



Universidad Autónoma de San Luis Potosí
Facultad de Ciencias



Coupled quantum wells as a novel source of optical anisotropies in nanostructured systems

Doctoral Thesis in Applied Sciences
submitted by:

Oscar Ruiz Cigarrillo

Supervisors:

Dr. Luis Felipe Lastras Martínez

Dr. Raul Eduardo Balderas Navarro

Dr. Edgar Armando Cerda Méndez

SAN LUIS POTOSÍ, S.L.P. MÉXICO
AUGUST 2022

Statement of authorship

I, Oscar Ruiz Cigarrillo, student of the Graduate Program in Applied Sciences of the School of Sciences of the Universidad Autonoma de San Luis Potosi, as author of the thesis "Coupled quantum wells as a novel source of optical anisotropies in nanostructured systems", declare that the thesis is an original, unpublished, authentic, personal work, that the corresponding sources have been cited and that in its execution the legal provisions in force that protect the copyright and intellectual and industrial property rights were respected. The ideas, doctrines, results and conclusions I have reached are my absolute responsibility.

Abstract

In the present work, it is proposed a new source of IOAs occurring in asymmetric coupled quantum wells ACQWs, namely a reduction of the symmetry from D_{2d} to C_{2v} as imposed by asymmetry along the growth direction. We report on reflectance anisotropy spectroscopy (RAS) of double GaAs quantum wells structures coupled by a thin (< 2 nm) tunneling barrier (CQWs). Two groups of DQWs systems were studied: one where both QWs have the same thickness (SCQWs) and another one where they have different thicknesses (ACQWs). RAS measures the in-plane optical anisotropies (IOAs) arising from the intermixing of the heavy- and light- holes in the valence band when the symmetry of the DQW system is lowered from D_{2d} to C_{2v} . If the CQWS are symmetric, residual IOAs stem from the asymmetry of the QW interfaces; for instance, associated to Ga segregation into the AlGaAs layer during the epitaxial growth process. In the case of an ACQWs with QWs with different thicknesses, the AlGaAs layers (that are sources of anisotropies) are not distributed symmetrically at both sides of the tunneling barrier. Thus, the system losses its inversion symmetry yielding an increase of the RAS strength. The RAS line shapes were compared with reflectance spectra in order to assess the heavy- and light- hole mixing induced by the symmetry breakdown. The energies of the optical transitions were calculated by numerically solving the one-dimensional Schrödinger equation using a finite-differences method. Our results are useful for interpretation of the transitions occurring in both, symmetric and asymmetric CQWs.

ACKNOWLEDGEMENT

CONTENTS

Abbreviations	II
List of codes and packages	III
Symbols	IV
List of Figures	V
List of Tables	VII
1 Physical model	1
1.1 The Symmetry Context	2
1.1.1 The symmetry and the Band Structure	5
1.2 Symmetry breaking in CQWs	7
1.2.1 Coupled Quantum Wells	9
1.2.2 Special symmetry reduction from $D_{2d} \rightarrow C_{2v}$	11
1.3 Numerical Calculations	13
1.3.1 Envelope Function and Effective Mass Aproximation Methods	16
1.3.2 Finite Difference Method	19
1.4 Numerical Results	22
1.5 Anisotropy model in CQWs	25
1.6 Summary	30
Bibliography	31

ABBREVIATIONS

BS	Band structure
BZ	<i>Brillouin zone</i>
QS	Quantum Structures
QW	Quantum Well
SQW	Single 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
2DEG	Two-dimensional electron gas
BL	Beer-Lambert-Law
TB	Tight-Binding method
PD	Photo-Detector
PEM	Photo-Elastic Modulator
QM	Quantum Mechanics
$k \cdot p$	Semiempirical theoretical tool to calculate band-structure
TB	Semiempirical Thight-Binding Method
DFT	Density Functional Theory
SOC	Spin-Orbit Coupling, also called Spin-Orbit interaction
LFLM	Dr. Luis Felipe Lastras Martinez group.
EFA	Envelope function Approximation
EMA	Effective Mass Approximation
FKOs	Franz Keldysh oscillations
IOA	In-plane Optical Anisotropy

LIST OF CODES AND PACKAGES

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

cqws-codes Repository of our codes implemented in this work. [1]

kp-lflm-group $k \cdot p$ julia [2] package developed by Our group research [3]

ASE The Atomic Simulation Environment (ASE) is a set of tools and Python modules for setting up, manipulating, running, visualizing and analyzing atomistic simulations. [4]

Spglib Software library for crystal symmetry search [5]

SOLCORE A multi-scale, Python-based library for modelling solar cells and semiconductor materials [6]

Aestimo One-dimensional (1D) self-consistent Schrödinger-Poisson solver for semiconductor heterostructures [7]

VESTA 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies. [8]

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 pdfTeXand dvips. It comes with a user-friendly syntax layer called TikZ. [9]

pst-optexp PStricks package to drawing optical experimental setups. [10]

SYMBOLS

X⁻ Negative Trion

X⁺ Positive Trion

X Direct Exciton

IX Indirect Exciton

$\text{Al}_x\text{Ga}_{1-x}\text{As}$ 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

E_g Energy bandgap

e electron

hh heavy-hole

lh light-hole

$e_n - hh_n$ **or** $e_n - lh_n$ Electronic transitions

LIST OF FIGURES

1.1	(a) GaAs crystal structure in “real space”, this region is known as <i>unit cell</i> , 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 <i>reciprocal space</i>	3
1.2	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.	7
1.3	General scheme to describe a SCQWs structure. In this case, the barriers are it composed by $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and the wells are of GaAs with the same width ($d_1 = d_2$), while the coupling barrier also composed by $\text{Al}_x\text{Ga}_{1-x}\text{As}$. In top (a) denotes both CB and VB edges profiles over z -axis (Real-space) direction. Then in bottom (b), it represents the atoms structure to CQWs.	9
1.4	General scheme corresponds to ACQWs structure. As in Figure 1.3(b), the structure is basically same both in barriers composition and dimensions as well as the coupling barrier, only changes the relative position of this. Then, result that one of QW is wider than other ($d_1 < d_2$), so, this reason causes the asymmetry in structure. Also, here in top (a) draws the potential profile along z , and bottom (b) scheme the atoms structure where is clear that only changes coupling barrier relative position with respect to Figure 1.3(b)	10
1.5	This roadmap it's developed around of QWs with remarkable potential profile, this mean posses a desire C_{2v} symmetry. It starts with asymmetric QW (a) [11, 12] specifically in potential, this is due to the semiconductor difference in adjacent barriers to well. At center left (b) and bottom left(c) are asymmetric QWs, in the first case the asymmetry [13, 14] it's caused by gradied concentration in a barrier and bottom while the other case the asymmetry it's originated by insert an atom specie different of the barrier [15]. At top center (d), it's show the QW under strain [16–18] which causes the reducing symmetry, while at bottom center(e) it shows the CQWs under applying electric field [19], the relation of both, it's the external perturbation which causes the breaking symmetry. Finally, at right (f) it's presented the ACQWs which has a symmetry breaking due to the relative width of QWs [20].	12

1.6	(a) The GaAs band structure calculated with 8-band Khane Hamiltonian [21, 22]	15
1.7	(a) it's tyhe focus over $\Gamma = 0$ and inside is the SQW VB $\mathbf{k} \cdot \mathbf{p}$ results, while the	17
1.8	Sketch of discrete potential band-edge profile which depends on spacial desplacement δz . HJ denotes the Heterojuntion boundary.	19
1.9	Doble Quantum Wells structure reproduce from Harrison et al. [23], (a) shows the plot to each energy calculate e_1 and e_2 , while in (b) the table exposes the comparison of numerical results from Harrison et. al., Nextnano software [24] and our results. The difference taken into account the Harrison's results practically are the same, but around of meV orders our results are precisely.	22
1.10	From (a) a to (d) shcemes the numerical results obtained to solved 1D-Schrödinger equation in both SQWs and ACQWs.	24
1.11	Diagram of three principal structures studied in this work, started with CQWs with the same width (bottom, $d_1 = d_2$), this sample structure is called as SCQWs, the second one the first asymmetric structure (top, $d_1 < d_2$), this means that one of the wells is slightly width than the other. Finally the third sample (right) it's more asymmetric, which means that one of the wells is double wider than the other.	26
1.12	Wave functions and confined energies calculated for (a) sample S1 (SCQWs sample) and (b) sample A2 (ACQWs sample 2)	29

LIST OF TABLES

1.1 Direct transitions (X) calculated for two ACQWs and one SCQW detailed in ?? and ?. From up to down shows the numerical (E) and experimental results, the experimental results was obtained from RAS experiments which are performed at 30K.	23
--	----

1

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.

Contents

1.1	The Symmetry Context	2
1.1.1	The symmetry and the Band Structure	5
1.2	Symmetry breaking in CQWs	7
1.2.1	Coupled Quantum Wells	9
1.2.2	Special symmetry reduction from $D_{2d} \rightarrow C_{2v}$	11
1.3	Numerical Calculations	13
1.3.1	Envelope Function and Effective Mass Aproximation Methods	16
1.3.2	Finite Difference Method	19
1.4	Numerical Results	22
1.5	Anisotropy model in CQWs	25
1.6	Summary	30

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 ??) 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 [25]. 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.

1.1 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 [26,27]. 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 [26].

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 [26, 28, 29]. It is important to remark which the heterostructure to will study is composed by GaAs/Al_xGa_{1-x}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 [30,31], from here arises two concepts: basis and lattice, where that

last is the set of mathematical points to which the basis is attached [30]. 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) [30].

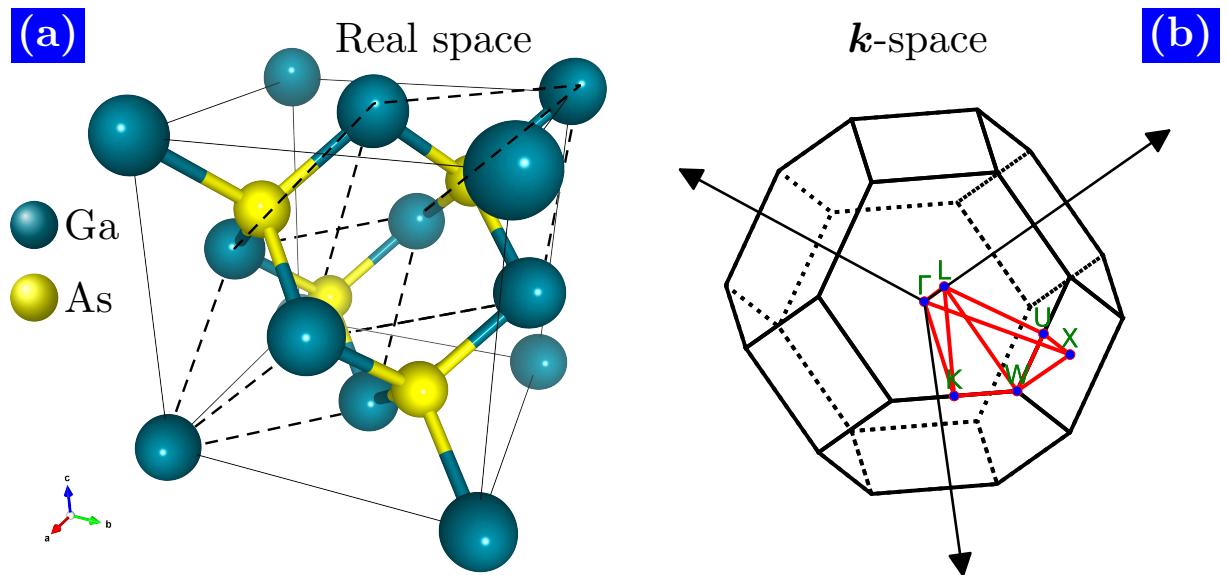


Figure 1.1: (a) GaAs crystal structure in “real space”, this region is known as *unit cell*, into that with dashed line is denoted the primitive cell. This lattice is well-defined by the vectors \mathbf{a} , \mathbf{b} and \mathbf{c} , these vectors are defined as the basis vectors. In (b) is schematized the GaAs crystal structure in 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” [32]. 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 [30, 33]. The Figure 1.1(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 [32]. 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" [32] 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 [26, 34]. 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 [35]. Then taken into account this, and the vectors \mathbf{a} , \mathbf{b} and \mathbf{c} in reciprocal space can describe the total unit cell [26, 35].

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} [26]*. In Figure 1.1(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 [36] equation (1.5)

1.1.1 The symmetry and the Band Structure

Returning to Figure 1.1(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* [37–40]. 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 ?? 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 1.1(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 [41].

Thus the band structure as a whole exhibits the symmetry characterized by the crystal [41]. 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 [42–44], in this case, the basis functions it's forming linear combinations of atomic orbitals (LCAO) to specific symmetry group [37].

