicular to a plane (hkl) [33].

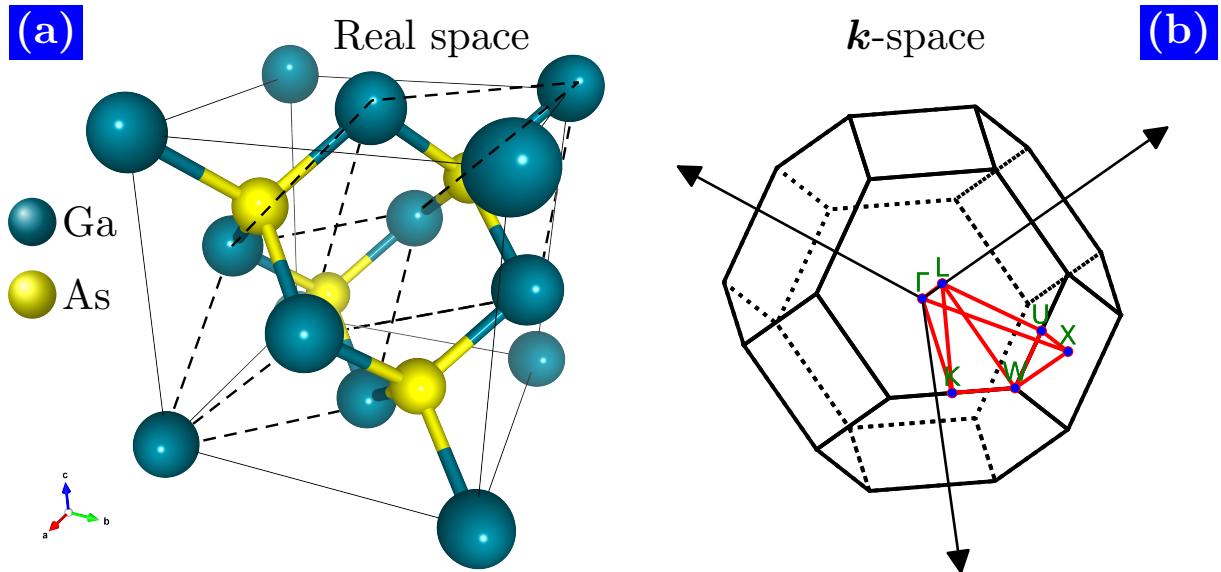


Figure 2.1: (a) GaAs crystal structure in “real space”, this region is known as *unit cell*, into that with dashed line is denoted the primitive cell. This lattice is well-defined by the vectors **a**, **b** and **c**, these vectors are defined as the basis vectors. In (b) is schematized the GaAs crystal structure in \mathbf{k} -space, also known as *reciprocal space*.

The lattice is an array of points which make the space lattice of a *crystal* and the repetitions or disposition of these points is controlled by “*symmetry* operations” [35]. The crystal is composed by a space lattice this is a plane lattice[†] which have three *symmetry* operations: *Rotation axes*, *Mirror plane* and *Centre of Symmetry*. If add a one dimension to plane lattice it gets a space lattice, which define the unit cell of a *crystal*, so this adds one more *symmetry* operation which is *Rotation Inversion* or *Roto-Inversion*. Then, can get *symmetry* elements of a *crystal* if apply the four *symmetry* operations and their possible combinations. If collect that *symmetry* elements obtains the *point symmetry* or the *point*

*This lattices are known as Bravais Lattices

[†]2D point pattern array

group of symmetry of a *crystal*. The GaAs crystal as before mentioned is a *cubic* system, but have a defined *cubic* structure called as *cubic zinc sulfide* or simply *zincblende*. This specific *cubic* structure is characterized by arrangement of two type atoms with places coordinates: $000, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0$ for one type of these as Zn in ZnS or Ga in GaAs structure. In case of the second one atom, it has coordinates : $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{3}{4}, \frac{3}{4}, \frac{3}{4}, \frac{1}{4}, \frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ for S in ZnS or As in GaAs [33, 36]. The Figure 2.1(a) shows the unit cell of GaAs structure and into them it dashed the primitive cell for the FCC lattice, also denoted the basis vectors \mathbf{a} , \mathbf{b} and \mathbf{c} .

In the case of symmetry of GaAs crystal, is important to remark that this symmetry can also denote in Hermann-Maguin notation $F\bar{4}3m$ which corresponds to three fourfold rotary inversion parallel to the edges of a cube, with four threefold rotation axes parallel to the body diagonal and six mirror planes, each containing a face diagonal [35]. The F label corresponds to cubic system FCC, following by the corresponds operations.

The symmetry context before exposed can view as a macroscopic symmetry about a crystal system, which means, is very interactive to think as a pattern well-ordered can conform a plane lattice and is intuitively work the symmetry operations. But it's not the only symmetry concept in crystal systems, if we enter into crystal it found atoms or molecules which conforms it. So, the internal study of a crystal add two symmetries to the actual worked before. These "microscopic symmetry" [35] the make reference to \mathbf{k} -space or reciprocal space. So, the previous concept of lattice it's also known as direct space lattice. Thanks to X-Ray, Electron or Neutron diffraction techniques, it was possible to study the internal structure o crystal symmetries in the reciprocal space, this trough diffraction phenomena, the propagation of waves into crystal can to form well defined pattern they which are explained by the wave-vector concept [29, 37]. Therefore, is expected that the electron wave function can be denoted with a lattice periodic part $u(\mathbf{r})$ and wavelike part $e^{i\mathbf{k}\cdot\mathbf{r}}$ so, the set of all wave vectors \mathbf{k} corresponds to plane waves due the lattice, this is known as reciprocal lattice [38]. Then taken into account this, and the vectors \mathbf{a} , \mathbf{b} and \mathbf{c} in reciprocal space can describe the total unit cell [29, 38].

Finally, as a result to get the unit cell in reciprocal space and known which this is composed by lattices, these lattices are called as *Brillouin zones*. Practically the *Brillouin zones* are constructed by drawing the vectors \mathbf{K} defining the reciprocal lattice and then bisecting each of these with planes perpendicular to \mathbf{K} [29]*. In Figure 2.1(b) it's schematized the *Brillouin zone* to GaAs crystal structure, specifically this representation is called as *first Brillouin zone*. To GaAs crystal it was defined the symmetry operations which compose the symmetry elements in Hermann-Maguin notation as the point group $F\bar{4}3m$, it's important to consider the Schoenflies notation also, this due people often speak in terms of both, although the Hermann-Maguin notation is consider as the International notation. In Schoenflies notation, the GaAs correspond to T_d point group.

*The wave vector \mathbf{K} is defined in [39] equation (1.5)

2.1.1 The symmetry and the Band Structure

Returning to Figure 2.1(b), the Brillouin zone have labels which they are, importantly, this is because each of these denote a point group symmetry. These points are: Gamma, X, L, W, U, K. In Schoenflies notation these correspond to: $\Gamma \rightarrow O_h$, $X \rightarrow C_{4v}$, $L \rightarrow D_{3d}$, $W \rightarrow C_{4v}$, $U \rightarrow C_{2v}$, being Γ the high symmetry point. Then, why is the importance of the **BZ** role in semiconductor band structure?, the answer is the aim of this subsection. We started with the first section of this work, in it refer the importance of solution of Schrödinger equation, specifically at crystal structures as semiconductors. Here, the most important tool is the Bloch's theorem, it which is developed from periodic property of crystal so, it's possible to approximate.

This context is introductory and general, because this doesn't possible if not consider the symmetry properties in crystals, in fact, *the symmetry of system define the basis function to get the electron band structure* [11, 40–42]. Remember that the concept of *basis function* is a mathematical concept, which in quantum mechanics it's known as *Wave functions*. Also, never to forget which the *symmetry* concept is inherent in physics. Therefore, the Group theory establishes the game rules. So, the **BZ** is the result of Group theory applied in crystal structures, then the **BZ** is the map to understand the electron behavior in crystal structures, this defined the \mathbf{k} points trough high symmetry paths, where this starts at Γ point or $\mathbf{k} = 0$. If observe the Section 1.1.1 the horizontal axis correspond to \mathbf{k} points and labeled the high-symmetry directions from Γ , then this is the \mathbf{k} paths in **BZ** as can see in Figure 2.1(b).