In this method, the importance is the arrangement of atoms and their orbitals considered, for ?? 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 [37, 41]. 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 [45, 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} [41]

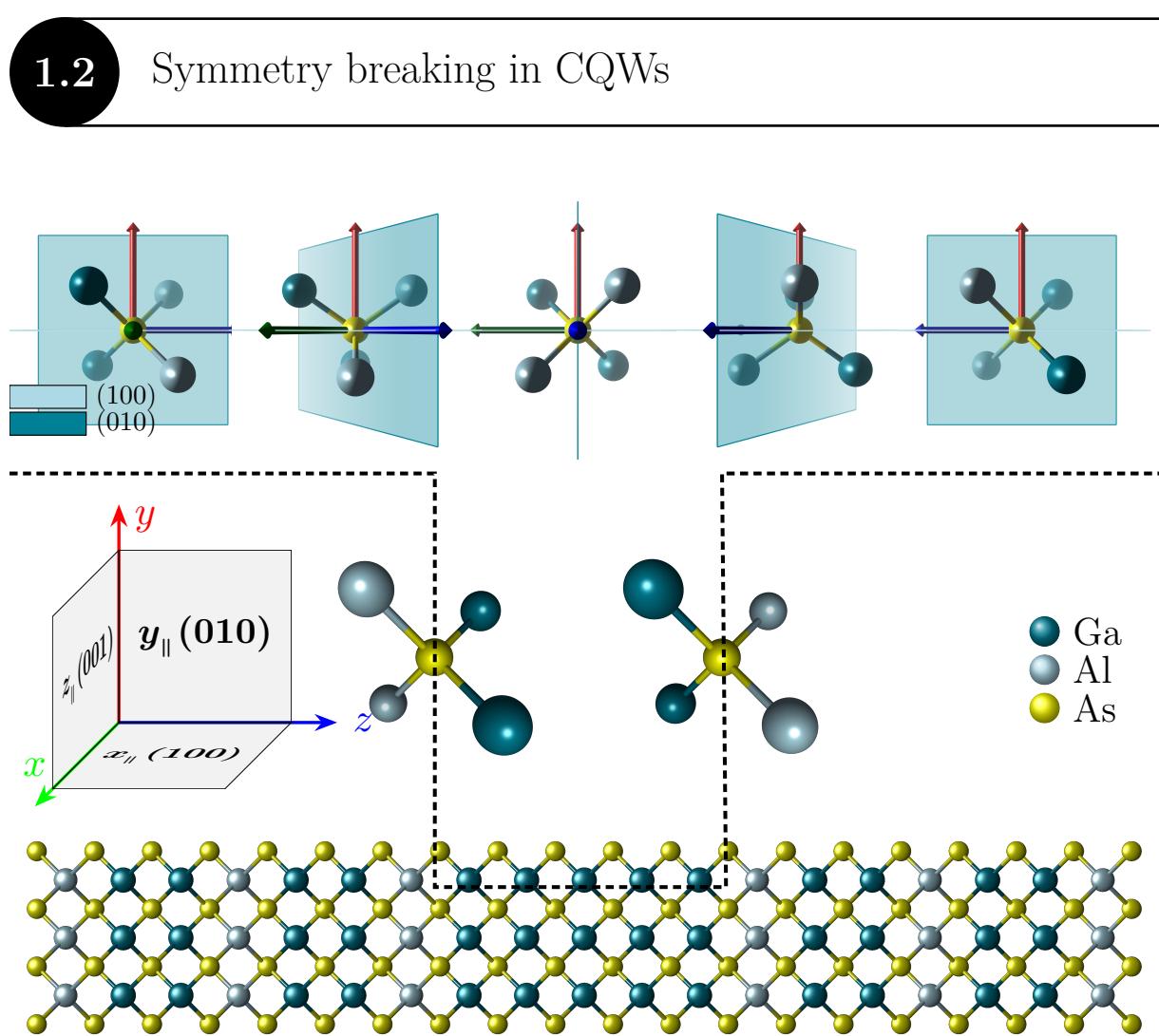


Figure 1.2: In this figure, it's schematized the atom arrangement of $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ single QW. At bottom can see the atom structure assuming the Al concentration to barriers, then, in middle of figure draws the conduction band edge 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 [37].

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 1.2 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 1.2. 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 1.2, 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 ?? 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 ?. 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 (EFA) can works, thanks to that the Schrödinger 's equation can solve as one dimensional equation over both CB and VB band under structure material parameters. Then, the facility of solve Schrödinger 's equation it's limited to only getting information about transitions, it is important to remember which this solution is over real-space, for this reason, it says that the potential profile is called a band edge profile and can't confuse with the band structure. So, this is the principle of symmetry reduction in QWs structures, in the next section will be addressed the symmetry in CQWs structures and the mechanisms to reduce it.

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

1.2.1 Coupled Quantum Wells

The symmetry breaking doesn't only wight in mathematical aspect, for physics this concept with leads to discover many important and exotic phenomena. When a system reduces its symmetry, their physical properties changes. It's the change in physical properties which reason to study it, in semiconductors as QWs the symmetry breaking starts with modify their band structure (fingerprint) splitting the valence band and reducing the degeneracy, although it can be the first one to appear their consequences get more relevance.

In therms to study changes in physical properties in this work it's focus on optical properties, the light matter interaction gets information about the symmetry breaking through transitions. The GaAs QWs as a direct band gap semiconductor are excellent platform to study light-matter interaction and the effects on symmetry. It's important to remark that from here the excitons played it an important role, in fact, over them falls the physical interpretation of optical properties.

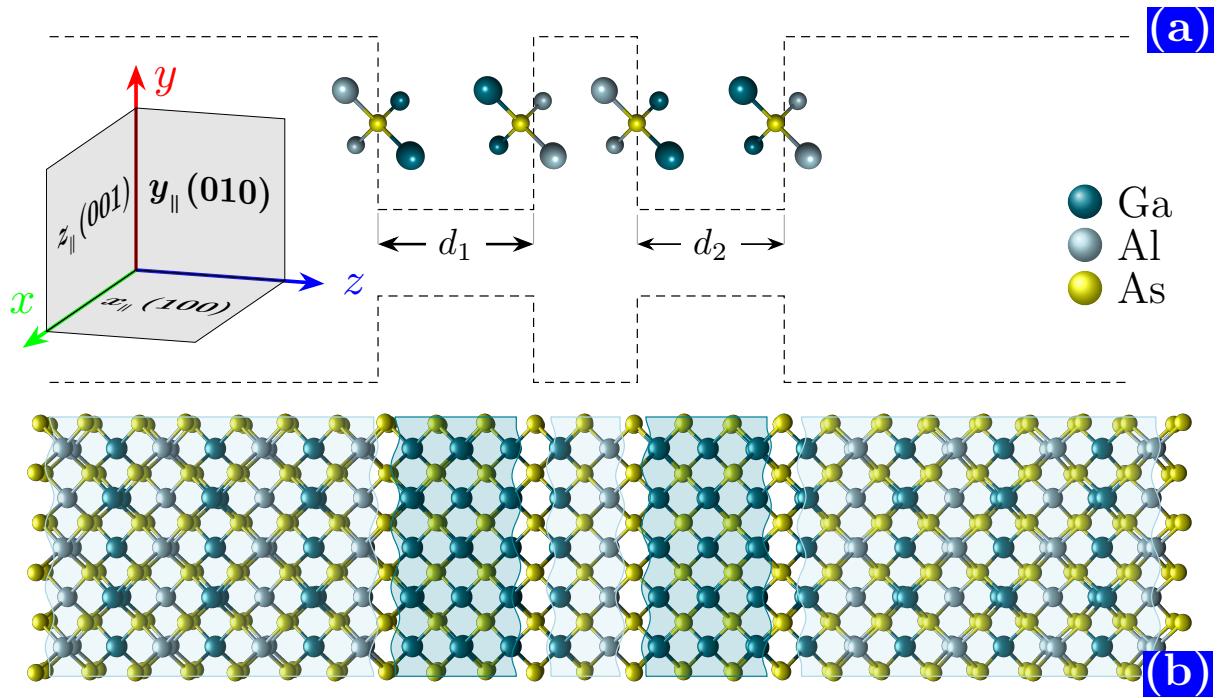


Figure 1.3: General scheme to describe a SCQWs structure. In this case, the barriers are composed by $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and the wells are of GaAs with the same width ($d_1 = d_2$), while the coupling barrier also composed by $\text{Al}_x\text{Ga}_{1-x}\text{As}$. In top (a) denotes both CB and VB edges profiles over z -axis (Real-space) direction. Then in bottom (b), it represents the atoms structure to CQWs.

Then, in the case, of Coupled Quantum Wells (CQWs) through excitons get optical properties really it's interesting, although, to get that properties the CQWs should get a double reduce symmetry from T_d , even if that's not obtained it's important to anisotropy

spectroscopy get it as a basis. Then, firstly, it's start with the symmetric coupled quantum wells (SCQWs), these are QWs with same width and coupled with a thin barrier, this barrier must be enough thinner so that electron wave function can be overlapping along potential of the two wells. For these structures the symmetry is also D_{2d} as in single QW, it's important to say which, if they aren't consider the interface defects as roughness it's possible to consider ideal interfaces, then the same symmetry operations works in both single QW like a SCQWs.

From Figure 1.3 it's possible to compare which in contrast with the SQW (??) is the same case with exception to the two QWs, although it's true that the technology of growth it's really accurate, the interfaces aren't be exempt free of them. Even, the rough by possible of Al impurity can cause the possible segregation of this, then it's important the Al concentration x [54, 55]. Even tought, an interface grown over (001) is C_{2v} , if consider structurally perfect as SQW or SCQWs, the overall symmetry of both interfaces is D_{2d} [47].

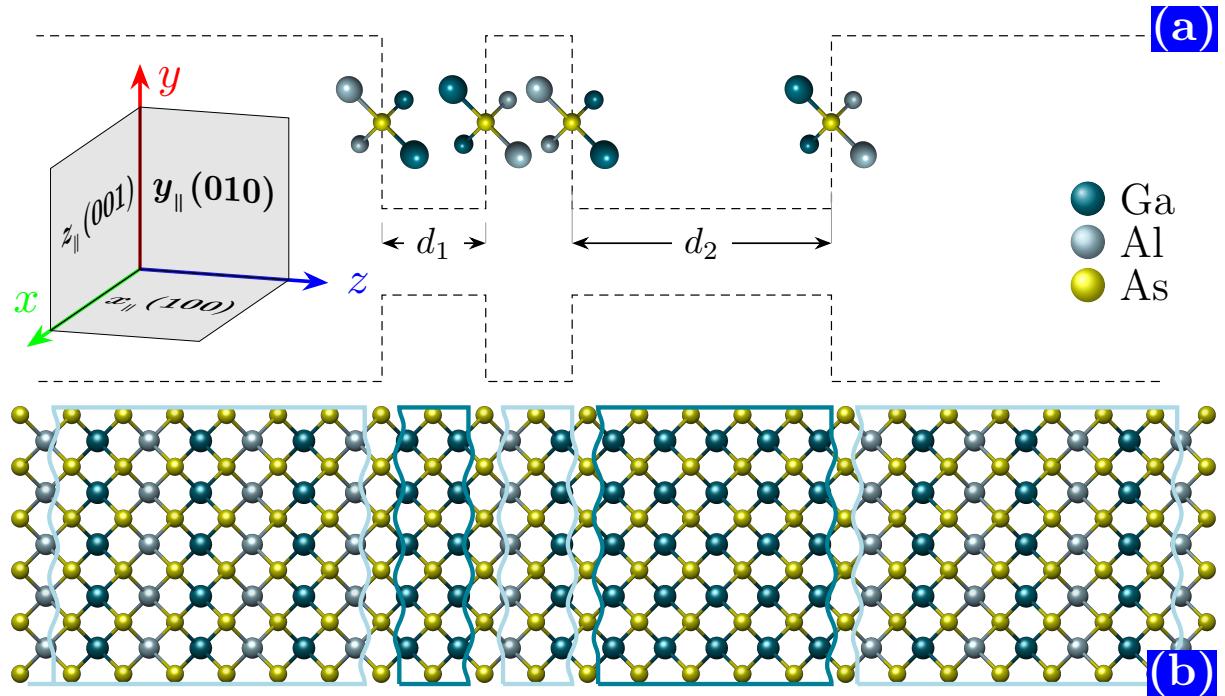


Figure 1.4: General scheme corresponds to ACQWs structure. As in Figure 1.3(b), the structure is basically same both in barriers composition and dimensions as well as the coupling barrier, only changes the relative position of this. Then, result that one of QW is wider than other ($d_1 < d_2$), so, this reason causes the asymmetry in structure. Also, here in top (a) draws the potential profile along z , and bottom (b) scheme the atoms structure where is clear that only changes coupling barrier relative position with respect to Figure 1.3(b)

Remember that as Courie mentioned [45, 46, 56]: a system under perturbation reduces their symmetry to a subgroup of original symmetry group, then, if now starts with D_2 symmetry

this subgroup can only reduce to a subgroup of six possibles, into them is C_{2v} subgroup. Previously it mentioned which, exist several mechanisms can reduce the symmetry, these are usually called perturbations. These perturbations can be nature by different sources, *in this work has been it found a novel source which reduces the symmetry, in other words, broken symmetry without needed external source as applied electric or magnetic fields.*

In the next section, it details the reason which it's called a novel source of reduce symmetry, therefore, before continue it's important to mentioned that the simple reason of modify the one well width in CQWs structures makes the system loses fourfold rotations over $z_{\parallel}(001)$ then, the symmetry it reduces.

If compares Figures 1.3 and 1.4 it's clearly that the representative part of the coupling barrier only shift over z , this allows to simulate a ACQWs heterostructure, this mean which QW is wider than the other, so, it gets an asymmetric structure which along z losses the rotation symmetry. Also, if it's uses symmetry code packages as ASE or Spglib which applies consecutively symmetry operations to both CQWs structures, it results in a D_{2d} and C_{2v} for SCQWs and ACQWs respectively.

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

The importance of C_{2v} point group around of QWs system is attractively to study properties of them, over all quantum properties as “spin” [12, 50, 53, 57–59]. Also, it's very important the quantum mixing which exhibits as a result of symmetry breaking, in fact, latter in ?? it presents the result of RAS experiments, which are the result of hole mixing. The anisotropy experimental measured it's caused due to the mixing at VB, therefore it's a direct cause of symmetry. Figure 1.5 shows and schematics the roadmap to get a QWs structures with C_{2v} symmetry. This starts at the left side with asymmetrical structures Figures 1.5(a) and 1.5(b), this asymmetry is related with the potential, exists a variety of them but the objective it's practically the same, the asymmetric potential profile it can be obtained by: asymmetric barrier, this can be due to the change of semiconductor type between adjacent barriers, i.e., AlAs/GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$ structure, this can interpret as high barrier/well/low barrier [11]. Another way of them, is caused of a barrier it's under gradient composition [13, 14]. The end case under asymmetric potential consideration shows in Figure 1.5(c), this case is due in one of the barriers is intentionally “inserted” an atom from other specie [15], this causes an asymmetric potential profile. Finally, it display the our CQWs structure, in comparison with all above firstly it has two wells, therefore reduced symmetry it be

Continued with the map, they have the perturbed structures, they are called like that due to they are under an external perturbation, at center top Figure 1.5(d) it's outlined a QW structure under strain applied, while at bottom center Figure 1.5(e) it's showing a QW structure under electric field applied. So that, in both exists, an external perturbation

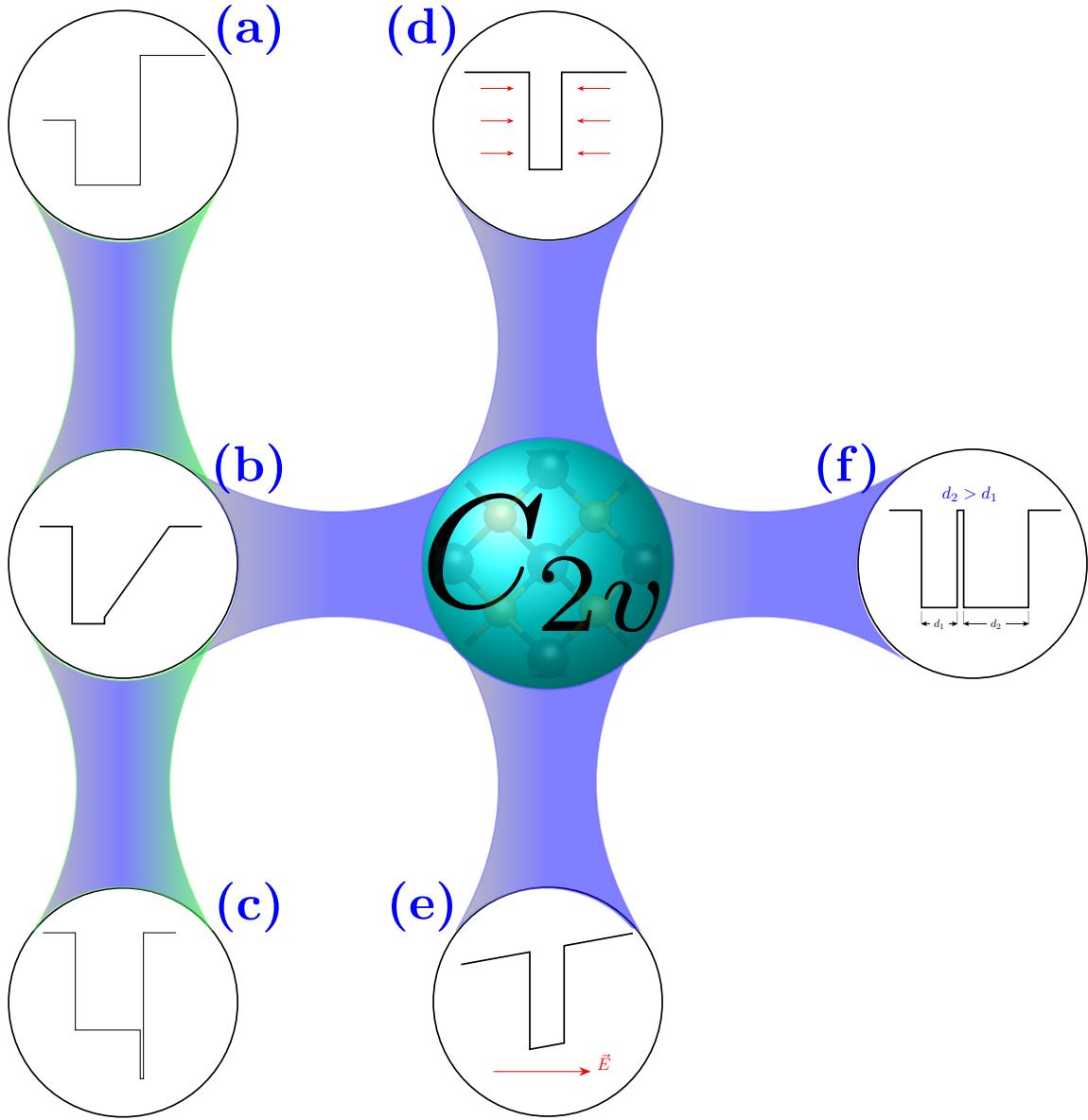


Figure 1.5: This roadmap it's developed around of QWs with remarkable potential profile, this mean posses a desire C_{2v} symmetry. It starts with asymmetric QW (a) [11, 12] specifically in potential, this is due to the semiconductor difference in adjacent barriers to well. At center left (b) and bottom left(c) are asymmetric QWs, in the first case the asymmetry [13, 14] it's caused by gradied concentration in a barrier and bottom while the other case the asymmetry it's originated by insert an atom specie different of the barrier [15]. At top center (d), it's show the QW under strain [16–18] which causes the reducing symmetry, while at bottom center(e) it shows the CQWs under applying electric field [19], the relation of both, it's the external perturbation which causes the breaking symmetry. Finally, at right (f) it's presented the ACQWs which has a symmetry breaking due to the relative width of QWs [20].

which causes a losses symmetry. Finally, it displays the ACQWs structureFigure 1.5(f), in comparison with all above. It's notably that this structures has two wells which are coupled by a thin barrier, by this reason as called Coupled Quantum Wells. Then, which is the reason by these structures are novels?.

To discuss this answer, it's important to mention the relevance of CQWs being that these structures are recurrent studied to observe quantum phenomena as exciton (**X**) condensation [60–62]. It's to be expected that in CQWs can measure indirect transitions, this means that in comparison with a single QWs whereby exists direct transitions (band to band) hardly can measure these. But, the reality of the importance of CQWs being that excitons are very interested to apply in semiconductor devices, the properties of excitons and their interactions really exhibit quantum attractive properties. So, unlike with single QW in CQWs the life of excitons increases [63, 64], in fact, this is one of the principal reasons which that are attractive structures [60, 65, 66]. Also, in terms of spin properties, the CQWs exhibit great potential [67]. Therefore, it being can discuss several interesting quantum properties in comparison that single structures. But, in comparison between CQWs, the symmetric structures need it perturbed to them exhibit these properties, while asymmetric structures are an excellent platform to study quantum properties such as holes mixing, spin, etc. It's then *ACQWs an interesting structure which part from being artificial, to get natural perturbation**, even though, as can see doesn't are the unique structures with “natural perturbation” which generates a symmetry breaking, all above mentioned it's reduced to confinement way. This, is the reason to call special symmetry reduction in a structure hardly studied in several sub-areas of solid state.

1.3 Numerical Calculations

All the above cool properties mentioned, could not have been predicted or observed without their knowing their electronic properties. This is many times mentioned, is the fingerprint of semiconductors, so, also mentioned the problem to calculate it. Here was implemented a *simple* model-based in EFA method to calculate the confined energies in CQWs structures. Before explaining the numerical method to obtain these solutions, it is important to discuss the reason which can apply this method, so, it starts with the definition of band-edge from energy dispersion. In ?? are discussed in general the concept of VB and CB, also is mentioned the significant methods to calculate them, in case of a heterostructure as CQWs the complexity is greater than bulk case. In bulk, the case is well-known several methods to calculate bandstructure, where all of them are developed by the symmetry properties of the system at stake. In the case of the heterostructure, the symmetry is also important, the problem is developed a Hamiltonian capable to describe all of the

*Thanks Dr. Raul for magnificent description.

system, this means, building a Hamiltonian which considers all properties as symmetry, perturbations, and in this case the potential. This work is very hard, even though exists general Hamiltonians to heterostructures, these don't warranty the correct solutions. The history and development of methods and techniques to calculate electronic properties is an area in constant evolution, from the fifties with Kane [21], Luttinger and Kohn [68] in perturbed methods as $\mathbf{k} \cdot \mathbf{p}$ to Slater and Koster [44] which proposed an atomistic method based on a linear combination of atomic orbitals called as TB, all of this already discussed and mentioned. So, we developed a model to calculate the confined energies in coupled structures. Even though exist analytical methods to calculate confined energies, in case of CQWs is more difficult to get an exact analytical method, while also exist some analytical methods under approximation description [69–71]. In the ?? it's developed the analytical solution of a simple quantum well taken into account the EFA method. It's possible to use this type of methods due to the symmetry reduction from bulk to QW, this due to the split in VB which passes from being a fourfold degenerate to be a twofold degenerate. It's precisely in VB where is it complicated to solved it.

The Figure 1.6 it's the result of apply $\mathbf{k} \cdot \mathbf{p}$ method, specifically taken into account 8-band model Hamiltonian [21, 72, 73] which is an extension of four band model [72] and even, this model is raised to bulk semiconductors, but in Figure 1.6(b) shows the results applied in a GaAs SQW heterostructure. To give support to these calculations is important to invoke EMA, this method is an efficient method to computational calculations [74, 75] and their basis allows developed electron solutions. In general, exist a variety of Hamiltonian intending to calculate the bandstructure of heterostructures. From conventional Luttinger-Kohn model, [68] to relatively recent models by Burt and Foreman [76–78], which they consider the basis functions depends on symmetry, this is the reason which Hamiltonian is associated to the bulk structure as in this case is Zinc-Blende type.

Although it has been discussed applying this method over heterostructures as the QWs, this work considers it as an “exploratory” tool. The reason for taking him into account in that way is basically their difficult and tedious way to get a correct Hamiltonian that describes our structures, in fact, $\mathbf{k} \cdot \mathbf{p}$ isn't the unique difficult method, also TB and others, have laboriousness way to build their Hamiltonians. So, we take the technic and equations from Vurgaftman [73] and solve it numerically to gets the GaAs bulk as shown in Figure 1.6(a) and in the same route, we take the Hamiltonian from Marchewka [22, 79] and solve under FDM, without major preamble the idea is to denote the split between heavy- and light-hole bands which is the justification to our numerical calculations proposed. In Equation (1.1) it's presents the 8×8 Hamiltonian solved to get bandstrcutre to GaAs SQW.

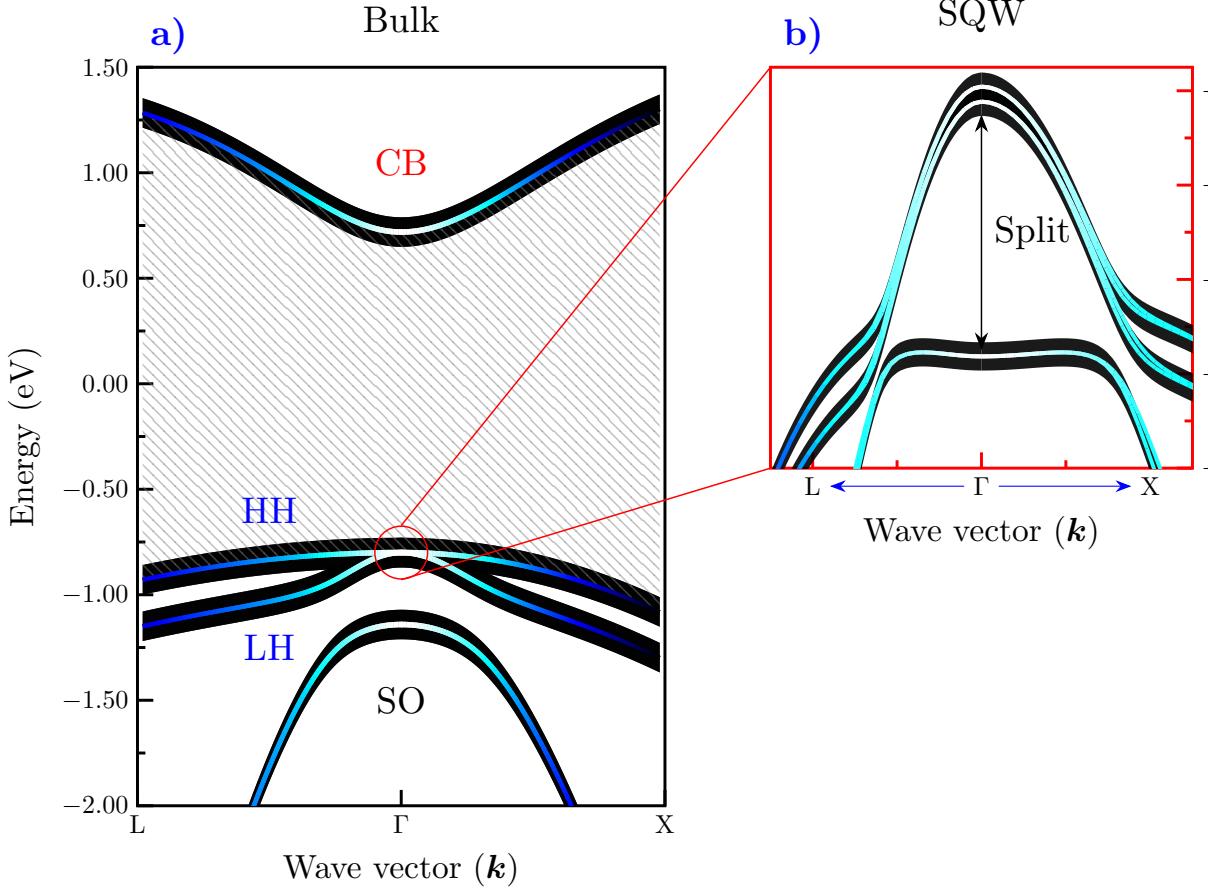


Figure 1.6: (a) The GaAs band structure calculated with 8-band Khane Hamiltonian [21, 22], therefore SOC is consider. At $\Gamma = 0$ in Bulk VB is closed by a circle, here observed the degeneracy, while in (b) it's denoted the split (Δ) between heavy- and light hole bands. Also due SOC consideration, it displays the spin up and down, bands.