Previously, it's continuously mentioned which band structure calculations are difficult, so, it will start to change the hard word to tricky, this because it's possible to make very good models and approximations taking into account the symmetry of the system. All to begins from symmetry, the well-known models to calculate band structure starts from symmetry arguments of crystal or the semiconductor studied, through succession of symmetry operations it knows until it's invariant, this mean doesn't change under transformation. Here, highlights the invariants concept, which is the connection of symmetry and Quantum Mechanics. The symmetry gets the information of the system, while the QM the information of the state electrons. The Hamiltonian of the crystal has a symmetry which depends on their potential, then the crystal potential posses a point group, which is invariant under any transformation. So, the solution of the Schrödinger equation contains the state of the system. From these tools, can propound the physics of electrons or another quasi-particle inside a semiconductor, for example in perturbation theory, starts from Hamiltonian \mathcal{H}_0 with it specific space group, but under perturbation the Hamiltonian of the system should be the sum of $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}'$, where this last has the symmetry correspond to a subgroup of the \mathcal{H}_0 group. This is, the principle of this work which after will be discussed with detail. While the solution of Schrödinger equation with the total Hamiltonian \mathcal{H} will result in the energy spectrum $E(\mathbf{k})$ along of the **BZ**.

Being a crystal system and the potential is the periodic, it's to hope which a multiband spectrum. Although here doesn't consider the degeneracy* term, it's evident which the Group Theory has the solution, in general words, are the irreducible representations of the symmetry group which determine the dimension of degeneracy [43].

Thus the band structure as a whole exhibits the symmetry characterized by the crystal [43]. All previous it's about of an ideal crystal, then it's possible to get exact solutions of Schrödinger equation. But, to determine in detail the spectrum $E(\mathbf{k})$ throughout the **BZ**, one needs a numerical solution of the Schrödinger equation. In previous sections, it shows the results of apply **TB** method to GaAs bulk, this method parts from Bond Orbital Model [14, 44, 45], in this case, the basis functions it's forming linear combinations of atomic orbitals (LCAO) to specific symmetry group [40].

In this method, the importance is the arrangement of atoms and their orbitals considered, for Figure 1.2 these are sp^3 . In another way, in the case of $\mathbf{k} \cdot \mathbf{p}$ method, apart from perturbed model, but in both the main idea it's found the \mathbf{k} -points correspond to the symmetry of the system. In another way, in the case of $\mathbf{k} \cdot \mathbf{p}$ method, apart from disturbance model, but in both the main idea it's found the \mathbf{k} -points correspond to the symmetry of the system. The difference apart from their basis is the efficiency in their applied over semiconductor structures, this means that the $\mathbf{k} \cdot \mathbf{p}$ -method is appropriate in a small region of **BZ** to describe $E(\mathbf{k})$, therefor is the preferred option to describe semiconductor bands around of Γ , while if the idea is describing $E(\mathbf{k})$ in an extended region of the **BZ** the **TB**-method is the correct [40, 43]. In any way, the symmetry establishes the basis to get semiconductor band structure, no matter the method this, includes the first principle methods as DFT, which requires the symmetry information of the system to get the pseudopotentials and the geometric optimization to enhance calculations.

Although the symmetry concept is the base, the principal objective in this work you have to see the consequences of symmetry under in a non-direct perturbation, this mean, if it has GaAs bulk-semiconductor this has one defined point group T_d . When applied it a perturbation, as an electromagnetic perturbation the principal symmetry group it's reducing to a subgroup of itself. This is to mean which the subgroup is also invariant. This conception is also knew or called *symmetry breaking*. It this concept, it was employed at first time by Pierre Curie at ended of nineteenth century [46], It this concept, it was employed at first time by Pierre Curie at ended of nineteenth century, he establishes that, if happens thing which doesn't allow system invariance, so the original symmetry it's lowered then, this mean which symmetry is broken. But, what is the importance to focussing on that?. The importance of symmetry breaking is the physical effects that are presents, the properties of semiconductors changes under reduce symmetry and this can observe in band structure. In the next section will be discussed the importance of symmetry breaking in semiconductors and above all over QWs.