$$H_0 = \begin{bmatrix} T & 0 & -\frac{1}{\sqrt{2}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \frac{1}{\sqrt{6}}Pk_- & 0 & -\frac{1}{\sqrt{3}}Pk_z & -\frac{1}{\sqrt{3}}Pk_- \\ 0 & T & 0 & -\frac{1}{\sqrt{6}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \frac{1}{\sqrt{2}}Pk_- & -\frac{1}{\sqrt{3}}Pk_+ & \frac{1}{\sqrt{3}}Pk_z \\ -\frac{1}{\sqrt{2}}k_-P & 0 & U + V & -\bar{S}_- & R & 0 & \frac{1}{\sqrt{2}}\bar{S}_- & -\sqrt{2}R \\ \sqrt{\frac{2}{3}}k_zP & -\frac{1}{\sqrt{6}}k_-P & -\bar{S}_-^\dagger & U - V & C & R & \sqrt{2}V & -\sqrt{\frac{3}{2}}\tilde{S}_- \\ \frac{1}{\sqrt{6}}k_+P & \sqrt{\frac{2}{3}}k_zP & R^\dagger & C^\dagger & U - V & \bar{S}_+^\dagger & -\sqrt{\frac{3}{2}}\bar{S}_+ & -\sqrt{2}V \\ 0 & \frac{1}{\sqrt{2}}k_+P & 0 & R^\dagger & \bar{S}_+ & U + V & \sqrt{2}R^\dagger & \frac{1}{\sqrt{2}}\bar{S}_+ \\ -\frac{1}{\sqrt{3}}k_zP & -\frac{1}{\sqrt{3}}k_-P & \frac{1}{\sqrt{2}}\bar{S}_-^\dagger & \sqrt{2}V & -\sqrt{\frac{3}{2}}\bar{S}_+^\dagger & \sqrt{2}R & U - \Delta & C \\ -\frac{1}{\sqrt{3}}k_+P & \frac{1}{\sqrt{3}}k_zP & -\sqrt{2}R^\dagger & -\sqrt{\frac{3}{2}}\bar{S}_-^\dagger & -\sqrt{2}V & \frac{1}{\sqrt{2}}\bar{S}_+^\dagger & C^\dagger & U - \Delta \end{bmatrix} \quad (1.1)$$

where

$$\begin{aligned}
k_{\parallel}^2 &= k_x^2 + k_y^2, \quad k_{\pm} = k_x \pm ik_y, \quad k_z = i\partial/\partial z, \\
T &= E_c(z) + \frac{\hbar^2}{2m_0} \left[(2F+1)k_{\parallel}^2 + k_z(2F+1)k_z \right], \\
U &= E_v(z) - \frac{\hbar^2}{2m_0} \left(\gamma_1 k_{\parallel}^2 + k_z \gamma_1 k_z \right), \\
V &= -\frac{\hbar^2}{2m_0} \left(\gamma_2 k_{\parallel}^2 - 2k_z \gamma_2 k_z \right), \\
R &= -\frac{\hbar^2}{2m_0} \sqrt{3} \left(\mu k_+^2 - \bar{\gamma} k_-^2, \right), \\
\bar{S}_{\pm} &= -\frac{\hbar^2}{2m_0} \sqrt{3} k_{\pm} \left(\{\gamma_3, k_z\} + [\kappa, k_z] \right), \\
\tilde{S}_{\pm} &= -\frac{\hbar^2}{2m_0} \sqrt{3} k_{\pm} \left(\{\gamma_3, k_z\}, \frac{1}{3} [\kappa, k_z] \right), \\
C &= \frac{\hbar^2}{2m_0} k_- [\kappa, k_z]
\end{aligned}$$

and each of these parameters taken from [73]. The Hamiltonian H_0 is defined for [001], and the principal idea is evaluating it in a “discrete” SQW structure, the ”discrete“ term refers to a numerical technique for solving it. The results it shows in fig. 1.6(b), this approximation is enough to evince the VB split, even, the results also CB information the importance falls on VB, this is due that difficult to solve there. Then, the VB split allows applying “simple” numerical methods without needing to define complex Hamiltonian and many parameters. In next section it will discuss the physical and mathematical formulation to calculate the electron energy confined, beginning with the symmetry reduce causes the VB split and developed all around of $\Gamma = 0$ this means we work over band-edge potential in real space.

1.3.1 Envelope Function and Effective Mass Aproximation Methods

Furthermore, to get a numerical method and solution robustness without any complex formalism but based on the essence of this work which is the effect of asymmetric width potential in CQWs which causes the symmetry breaking and this physical property involve important optical phenomena, as increase Anisotropy depending on relative width in these. The EFA is the mathematical justification to model electron behavior under periodic potential as a crystal, while the EMA is the physical model and the considerations to study the electron behavior inside a periodic potential from a crystal [75]. Under that

*Frequently the EFA and EMA approximations are considered as the same term, although maybe being correct, given that one depends on the another, is important to remark that the EMA depends on the formalism of EFA.

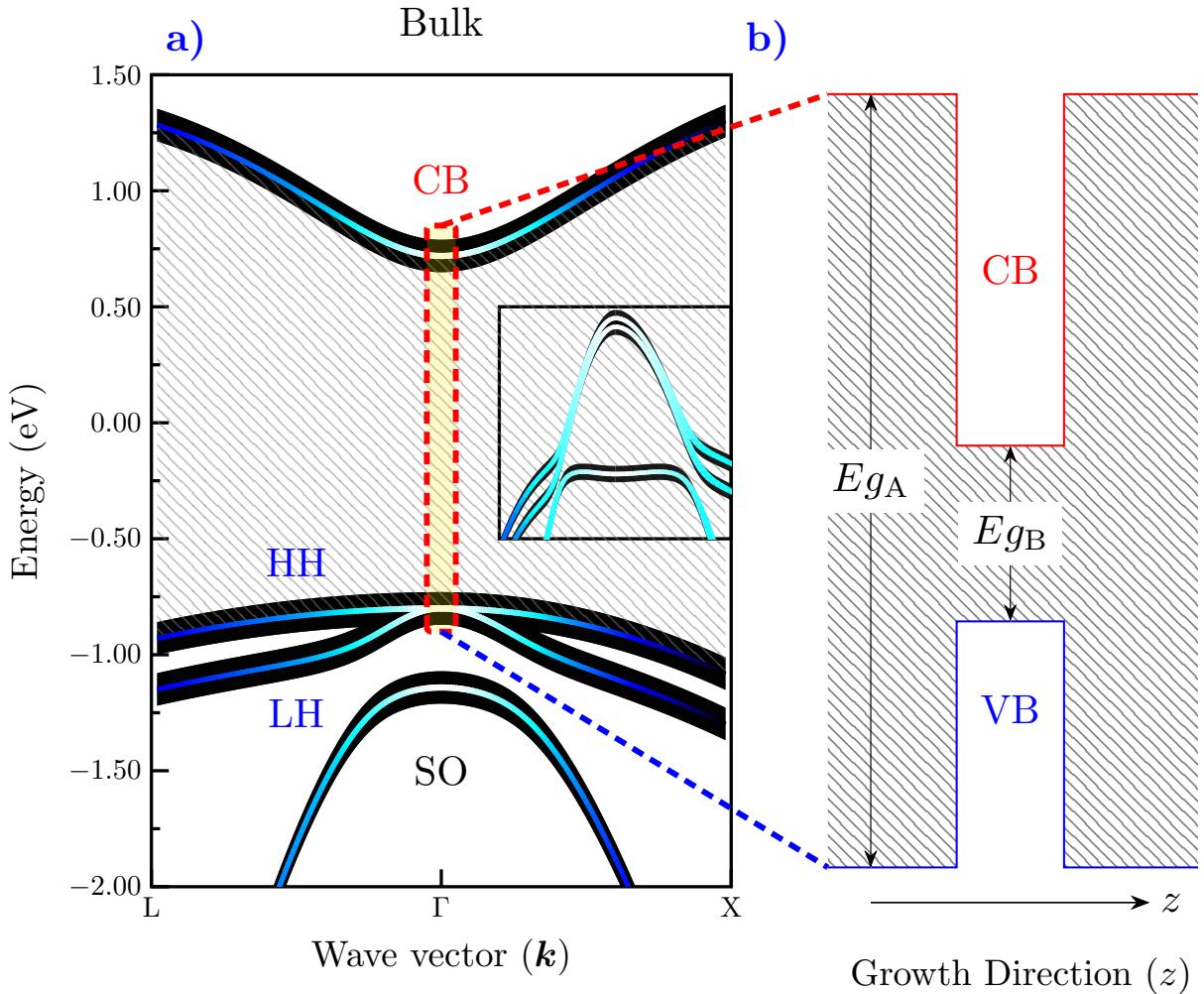


Figure 1.7: (a) it's tyhe focus over $\Gamma = 0$ and inside is the SQW $\mathbf{V}\mathbf{B} \cdot \mathbf{p}$ results, while the

assumptions, it's possible to review several considerations, that considerations reduce the complexity of solutions and allow simplifying the calculations. Then, in all of this work it develops around of $\Gamma = 0$, this means that will use a one-band model. To resume this last context, it's importantly to taken into account the next considerations. Firstly, from here we can study the electron and holes behavior by separately, from basic assumption which $\Gamma = 0$ this enables to pass from electronic band to band edge (see Figure 1.7). So, it's important to define that tools previosuly mentioned. The EMA is a valid approximation in bulk materials, in fact this is an elemental model which due to the good results and simplicity it's can be applied over heterostructures. About of this last, the heterostructures are complex, the dissimilar matched semiconductors which conformed that it, posses doesn't only difference in band-gap energy but also the effective mass.

If join all of that parameters involved it, the model to solve should being proportional to the considers in it, by this reason models as TB are complex due to the difficult to define

all that parameters, while in $\mathbf{k} \cdot \mathbf{p}$ are well-defined, but contrary, the method frequently is submitted to discussion due to the assumptions as the doesn't "see" the correct point-group symmetries, in fact, frequently assumes which the system already owns it. We can introduce ourselves in a severe discussion about of bandstructure calculations methods, but the reality is can't define a standard method, so that, doing reference to Harrison et al. [75], we can apply the simplicity method. Then, assuming the simplicity term, in which practically mentioned that, it's important to consider the simple way to get a result as a long as this works. So, in this work, will discuss the increase of the IOA due to the relative width in the wells of the coupled system, then here only considers the potential profile as a really significant parameter, of course, the effective mass and the band-gap are also essential, but these are considered as a part of the model. Being this the basis of the model, this work will employ the formalism of EFA where in a general explain, this it gives the envelope functions to calculate the single electron behavior under periodic potential as a heterostructure, therefore, this can allow describing it through position-depend material properties [80–82], then it's also indispensable to declare the boundary conditions owned by the EFA. Therefore with a mathematical formalism, then it's employed the EMA which parts of the fundamental parameter which is the effective-mass, then it can work with the 1D-Schrödinger 's equation as a function of effective-mass, as traditional egen-value equation:

$$\mathbf{H}\psi(z) = E\psi(z) \quad (1.2)$$

Then, the Hamiltonian of EMA it's developed mainly by the effective-mass, this has the advantage of evaluated along of heterostructure, allowing the change of semiconductors which composed that, so, this makes it a great method. Therefore the Hamiltonian for a particle is given by [80, 82, 83]:

$$H_z = \frac{p_z^2}{2m^*(z)} + V(z). \quad (1.3)$$

In Equation (1.3) it's taken z -axis as a direction perpendicular to interface of QWs, or simply as the growth direction, consequently the potential $V(z)$ it's depend on, and the effective-mass $m^*(z)$ also depends on position z . The Equation (1.3) it's taken z -axis as a direction perpendicular to interface of QWs, or simply as the growth direction, consequently the potential $V(z)$ it's depend on, and the effective-mass $m^*(z)$ also depends on position z . As can see in Figure 1.7(b), it's showing the band-edge profile as a potential profile which depends on semiconductor band-gap along of heterostructure. Also in Equation (1.3), it considers the momentum as p_z^2 as a 1D, due to the before discussed. Then it's allow to developed a method to solution which depends of position z . Finally, it can denote a 1D Scrödinger quation under EMA to electron also heavy- and light-holes :

$$\left[-\frac{\hbar^2}{2m_{jz}^*} \frac{d^2}{dz^2} + V(z) \right] \psi_{nj}(z) = E_{nj} \psi_{nj}(z), \quad (1.4)$$

$j = e, hh, lh.$

The Equation (1.4) it's then the effective-mass equation implemented in this work. The solution of that, it's detailed in next section where explains the numerical method to solve it. Before to continue, it's important to discuss the 1D equation. This equation will be applied over each particle ($j = e, hh, lh$), this means, over electron, heavy- and light-holes, where only considers the effective-mass (m_{jz}^*) trough each semiconductor in heterostructure studied and the most important in this work, the potential profile $V(z)$ which depends on relative widths of coupled wells.

1.3.2 Finite Difference Method

In this section it will discuss the numerical method to solve the 1D Schrödinger's equation, even though this is a large discussed theme, here focus on a simple but powerful numerical method. Started from the fact that the Equation (1.4) can it solve along of heterostructure and taken into account each semiconductor with compose it, this means that can discretize that and solved it for electron and holes. Although this, being a 1D equation, doesn't remove importance in the solution, that is to say, it's needing a robust method. It's important to remark which the spacial discretization depends on δz .

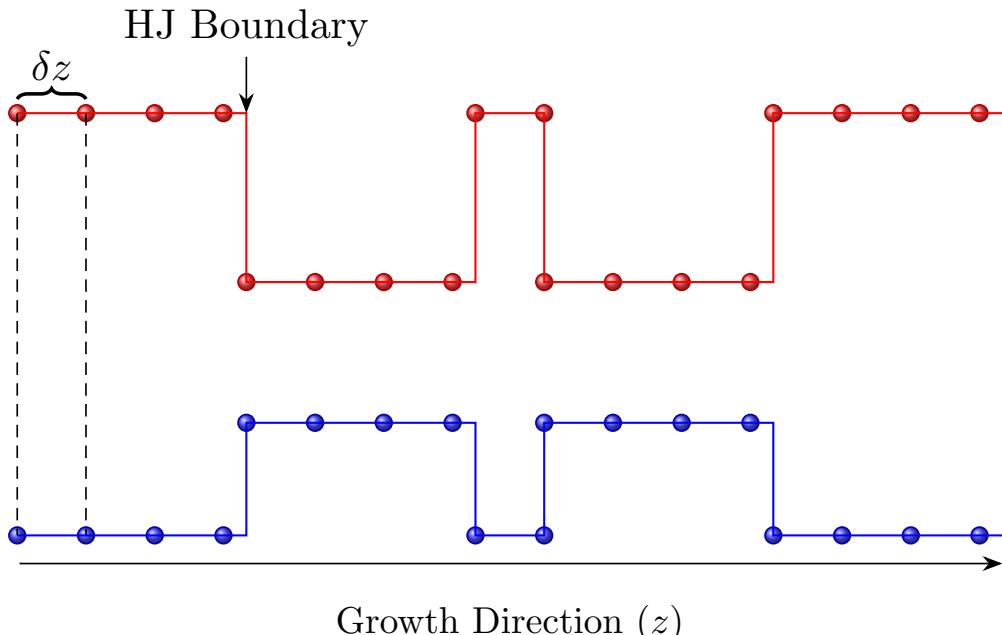


Figure 1.8: Sketch of discrete potential band-edge profile which depends on spacial desplacement δz . HJ denotes the Heterojunction boundary.

In Figure 1.8 schemes the discrete potential profile considers, this band-edge profile corresponds to a SCQWs structure. Remember that the potential $V(z)$ comes from the bend-edge Energy E_{edge} , like in the CB and VB, from that take the effective mass which corresponds to each semiconductor which compounds all heterostructure. Then, we can divide a heterostructure with coupled quantum wells basically into two parts, the adjacent barriers and the zone of wells which is considered the coupled barrier and their width as well as the relative widths of each well. So, if consider the discrete structure we can apply Equation (1.4) in each point which composes that.

The solution of Equation (1.4) it's the central discussion, although exist several numerical methods to solve it, in this work is employed the *Finite Difference Method* (FDM), which begin characterized by the easy computational application. Even if, this method doesn't unique in applied discretization in comparison with the other method as Shooting [75, 84], reduce the computational time and assure the correct convergence as long as the boundary conditions are correct. In other words, the FDM is a non-sensible convergence method, being focused on matrix solution. Taking the Equation (1.4) and reformulated as a *difference equation* [75]:

$$-\frac{\hbar^2}{2m^*} \left[\frac{\psi(z + \delta z) - 2\psi(z) + \psi(z - \delta z)}{(\delta z)^2} \right] + V(z)\psi(z) = E\psi(z). \quad (1.5)$$

In the Equation (1.5) it's denoted the derivative change by numerical difference, being a discrete equation. Something that it's important to consider is the boundary conditions which depend on the number of semiconductors involves in the structure and their dimensions, then, if it requires high precision it's important two factors: the total dimension of the structure, which contemplates each heterojunction boundary and the spatial step defined by δz . Either way, if considering a wide structure, as well as a very small step ($\delta z \approx 1\text{\AA}$) the computational effort, is high, for this reason, the compute considered memory should be reasonable. Then, taking into account these two factors and considering the computational work, the best choose a Matrix solution.

The Matricial solution allows solving the system of equations naturally as an eigenvalue problem, then it has several numerical alternatives* to solve the system. The reason to assert these has to do with the discrete solution as large as the ratio between structure width and spatial step. This means the matrix has dimensions as : $N = \text{total width}/\delta z$. Then, the way to get matrix (\mathbf{H}), from Harrison et al. [75], consists in reformulate Equation (1.5) as function of spatial potential band edge taken into account the variable effective mass, then:

$$a_i\psi_{i-1} + b_i\psi_i + c_i\psi_{i+1} = E\psi_i \quad (1.6)$$

*This refers to linear algebra techniques [75, 85]

where the coefficients are:

$$a_{i+1} = c_i = -\frac{\hbar^2}{2m_{i+\frac{1}{2}}^*(\delta z)^2} \quad \text{and} \quad b_i = \frac{\hbar^2}{2(\delta z)^2} \left(\frac{1}{m_{i+\frac{1}{2}}^*} + \frac{1}{m_{i-\frac{1}{2}}^*} \right) + V_i \quad (1.7)$$

From Equation (1.2), then the matrix \mathbf{H} is conformed by the system of equations which is evaluated in each point os structure, then \mathbf{H} is:

$$\mathbf{H} = \begin{pmatrix} b_1 & c_1 & 0 & \cdots & 0 \\ a_2 & b_2 & c_2 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \cdots & a_{N-1} & b_{N-1} & c_{N-1} \\ 0 & \cdots & 0 & a_N & b_N \end{pmatrix} \quad (1.8)$$

then ψ is in Equation (1.2) is a vector column which containing all the samples of the wave function.

Then, for the solution of the $N \times N$ matrix it's represents a computation work, but due to the *tridiagonal* nature it reduces that effort and thanks to exist great algebraic algorithms to solve [86, 87], this work can simplify enormous. Therefore, this method simplifies the solution of any structure with arbitrary or in our case dependent on band-edge potential. The next task is over to define the potential profile and their dependence of effective-mass and band gap energy (E_g). Firstly, we take as reference the double quantum wells propose by Harrison et al. [23] and reproduce the eigenenergies and wave functions as shows in Figure 1.9. For this structure, it takes into account symmetric double wells, that is to say, with same width $l_w = 6\text{nm}$, $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ central barrier of $l_b = 4$. For the semiconductor parameters with compose that structure, as the model like shows in the Equation (1.4) doesn't take into account the effective mass as energy function and not taken into account the nonparabolicity [88, 89]. Then, to define potential profile $V(z)$ uses the Varshni's model [90], to calculate bandgap energy to $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$, how doesn't consider the mass-effective as energy dependence then it uses paramaters from: [91–94], finally it employs the Vegard's law to define the thernary semiconductors [95, 96]. If defines the potential profile as:

$$V(z), m^*(z) = \begin{cases} \text{Al}_{0.2}\text{Ga}_{0.8}\text{As} & 0 < z < 20 \text{ nm} \\ \text{GaAs} & 20 < z < 26 \text{ nm} \\ \text{Al}_{0.2}\text{Ga}_{0.8}\text{As} & 26 < z < 32 \text{ nm} \\ \text{GaAs} & 32 < z < 38 \text{ nm} \\ \text{Al}_{0.2}\text{Ga}_{0.8}\text{As} & 38 < z < 58 \text{ nm} \end{cases} \quad (1.9)$$

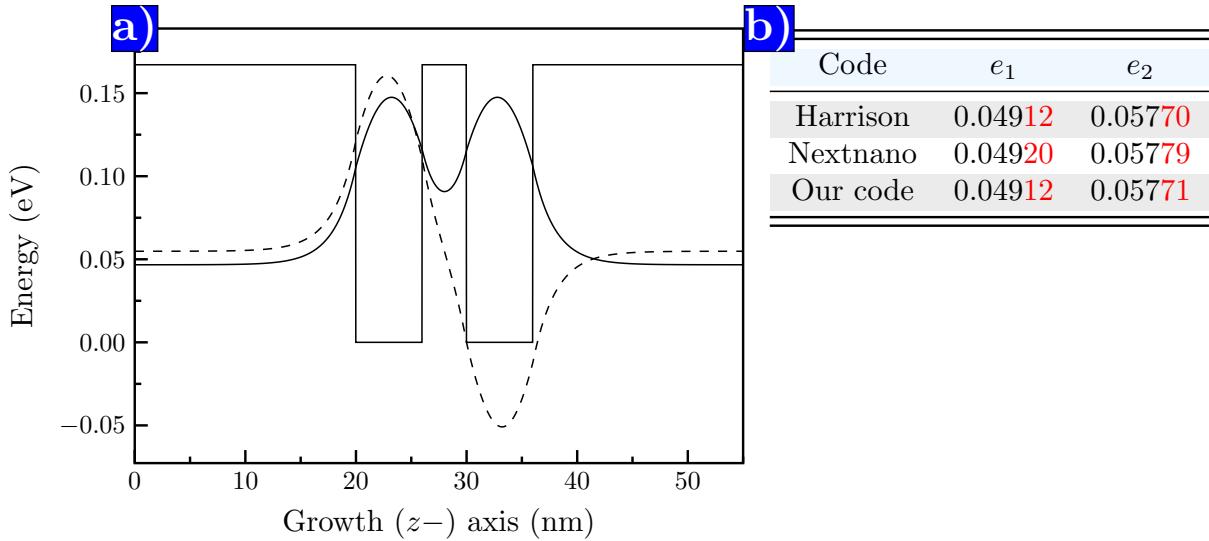


Figure 1.9: Doble Quantum Wells structure reproduce from Harrison et al. [23], (a) shows the plot to each energy calculate e_1 and e_2 , while in (b) the table exposes the comparison of numerical results from **Harrison** et. al., **Nextnano** software [24] and our results. The difference taken into account the Harrison's results practically are the same, but around of meV orders our results are precisely.

where the $V(z)$ it defines by the correspond value of E_g and the effective-mass $m^*(z)$, both with the spatial z dependence. But, this work as only in take **Harrison** et al. [75] like a reference, the **Nextnano** software [24, 97] also take that, in the Figure 1.9 and Figure 1.9(b) shows the table of comparison results, taken as basis **Harrison** et al. and compare also with **Nextnano** software and the codes developed in this work [1]. As can see, the results getting in this work are precise with respect to Harrison, and it's important to remark this work doesn't intend to denote supremacy since that fall short of sense, the intent is only the comparison to demonstrate that our codes works. The table in Figure 1.9(b) it denotes (with red) the precision around of meV, this is what we mean when say the major precision with respect to Harrison's results. Thus, we can trust the codes and model here present, do they work concerning with computational aspect and the physical results, and although only focused over electrons' solution in the band-edge profile, the next part of this works presents the results obtained in the interest structures.

1.4 Numerical Results

Here, we introduce the results obtained in CQWs studied in this work.?? it's detailed of the structures' composition as well as the properties of these. Then, here focus only in the numerical and computational results, over all, in the calculation of confined energies

it remembers that our model is oriented only about energies, so that, frequently explain many parameters and arguments that doesn't consider here. But, that doesn't mean which the obtained results minimize the quality of this work, in fact, we achieve very interest results without need to draw on to the very hard models. The Figure 1.10 shows the plot of wave functions for electrons, heavy- and light-holes resultant of numerical calculations, here taken into account only four samples detailed in ?? at the ??, all of these samples are the CQWs structures studied in this work, then over each of these was calculated the confined energies and the wave functions profiles. In the Figure 1.10 it's calculated ψ to denoted more clarify the overlapping wave functions over two coupled wells, even tough here doesn't show the total table of confinement energies results, later these will compare with the experimental transitions. Therefore, in this section, we limited to specify the numerical results in accordance with the published work [20].

Sample	e1-hh1	e1-lh1	e2-hh2	e2-lh2	e3-hh3
SCQWs	(N)1.5328 (E)1.5297	(N)1.5380 (E)1.5341	(N)1.5394	(N)1.5499	(N)1.5948
ACQWs-1	(N)1.5265 (E)1.5273	(N)1.5296 (E)1.5314	(N)1.5368	(N)1.5460	(N)1.5837
ACQWs-2	(N)1.5181 (E)1.5190	(N)1.5206 (E)1.5210	(N)1.5330	(N)1.5394	(N)1.5460

Table 1.1: Direct transitions (**X**) calculated for two ACQWs and one SCQW detailed in ?? and ???. From up to down shows the numerical (E) and experimental results, the experimental results was obtained from RAS experiments which are performed at 30K.

In the Table 1.1 exposes and compares the numerical results obtained, it's importantly to remark that the calculations were performed at 30K, this due to the central experiments (RAS) are performed to that temperature, by this reason the parameters involves are well-defined as a function of temperature. These calculations taken into account the conduction and valence-band offsets of 65% and 35% respectively. Both electron and hole effective masses for GaAs and AlAs can be found in Refs. [91–93], whereas the ternary $\text{Al}_x\text{Ga}_{1-x}\text{As}$ we used the Vegard's law [95]. For the numerical direct transitions (**X**) calculated, it's consider the exciton binding energy as a function of well width [98, 99], as commonly only shows the direct transitions in a range of wells widths, we interpolate these energies to used in accordance with the structures used in this work. The Figure 1.10 denotes some interesting physical issues, one of these with principal role in this work it's a linked between barrier width and the relative width of the coupled wells.

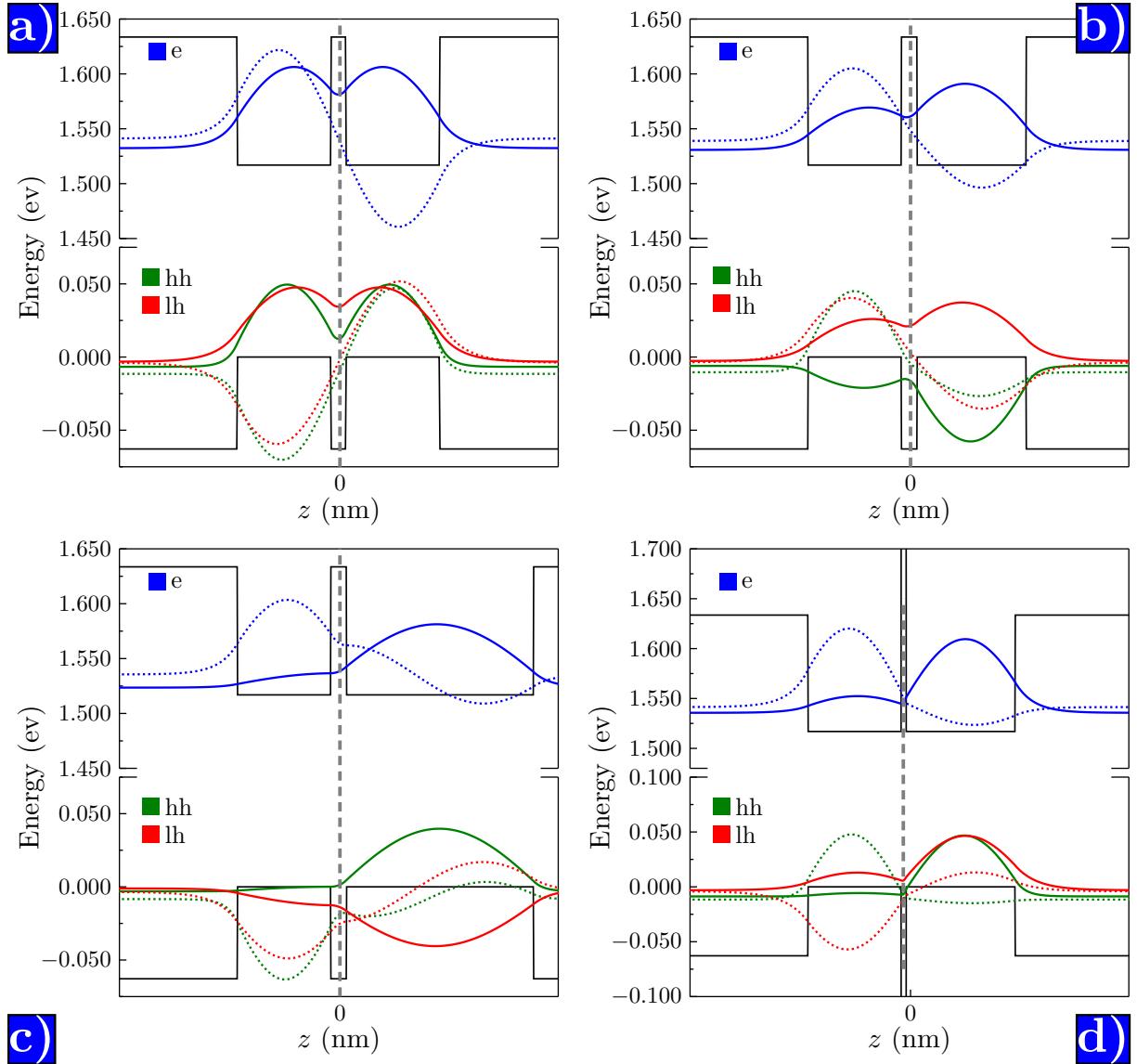


Figure 1.10: From (a) to (d) shcemes the numerical results obtained to solved 1D-Schrödinger equation in both SQWs and ACQWs.