*This is due to the linear independent solutions, which corresponds to one energy, this mean m -fold band degeneracy at the point \mathbf{k} [43]

2.2

Symmetry breaking in Semiconductor Structures

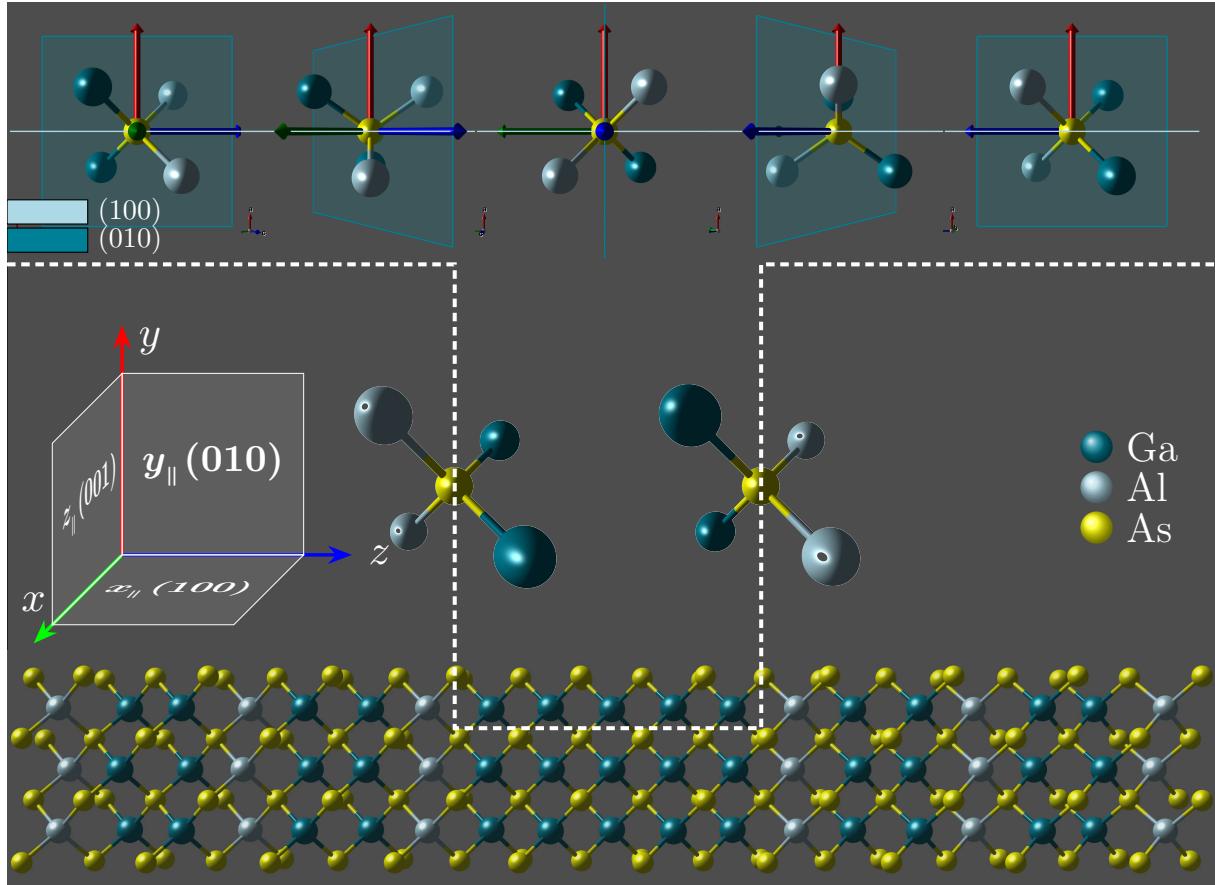


Figure 2.2: In this figure, it's schematized the atom arrangement of $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ single QW. At bottom can see the atom structure assuming the Al concentration to barriers, then, in middle of figure draws the conduction band edge as a potential profile, at interfaces between the change from barrier to well and vice versa, are located the matched atoms, here it can observe that at these positions (interface) the symmetry of changed. At top, it's added the atoms' basis where it has taken the Arsenic as central atom, and scheme the continues rotation over the y -axis.