The barrier width as can see plays an important role, because the width define tunneling of electrons and holes, for example Figure 1.10(b) and Figure 1.10(d) structures has the same wells widths with exception to barrier type, the first one is Al_{0.15}Ga_{0.9}As and the width is $b_w = 1.98\text{nm}$ while the second one is AlAs type with a width of $b_w = 0.565\text{nm}$. It's known that the difference between these is the bandgap energy then, as is expected, the tunneling is less than the Al_{0.15}Ga_{0.9}As barrier. Concerning tunneling, if compares the Figure 1.10(a) and Figure 1.10(c) structures, which basically are the same structures except for the width of the second well, the wave function in one of these, are symmetrically localized as a doublets states, while the other the wave function practically is well localized

in one of the wells as single state energy of a single QW [100]. While if compares with Figure 1.10(b) where one of the coupled wells is slightly width than the other, the wave function distribution seems an SQCWs under applied external electric field [65], later in ?? this take a sense, in PR experiments appear transitions which we associated to three-body particles known as trions (\mathbf{X}^- or \mathbf{X}^+). Trions are particular particles that consist of the bound of two electrons and one hole (\mathbf{X}^-) or vice versa, two holes and one electron (\mathbf{X}^+). The fact of one of the wells is slightly width, entails quantum interactions measured experimentally. But, this doesn't only the unique, interesting phenomena observed in these structures. As before mentioned this work, focuses on the optical properties consequent of the structural asymmetry, this means, the relative width in double wells.

1.5

Anisotropy model in CQWs

Now, we focus on the central part either, the core of this work. The asymmetry in structure entails a very interesting quantum process in these semiconductor structures. The symmetry reduction is the basis of the model in this work, as explained before, symmetry is the cause of many quantum phenomena its exhibits in solids, and the fact, that symmetry breaking in CQWs increases the optical anisotropy, which among many properties this opens the field of spin properties [65, 101–104].

Generalizing the before discussed in the symmetry section exists several mechanisms to reduce symmetry in QWs structures, principally in the single QWs with external perturbations such as electric or magnetic field, mechanics perturbations as applied strain among others. But, the objective is the same, reduce the symmetry in these structures from T_d which is the symmetry group to cubic crystals to C_{2v} which in turn a subgroup of this. As the result of the symmetry breaking, it originates an OA which was measured through RAS experiments results in a peculiar way, this refers to the spectral results. In our case, it compares the experimental results of RAS experiments (later discussed) about three CQWs structures, in which the difference between these is only the width of one of the wells (as many times mentioned), the RAS spectra increase as the relative width also, this, come back to these structures very interesting. Therefore, it will discuss the Anisotropy Model which includes all of the previous contained and focused on the CQWs. The IOA was borns as of the Quantum-mechanically effect of mixing between holes states, the theoretical formalism frequently is developed around effective mass but it's important to remember the difficulty of solid physics, now if it adds the physics of the interface this is so crazy. The role of interfaces is crucially in heterostructures in point of fact is the principal cause, then, having a standard model which explains it, is practically impossible. Therefore the *simplicity method is ever the good choice*.

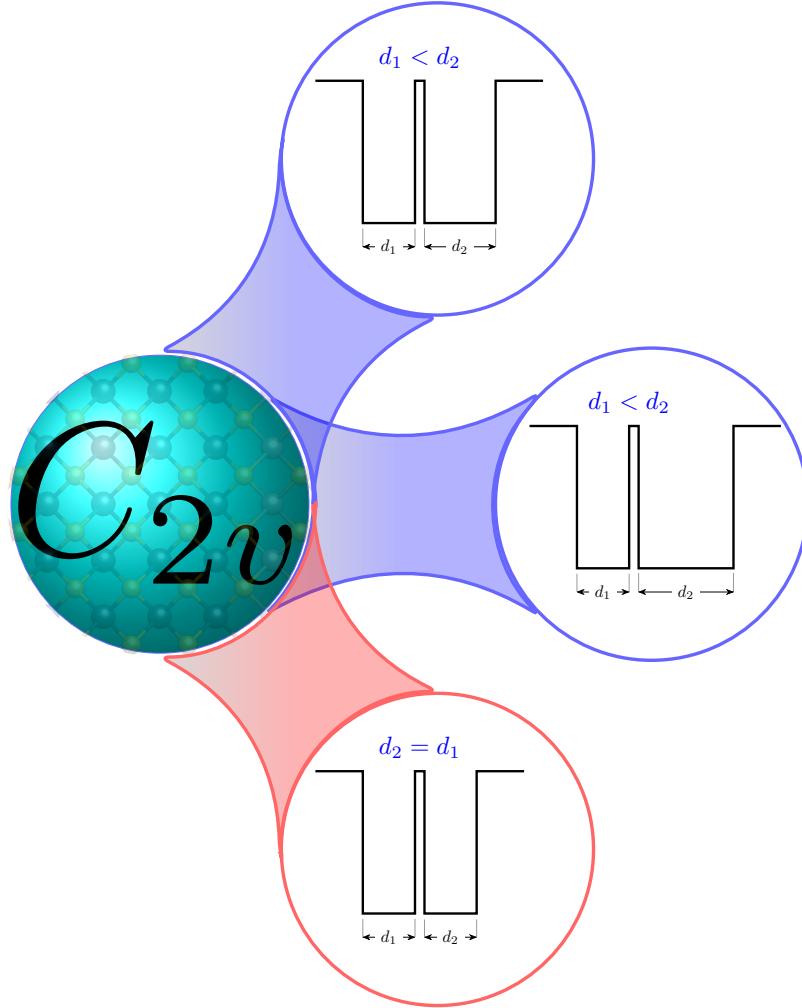


Figure 1.11: Diagram of three principal structures studied in this work, started with CQWs with the same width (bottom, $d_1 = d_2$), this sample structure is called as SCQWs, the second one the first asymmetric structure (top, $d_1 < d_2$), this means that one of the wells is slightly width than the other. Finally the third sample (right) it's more asymmetric, which means that one of the wells is double wider than the other.

The EFA usually employs the analytical method to explain the heavy- and light- holes states lack of interface contribution [105]. In the fact, always it desires high-quality interfaces but even though the growth technologies are very precise and powerful this remains a natural atom process. It's important to say that the quality of structures studied it's amazing, even in the SCQWs were expected a non-observable anisotropy due to the conserve of D_{2d} symmetry, experimentally observes a remanent of anisotropy. As it's exposed in the Figure 1.11 the three CQWs structures studied, including the symmetric double wells sample which remarks in red because this is the basis to demonstrate the evolution of anisotropy as increases as the asymmetry in wells also to. If we inside into discussion we increase the uncertainty of who is the best method to explain the IOA increases, on the one hand, the perturbative methods like the $\mathbf{k} \cdot \mathbf{p}$ have a powerful several Hamiltonians while

the “atomistic” as TB which advantage is the consideration symmetry intrinsically. Then as mentioned before we employs one method based on EFA, which consider each interfaz a scalar potential [48, 52, 105, 106]. Then, to deal measure the hole-mixing caused by interface anisotropy it’s important that this be sensitive to changes in polarization, by this reason, the models by a QW’s consider a hole-mixing Hamiltonian H' as [52, 105, 107]:

$$H' = \{E_p + [P_0\delta(z - w/2) - P_0\delta(z + w/2)]\} \{\hat{J}_x \hat{J}_y\} \quad (1.10)$$

with

$$\{\hat{J}_x \hat{J}_y\} = \begin{pmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}. \quad (1.11)$$

The Equation (1.10) is employs in a SQW [52], here, we denoted E_p as the external perturbations parameter, this parameter usually involves the multiplication of electric field along z direction, D as deformation potential and other as the piezo-electric constant d_{14} . The δ is the “abrupt” interface as a function of position z and well width w and P_0 is the potential parameter, finally considers the angular momentum operators with basis [52]:

$$\left| \frac{3}{2}, \frac{3}{2} \right\rangle, \left| \frac{3}{2}, -\frac{1}{2} \right\rangle, \left| \frac{3}{2}, \frac{1}{2} \right\rangle, \text{ and } \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \quad (1.12)$$

This Hamiltonian is usually implemented to explain the interface anisotropy, of course, doesn’t only limit to SQW, also is implemented to superlattice structures [107], where is considered a summation of interfaces contribution. In our case, this Hamiltonian H' it’s not enough to explain the hole mixing which origins the OA, the principal reason is that this H' considers the interface sign \pm refers to BA or AB interfaces, then the total mixing would be canceled by that reason. Also, this last is not necessarily true, remember that this would occur in an ideal interface where is expected a structure with D_{2d} symmetry then the IOA should be zero. Then, the non-abrupt interfaces should be generated a residual IOA [18, 52, 106]. RAS spectra of single QWs have been reported extensively in the literature [11, 15, 17, 18, 52].

The thickness of the QW plays a fundamental role in the amplitude of the RAS signal. For the anisotropies originating at the interfaces and the ones induced by the segregation of Ga or In (in the case of the inclusion of a thin InAs layer), the RAS amplitude decreases when the thickness of the QW increases [52]. Contrary to this behavior, for the IOA induced by strain, the RAS signal increases with the thickness of the QW [17]. In any case, the RAS

signal is associated with the mixing between the heavy- and light-hole valence subbands of the QW [48]. In a perturbative approach, the IOA strength is proportional to

$$\frac{\langle \psi_{\text{en}} | \psi_{\text{hhn}} \rangle \langle \psi_{\text{hhn}} | \mathcal{H} | \psi_{\text{lhn}} \rangle \langle \psi_{\text{lhn}} | \psi_{\text{en}} \rangle}{\Delta E_n}, \quad (1.13)$$

where $\langle \psi_{\text{en}} | \psi_{\text{hhn}} \rangle$ and $\langle \psi_{\text{lhn}} | \psi_{\text{en}} \rangle$ are the overlap integrals between the $|\psi_{\text{en}}\rangle$ electron state in the conduction band and the $|\psi_{\text{hhn}}\rangle$ and $|\psi_{\text{lhn}}\rangle$ hole states in the valence band respectively. The mixing between heavy- and light-hole subbands is $\langle \psi_{\text{hhn}} | \mathcal{H} | \psi_{\text{lhn}} \rangle$, \mathcal{H} being the perturbative Hamiltonian. The difference in energy between the hole states before their mixing is $\Delta E_n = E_{\text{hhn}} - E_{\text{lhn}}$.

As previously mentioned, \mathcal{H} could account for a perturbation by applied uniaxial stresses, electric fields (built-in or external) and abrupt or smooth interfaces. In the case of CQWs system, \mathcal{H} is a measure of the asymmetry of the two QWs. In a CQWs, if both QWs have the same thickness, the electron and hole energy levels are brought into resonance and their probability density is distributed symmetrically at both sides of the barrier that connects both QW, as can be seen in Figure 1.10. If the AlGaAs/GaAs interfaces of the DQW are equivalent the symmetry of the DQW structure belongs to the D_{2d} crystallographic point group. However, as we mentioned, if the GaAs/AlGaAs interfaces (sources of anisotropies) are non-equivalent, and a residual IOA is induced by the symmetry reduction from D_{2d} to C_{2v} of the whole CQWs structure. In this case the number of symmetry operations is reduced to four: the operations that inverts the z -axis, are excluded, thus leading to a mixing of heavy- and light- holes in the valence band, and hence an IOA. When the thickness of one QW is larger than the other QW (ACQWs), the energy of the electron and hole states of each QW become different and are no longer in resonance. In this case, the probability density is distributed asymmetrically as can be seen in Figure 1.12(a). Besides of the anisotropic source induced by the GaAs/AlGaAs interfaces as in the symmetric case, for the asymmetric CQWs system another mechanism of IOA should be considered. Suppose that the AlGaAs/GaAs interfaces are equivalent. As we mentioned, in this case a symmetric CQWs system belongs to the D_{2d} symmetry. If the thickness of one QW is modified, the system changes symmetry from D_{2d} to C_{2v} . As can be seen in Figure 1.12(b), the symmetry operations that change the sign of the z -axis (i.e., a reflection on a plane perpendicular to z), are no longer possible because the AlGaAs/GaAs interfaces are located at different distances from the barrier. The number of symmetry operations of the ACQWs structure is reduced to the four operations of the symmetry group C_{2v} [50, 53]. In this case the IOA strength can be modulated by changing the relative thicknesses of the QWs in the CQWs system. This anisotropy is added to the residual IOA produced by the non-equivalence of the interfaces.