The symmetry breaking, it's the basis for the physical model in this work. Starting from the general and brief concept of the symmetry importance in the Solid State viewed in the past section will arise the symmetry role and the reduced symmetry in CQWs. Before starting the history, it's important to clarify that the SOC isn't considered in this work, although in the future works of the **LFLM** are considered, and they study spin phenomena in CQWs. Then, to start in terms of symmetry the GaAs bulk has T_d point group, without intention to minimize the operations only focussing on their subgroups this due as before mentioned if the symmetry is lowered then the point group reduces to one of subgroup [40].

So, in the superlattice case the symmetry reduces at interfaces due to the change of atom species, that is to say, if it parts from GaAs and added an AlAs or $\text{Al}_x\text{Ga}_{1-x}\text{As}$ lattice the new atom structure reduce symmetry elements that can be done then the point group T_d it's reduce. Let's discuss first the simple QW GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$ structure grown over [001] direction, if suppose that the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ /GaAs and GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$ interfaces* are “perfect”, this mean the QWs structurally are perfect, the symmetry of system it's reduced to from $T_d \rightarrow D_{2d}$ [47, 48].

If taken into account a common atom as in this case the As atom as can see in Figure 2.2 and consider that structures growth (001)-oriented lack of translational symmetry [48], then in a single QW, the translational invariance along z axis is lost [49] as can see in Section 2.2. Is so fact which the visualization of symmetry operations isn't trivial, it can support each other with open software library as **Spglib** or **ASE** symmetry functions, these are great tool which has an iterative algoritm under applied recursive operations. If set the arrangement of atoms as the bottom of Figure 2.2, sorting the atoms positions as As-Al-Ga-Ga-As-Al super lattice then at the center of heterostructure the GaAs atoms to finally complement with the heterostructure composed by the first super lattice. Then, it's applies over these the continuous operations under **ASE** package the result is the $P\bar{4}m2$ symmetry in terms of international notation, therefore the D_{2d} point symmetry group. Although that is well-known and described at [47–53], the use of package software will be got a powerful tool to developed future works. So, in order to understand reducing symmetry from $T_d \rightarrow D_{2D}$ of QW grown on the (001), the $z_{\parallel}(001)$ direction becomes inequivalent to both $x_{\parallel}(100)$ and $y_{\parallel}(010)$ directions, hence the symmetry is reducing.

In therm of band structure the symmetry breaking, or symmetry reducing, generate changes, above all over the VB of QWs. This was expected, the reason is the due to the **BZ** zone is reduce to Γ point. From here starts the relevance of Γ and the events which occurs are the next: the first one event which occurs is over VB, due to the **BZ** is reduces to Γ the **VB** it splits for heavy- and light-holes. This is, from bulk as show the band structure in Section 1.1.1 the **VB** is four-fold degenerate, then in QWs the heavy- and light- holes bands splits, so, it gets two-fold degeneracy as shows in Figure 1.9. In fact, when refer to Γ in really it's refer to near band extrema, in case of GaAs and $\text{Al}_x\text{Ga}_{1-x}\text{As}$ being direct band gap semiconductors this really clearly. The consequences of bands split it's the reazon which the effective mass approximation can works, thanks to that the Scrödinger 's equation can solve as one dimensional equation over both **CB** and **VB** band under structure material parameters.

2.2.1 Special symmetry reduction from $D_{2d} \rightarrow C_{2v}$

*Another nomenclature usually used is A/B interfaces, being reference to two dissimilar atoms.

2.3General revision of numerical methods

Some physical systems can be explained through models that can solved analytically assume nearby experimental parameters but in realistic cases analytical models doesn't enough to obtain approximation of the experimental results. In past computational time and technology limitations they did not allow solving numerically large system of equations. Nowadays, numerical solutions do not represent a problem because computational systems allows solving large system of equations in a few time. In this work was implemented a numerical solution of one-dimensional Scrödinger using finite-difference method the principal reason to use this is that, basically represent the solution of an eigen-value problem.

The solution of typical problem in quantum mechanics is the single well with infinite barriers, this is a one electron trapping inside a well like a see in the next figure

The electron has zero potential energy in the region $0 < x < a$ where a is the width of well, how previously comment the Scrödinger equation

2.3.1Finite Difference Method

2.4Structural Parameters

2.5Anisotropy model in CQWs

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