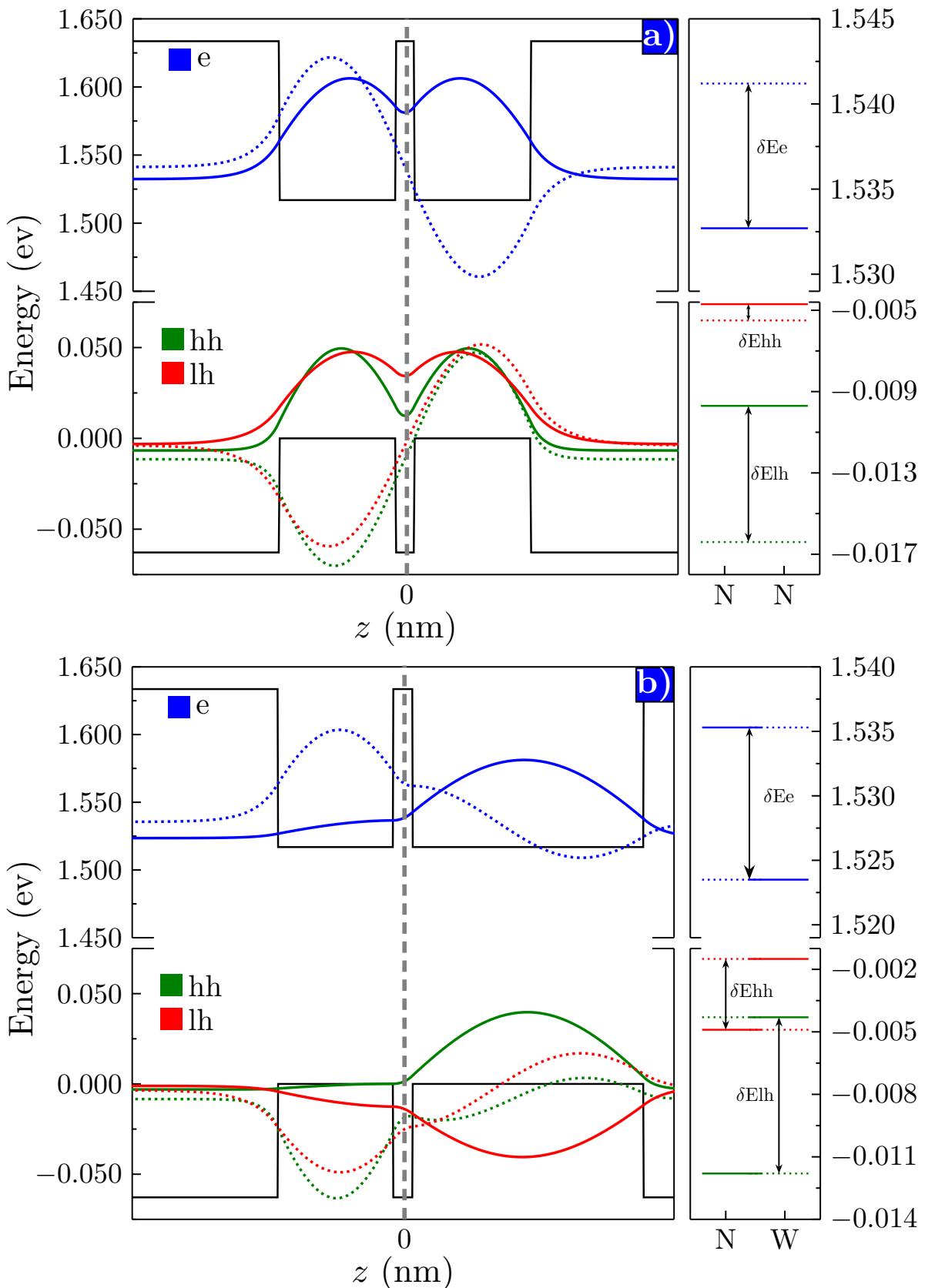


Figure 1.12: Wave functions and confined energies calculated for (a) sample S1 (SCQWs sample) and (b) sample A2 (ACQWs sample 2)

1.6 Summary

In this chapter explains and discusses the physics which involves this work, started from relation between symmetry and the bandstructure in semiconductors, the importance which understand the symmetry context and the importance of the “breaking” in it (symmetry reduction). We focus on enhance the particular symmetry “breaking” in CQWs which occurs practically natural, this means, in this work we don’t appeal to apply and external perturbation to success.

BIBLIOGRAPHY

- [1] O. Ruiz-Cigarrillo and G. Martinez-Cepeda, “Coupled quantum wells codes,” 2018. [Online]. Available: <https://github.com/lflmgroup/cqws-codes.git> (Cited on pages III and 22.)
- [2] J. Bezanson, A. Edelman, S. Karpinski, and V. B. Shah, “Julia: A fresh approach to numerical computing,” *SIAM Review*, vol. 59, no. 1, pp. 65–98, 2017. [Online]. Available: <https://pubs.siam.org/doi/10.1137/141000671> (Cited on page III.)
- [3] G. Martinez-Cepeda and O. Ruiz-Cigarrillo, “ $\mathbf{k} \cdot \mathbf{p}$ julia package,” 2022. [Online]. Available: <https://github.com/lflmgroup/kp-lflm-group.git> (Cited on page III.)
- [4] A. H. Larsen, J. J. Mortensen, J. Blomqvist, I. E. Castelli, R. Christensen, M. Dułak, J. Friis, M. N. Groves, B. Hammer, C. Hargus, E. D. Hermes, P. C. Jennings, P. B. Jensen, J. Kermode, J. R. Kitchin, E. L. Kolsbjerger, J. Kubal, K. Kaasbjerger, S. Lysgaard, J. B. Maronsson, T. Maxson, T. Olsen, L. Pastewka, A. Peterson, C. Rostgaard, J. Schiøtz, O. Schütt, M. Strange, K. S. Thygesen, T. Vegge, L. Vilhelmsen, M. Walter, Z. Zeng, and K. W. Jacobsen, “The atomic simulation environment—a python library for working with atoms,” *Journal of Physics: Condensed Matter*, vol. 29, no. 27, p. 273002, 2017. [Online]. Available: <http://stacks.iop.org/0953-8984/29/i=27/a=273002> (Cited on page III.)
- [5] A. Togo and I. Tanaka, “Spglib: a software library for crystal symmetry search,” 2018. (Cited on page III.)
- [6] D. Alonso-Álvarez, T. Wilson, P. Pearce, M. Führer, D. Farrell, and N. Ekins-Daukes, “Solcore: a multi-scale, python-based library for modelling solar cells and semiconductor materials,” *Journal of Computational Electronics*, vol. 17, no. 3, pp. 1099–1123, 2018. (Cited on page III.)
- [7] H. Hebal, Z. Koziol, S. Lisesivdin, and R. Steed, “General-purpose open-source 1d self-consistent schrödinger-poisson solver: Aestimo 1d,” *Computational Materials Science*, vol. 186, p. 110015, 2021. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0927025620305061> (Cited on page III.)
- [8] K. Momma and F. Izumi, “it VESTA3 for three-dimensional visualization of crystal, volumetric and morphology data,” *Journal of Applied Crystallography*, vol. 44, no. 6, pp. 1272–1276, Dec 2011. [Online]. Available: <https://doi.org/10.1107/S0021889811038970> (Cited on page III.)
- [9] T. Tantau, “Pgf/tikz,” 2007. [Online]. Available: <https://github.com/pgf-tikz/pgf.git> (Cited on page III.)

- [10] C. Bersch, “pst-optexp, drawing optical experimental setups,” 2022. [Online]. Available: <https://github.com/cbersch/pst-optexp> (Cited on page III.)
- [11] B. Koopmans, B. Koopmans, P. Santos, P. Santos, and M. Cardona, “Microscopic reflection difference spectroscopy on semiconductor nanostructures,” *physica status solidi (a)*, vol. 170, no. 2, pp. 307–315, 1998. (Cited on pages V, 11, 12, and 27.)
- [12] E. A. de Andrade e Silva, G. C. La Rocca, and F. Bassani, “Spin-orbit splitting of electronic states in semiconductor asymmetric quantum wells,” *Phys. Rev. B*, vol. 55, pp. 16 293–16 299, Jun 1997. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.55.16293> (Cited on pages V, 11, and 12.)
- [13] D. J. English, J. Hübner, P. S. Eldridge, D. Taylor, M. Henini, R. T. Harley, and M. Oestreich, “Effect of symmetry reduction on the spin dynamics of (001)-oriented gaas quantum wells,” *Phys. Rev. B*, vol. 87, p. 075304, Feb 2013. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.87.075304> (Cited on pages V, 11, and 12.)
- [14] P. S. Eldridge, J. Hübner, S. Oertel, R. T. Harley, M. Henini, and M. Oestreich, “Spin-orbit fields in asymmetric (001)-oriented gaas/ $\text{al}_x\text{ga}_{1-x}\text{as}$ quantum wells,” *Phys. Rev. B*, vol. 83, p. 041301, Jan 2011. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.83.041301> (Cited on pages V, 11, and 12.)
- [15] J. L. Yu, S. Y. Cheng, Y. F. Lai, Q. Zheng, Y. H. Chen, and C. G. Tang, “Tuning of in-plane optical anisotropy by inserting ultra-thin inas layer at interfaces in (001)-grown gaas/algaas quantum wells,” *Journal of Applied Physics*, vol. 117, no. 1, p. 015302, 2015. (Cited on pages V, 11, 12, and 27.)
- [16] D. J. English, P. G. Lagoudakis, R. T. Harley, P. S. Eldridge, J. Hübner, and M. Oestreich, “Strain-induced spin relaxation anisotropy in symmetric (001)-oriented gaas quantum wells,” *Phys. Rev. B*, vol. 84, p. 155323, Oct 2011. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.84.155323> (Cited on pages V and 12.)
- [17] C. G. Tang, Y. H. Chen, B. Xu, X. L. Ye, and Z. G. Wang, “Well-width dependence of in-plane optical anisotropy in (001) gaas/algaas quantum wells induced by in-plane uniaxial strain and interface asymmetry,” *Journal of Applied Physics*, vol. 105, no. 10, p. 103108, 2009. (Cited on pages V, 12, and 27.)
- [18] Y. Li, F. Liu, X. Ye, Y. Liu, J. Wang, and Y. Chen, “Quantitative investigation of intrinsic shear strain and asymmetric interface conditions in semiconductor superlattices,” *Journal of Applied Physics*, vol. 126, no. 6, p. 065704, 2019. (Cited on pages V, 12, and 27.)

- [19] S. H. Kwok, H. T. Grahn, K. Ploog, and R. Merlin, “Giant electropleochroism in gaas-(al,ga)as heterostructures: The quantum-well pockels effect,” *Phys. Rev. Lett.*, vol. 69, pp. 973–976, Aug 1992. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.69.973> (Cited on pages V and 12.)
- [20] O. Ruiz-Cigarrillo, L. F. Lastras-Martínez, E. A. Cerdá-Méndez, G. Flores-Rangel, C. A. Bravo-Velazquez, R. E. Balderas-Navarro, A. Lastras-Martínez, N. A. Ulloa-Castillo, K. Biermann, and P. V. Santos, “Optical anisotropies of asymmetric double gaas (001) quantum wells,” *Phys. Rev. B*, vol. 103, p. 035309, Jan 2021. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.103.035309> (Cited on pages V, 12, and 23.)
- [21] E. O. Kane, “Band structure of indium antimonide,” *Journal of Physics and Chemistry of Solids*, vol. 1, no. 4, pp. 249–261, 1957. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/0022369757900136> (Cited on pages VI, 14, and 15.)
- [22] E. G. Novik, A. Pfeuffer-Jeschke, T. Jungwirth, V. Latussek, C. R. Becker, G. Landwehr, H. Buhmann, and L. W. Molenkamp, “Band structure of semimagnetic $hg_{1-y}mn_yte$ quantum wells,” *Phys. Rev. B*, vol. 72, p. 035321, Jul 2005. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.72.035321> (Cited on pages VI, 14, and 15.)
- [23] P. Harrison and A. Valavanis, *Numerical solutions*. John Wiley & Sons, Ltd, 2016, ch. 3, pp. 81–130. (Cited on pages VI, 21, and 22.)
- [24] Nextnano, “Nextnano software.” [Online]. Available: https://www.nextnano.com/manual/nextnanoplus_tutorials/1D/double_qw.html (Cited on pages VI and 22.)
- [25] B. C. Van Fraassen, *Laws and symmetry*. Clarendon Press, 1989. (Cited on page 2.)
- [26] R. C. Powell, *Symmetry, group theory, and the physical properties of crystals*. Springer, 2010, vol. 824. (Cited on pages 2 and 4.)
- [27] K. Tapp, *Symmetry: A mathematical exploration*. Springer Nature, 2021. (Cited on page 2.)
- [28] J. F. Cornwell, *Group theory in physics: An introduction*. Academic press, 1997. (Cited on page 2.)
- [29] U. Müller, *Symmetry relationships between crystal structures: applications of crystallographic group theory in crystal chemistry*. OUP Oxford, 2013, vol. 18. (Cited on page 2.)
- [30] C. Kittel and P. McEuen, *Kittel’s Introduction to Solid State Physics*. John Wiley & Sons, 2018. (Cited on pages 2, 3, and 4.)

- [31] J. Sólyom, *Fundamentals of the Physics of Solids: Volume 1: Structure and Dynamics*. Springer Science & Business Media, 2007, vol. 1. (Cited on page 2.)
- [32] S. K. Chatterjee, *Crystallography and the World of Symmetry*. Springer Science & Business Media, 2008, vol. 113. (Cited on pages 3 and 4.)
- [33] J. McKelvey, *Solid State and Semiconductor Physics*, ser. A Harper international edition. Harper & Row, 1966. [Online]. Available: <https://books.google.com.mx/books?id=MQNRAAAAMAAJ> (Cited on page 4.)
- [34] C. Malgrange, C. Ricolleau, and M. Schlenker, *Symmetry and Physical Properties of Crystals*. Springer, 2014. (Cited on page 4.)
- [35] N. Ashcroft, A. W. N. Mermin, W. Ashcroft, D. Mermin, N. Mermin, and B. P. Company, *Solid State Physics*, ser. HRW international editions. Holt, Rinehart and Winston, 1976. [Online]. Available: <https://books.google.com.mx/books?id=1C9HAQAAIAAJ> (Cited on page 4.)
- [36] R. C. Powell, *Symmetry in Solids*. New York, NY: Springer New York, 2010, pp. 1–24. [Online]. Available: https://doi.org/10.1007/978-1-4419-7598-0_1 (Cited on page 4.)
- [37] M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group theory: application to the physics of condensed matter*. Springer Science & Business Media, 2007. (Cited on pages 5, 6, and 7.)
- [38] M. Cardona and Y. Y. Peter, *Fundamentals of semiconductors*. Springer, 2005, vol. 619. (Cited on page 5.)
- [39] R. H. Parmenter, “Symmetry properties of the energy bands of the zinc blende structure,” *Phys. Rev.*, vol. 100, pp. 573–579, Oct 1955. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRev.100.573> (Cited on page 5.)
- [40] P. N. Butcher, N. H. March, and M. P. Tosi, *Crystalline semiconducting materials and devices*. Springer Science & Business Media, 2013. (Cited on page 5.)
- [41] G. Bir and G. Pikus, *Symmetry and Strain-induced Effects in Semiconductors*, ser. A Halsted Press book. Wiley, 1974. [Online]. Available: <https://books.google.com.mx/books?id=38m2QgAACAAJ> (Cited on page 6.)
- [42] W. A. Harrison, “Bond-orbital model and the properties of tetrahedrally coordinated solids,” *Phys. Rev. B*, vol. 8, pp. 4487–4498, Nov 1973. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.8.4487> (Cited on page 6.)

- [43] P. Vogl, H. P. Hjalmarson, and J. D. Dow, “A semi-empirical tight-binding theory of the electronic structure of semiconductors†,” *Journal of Physics and Chemistry of Solids*, vol. 44, no. 5, pp. 365–378, 1983. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/0022369783900641> (Cited on page 6.)
- [44] J. C. Slater and G. F. Koster, “Simplified lcao method for the periodic potential problem,” *Phys. Rev.*, vol. 94, pp. 1498–1524, Jun 1954. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRev.94.1498> (Cited on pages 6 and 14.)
- [45] P. Curie, “Sur la symétrie dans les phénomènes physiques, symétrie d'un champ électrique et d'un champ magnétique,” *Journal de physique théorique et appliquée*, vol. 3, no. 1, pp. 393–415, 1894. (Cited on pages 6 and 10.)
- [46] K. Brading, E. Castellani, and N. Teh, “Symmetry and Symmetry Breaking,” in *The Stanford Encyclopedia of Philosophy*, Fall 2021 ed., E. N. Zalta, Ed. Metaphysics Research Lab, Stanford University, 2021. (Cited on pages 6 and 10.)
- [47] R. Magri and A. Zunger, “Anticrossing and coupling of light-hole and heavy-hole states in (001) GaAs/ $\text{al}_x\text{ga}_{1-x}\text{As}$ heterostructures,” *Phys. Rev. B*, vol. 62, pp. 10 364–10 372, Oct 2000. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.62.10364> (Cited on pages 8 and 10.)
- [48] E. L. Ivchenko, A. Y. Kaminski, and U. Rössler, “Heavy-light hole mixing at zinc-blende (001) interfaces under normal incidence,” *Phys. Rev. B*, vol. 54, pp. 5852–5859, Aug 1996. (Cited on pages 8, 27, and 28.)
- [49] P. Tronc, Y. E. Kitaev, A. G. Panfilov, M. F. Limonov, G. Wang, and V. P. Smirnov, “Bound-state symmetries and optical transitions in gaas/ala_s quantum wells and superlattices with impurities and defects,” *Phys. Rev. B*, vol. 61, pp. 1999–2007, Jan 2000. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.61.1999> (Cited on page 8.)
- [50] M. Glazov, *Electron & Nuclear Spin Dynamics in Semiconductor Nanostructures*, ser. Series on Semiconductor Scienc. OXFORD University Press, 2018. (Cited on pages 8, 11, and 28.)
- [51] O. Krebs and P. Voisin, “Giant optical anisotropy of semiconductor heterostructures with no common atom and the quantum-confined pockels effect,” *Phys. Rev. Lett.*, vol. 77, pp. 1829–1832, Aug 1996. (Cited on page 8.)
- [52] Y. H. Chen, X. L. Ye, J. Z. Wang, Z. G. Wang, and Z. Yang, “Interface-related in-plane optical anisotropy in gaas/ $\text{al}_x\text{ga}_{1-x}\text{As}$ single-quantum-well structures studied by reflectance difference spectroscopy,” *Phys. Rev. B*, vol. 66, p. 195321, Nov 2002. (Cited on pages 8 and 27.)

- [53] E. L. Ivchenko and S. D. Ganichev, *Spin-Photogalvanics*. Berlin, Heidelberg: Springer Berlin Heidelberg, 2008, pp. 245–277. (Cited on pages 8, 11, and 28.)
- [54] N. Chand and S. N. G. Chu, “Origin and improvement of interface roughness in algaas/gaas heterostructures grown by molecular beam epitaxy,” *Applied Physics Letters*, vol. 57, no. 17, pp. 1796–1798, 1990. [Online]. Available: <https://doi.org/10.1063/1.104025> (Cited on page 10.)
- [55] K. Tillmann, M. Luysberg, P. Specht, and E. Weber, “Direct compositional analysis of algaas/gaas heterostructures by the reciprocal space segmentation of high-resolution micrographs,” *Ultramicroscopy*, vol. 93, no. 2, pp. 123–137, 2002. [Online]. Available: [https://doi.org/10.1016/S0304-3991\(02\)00153-5](https://doi.org/10.1016/S0304-3991(02)00153-5) (Cited on page 10.)
- [56] A. SHUBNIKOV, “On the works of pierre curie on symmetry††originally appeared in russian in uspekhi fizicheskikh nauk 59, 591-602 (1956). translated by l. i. man.” in *Crystal Symmetries*, ser. International Series in Modern Applied Mathematics and Computer Science, I. HARGITTAI and B. VAINSSTEIN, Eds. Amsterdam: Pergamon, 1988, pp. 357–364. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/B9780080370149500078> (Cited on page 10.)
- [57] J.-W. Luo, G. Bester, and A. Zunger, “Supercoupling between heavy-hole and light-hole states in nanostructures,” *Phys. Rev. B*, vol. 92, p. 165301, Oct 2015. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.92.165301> (Cited on page 11.)
- [58] R. Winkler, *Spin-orbit coupling effects in two-dimensional electron and hole systems*. Springer, 2003, vol. 191. (Cited on page 11.)
- [59] S. Döhrmann, D. Hägele, J. Rudolph, M. Bichler, D. Schuh, and M. Oestreich, “Anomalous spin dephasing in (110) gaas quantum wells: Anisotropy and intersubband effects,” *Phys. Rev. Lett.*, vol. 93, p. 147405, Sep 2004. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.93.147405> (Cited on page 11.)
- [60] L. V. Butov, A. Zrenner, G. Abstreiter, G. Böhm, and G. Weimann, “Condensation of indirect excitons in coupled alas/gaas quantum wells,” *Phys. Rev. Lett.*, vol. 73, pp. 304–307, Jul 1994. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.73.304> (Cited on page 13.)
- [61] L. Butov, C. Lai, A. Ivanov, A. Gossard, and D. Chemla, “Towards bose-einstein condensation of excitons in potential traps,” *Nature*, vol. 417, no. 6884, pp. 47–52, 2002. (Cited on page 13.)

- [62] G. Grosso, J. Graves, A. Hammack, A. High, L. Butov, M. Hanson, and A. Gossard, “Excitonic switches operating at around 100 k,” *Nature Photonics*, vol. 3, no. 10, pp. 577–580, 2009. (Cited on page 13.)
- [63] A. T. Hammack, L. V. Butov, J. Wilkes, L. Mouchliadis, E. A. Muljarov, A. L. Ivanov, and A. C. Gossard, “Kinetics of the inner ring in the exciton emission pattern in coupled gaas quantum wells,” *Phys. Rev. B*, vol. 80, p. 155331, Oct 2009. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.80.155331> (Cited on page 13.)
- [64] J. E. Golub, K. Kash, J. P. Harbison, and L. T. Florez, “Long-lived spatially indirect excitons in coupled gaas/al_xga_{1-x}as quantum wells,” *Phys. Rev. B*, vol. 41, pp. 8564–8567, Apr 1990. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.41.8564> (Cited on page 13.)
- [65] K. Sivalertporn, L. Mouchliadis, A. L. Ivanov, R. Philp, and E. A. Muljarov, “Direct and indirect excitons in semiconductor coupled quantum wells in an applied electric field,” *Phys. Rev. B*, vol. 85, p. 045207, Jan 2012. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.85.045207> (Cited on pages 13 and 25.)
- [66] A. G. Winbow, J. R. Leonard, M. Remeika, Y. Y. Kuznetsova, A. A. High, A. T. Hammack, L. V. Butov, J. Wilkes, A. A. Guenther, A. L. Ivanov, M. Hanson, and A. C. Gossard, “Electrostatic conveyer for excitons,” *Phys. Rev. Lett.*, vol. 106, p. 196806, May 2011. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.106.196806> (Cited on page 13.)
- [67] C. A. Bravo-Velázquez, L. F. Lastras-Martínez, O. Ruiz-Cigarrillo, G. Flores-Rangel, L. E. Tapia-Rodríguez, K. Biermann, and P. V. Santos, “Photoluminescence of double quantum wells: Asymmetry and excitation laser wavelength effects,” *physica status solidi (b)*, vol. n/a, no. n/a, p. 2100612. [Online]. Available: <https://onlinelibrary.wiley.com/doi/abs/10.1002/pssb.202100612> (Cited on page 13.)
- [68] J. M. Luttinger and W. Kohn, “Motion of electrons and holes in perturbed periodic fields,” *Phys. Rev.*, vol. 97, pp. 869–883, Feb 1955. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRev.97.869> (Cited on page 14.)
- [69] A. Yariv, C. Lindsey, and U. Sivan, “Approximate analytic solution for electronic wave functions and energies in coupled quantum wells,” *Journal of Applied Physics*, vol. 58, no. 9, pp. 3669–3672, 1985. [Online]. Available: <https://doi.org/10.1063/1.335726> (Cited on page 14.)
- [70] T. Fromherz, “Floquet states and intersubband absorption in strongly driven double quantum wells,” *Phys. Rev. B*, vol. 56, pp. 4772–4777, Aug 1997. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.56.4772> (Cited on page 14.)

- [71] E. Rosencher and B. Vinter, *Optoelectronics*. Cambridge University Press, 2002. (Cited on page 14.)
- [72] C. Galeriu, “ $k \cdot p$ theory of semiconductor nanostructures,” *PhD Dissertations. Worcester Polytechnic Institute, Worcester*, 2005. (Cited on page 14.)
- [73] I. Vurgaftman, M. P. Lumb, and J. R. Meyer, *Bands and Photons in III-V Semiconductor Quantum Structures*. Oxford University Press, 2020, vol. 25. (Cited on pages 14 and 16.)
- [74] H. Yeo, J. S. Lee, M. E. Khan, H. S. Kim, D. Y. Jeon, and Y.-H. Kim, “First-principles-derived effective mass approximation for the improved description of quantum nanostructures,” *Journal of Physics: Materials*, vol. 3, no. 3, p. 034012, jul 2020. [Online]. Available: <https://doi.org/10.1088/2515-7639/ab9b61> (Cited on page 14.)
- [75] P. Harrison and A. Valavanis, *Quantum wells, wires and dots: theoretical and computational physics of semiconductor nanostructures*. John Wiley & Sons, 2016. (Cited on pages 14, 16, 18, 20, and 22.)
- [76] M. G. Burt, “A new effective-mass equation for microstructures,” *Semiconductor Science and Technology*, vol. 3, no. 12, pp. 1224–1226, dec 1988. [Online]. Available: <https://doi.org/10.1088/0268-1242/3/12/013> (Cited on page 14.)
- [77] B. A. Foreman, “Effective-mass hamiltonian and boundary conditions for the valence bands of semiconductor microstructures,” *Phys. Rev. B*, vol. 48, pp. 4964–4967, Aug 1993. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.48.4964> (Cited on page 14.)
- [78] M. G. Burt, “The justification for applying the effective-mass approximation to microstructures,” *Journal of Physics: Condensed Matter*, vol. 4, no. 32, pp. 6651–6690, aug 1992. [Online]. Available: <https://doi.org/10.1088/0953-8984/4/32/003> (Cited on page 14.)
- [79] M. Marchewka, “Finite-difference method applied for eight-band kp model for $Hg_{1-x}Cd_xTe/HgTe$ quantum well,” *International Journal of Modern Physics B*, vol. 31, no. 20, p. 1750137, 2017. [Online]. Available: <https://doi.org/10.1142/S0217979217501375> (Cited on page 14.)
- [80] B. A. Foreman, “Envelope-function formalism for electrons in abrupt heterostructures with material-dependent basis functions,” *Phys. Rev. B*, vol. 54, pp. 1909–1921, Jul 1996. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.54.1909> (Cited on page 18.)
- [81] D. J. BenDaniel and C. B. Duke, “Space-charge effects on electron tunneling,” *Phys. Rev.*, vol. 152, pp. 683–692, Dec 1966. (Cited on page 18.)

- [82] G. Bastard, *Wave mechanics applied to semiconductor heterostructures*. Wiley, 1990. (Cited on page 18.)
- [83] T. Kamizato and M. Matsuura, “Excitons in double quantum wells,” *Phys. Rev. B*, vol. 40, pp. 8378–8384, Oct 1989. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.40.8378> (Cited on page 18.)
- [84] J. P. Killingbeck, *Microcomputer algorithms: action from algebra*. CRC Press, 2020. (Cited on page 20.)
- [85] E. R. Davidson and W. J. Thompson, “Monster matrices: their eigenvalues and eigenvectors,” *Computers in Physics*, vol. 7, no. 5, pp. 519–522, 1993. (Cited on page 20.)
- [86] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen, *LAPACK Users’ Guide*, 3rd ed. Philadelphia, PA: Society for Industrial and Applied Mathematics, 1999. (Cited on page 21.)
- [87] C. R. Harris, K. J. Millman, S. J. van der Walt, R. Gommers, P. Virtanen, D. Cournapeau, E. Wieser, J. Taylor, S. Berg, N. J. Smith, R. Kern, M. Picus, S. Hoyer, M. H. van Kerkwijk, M. Brett, A. Haldane, J. F. del Río, M. Wiebe, P. Peterson, P. Gérard-Marchant, K. Sheppard, T. Reddy, W. Weckesser, H. Abbasi, C. Gohlke, and T. E. Oliphant, “Array programming with NumPy,” *Nature*, vol. 585, no. 7825, pp. 357–362, Sep. 2020. [Online]. Available: <https://doi.org/10.1038/s41586-020-2649-2> (Cited on page 21.)
- [88] D. F. Nelson, R. C. Miller, and D. A. Kleinman, “Band nonparabolicity effects in semiconductor quantum wells,” *Phys. Rev. B*, vol. 35, pp. 7770–7773, May 1987. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.35.7770> (Cited on page 21.)
- [89] J. D. Cooper, A. Valavanis, Z. Ikonić, P. Harrison, and J. E. Cunningham, “Finite difference method for solving the schrödinger equation with band nonparabolicity in mid-infrared quantum cascade lasers,” *Journal of Applied Physics*, vol. 108, no. 11, p. 113109, 2010. [Online]. Available: <https://doi.org/10.1063/1.3512981> (Cited on page 21.)
- [90] Y. Varshni, “Temperature dependence of the energy gap in semiconductors,” *Physica*, vol. 34, no. 1, pp. 149–154, 1967. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/0031891467900626> (Cited on page 21.)
- [91] I. Vurgaftman, J. R. Meyer, and L. R. Ram-Mohan, “Band parameters for iii–v compound semiconductors and their alloys,” *Journal of Applied Physics*, vol. 89, no. 11, pp. 5815–5875, 2001. (Cited on pages 21 and 23.)

- [92] L. W. Molenkamp, R. Eppenga, G. W. 't Hooft, P. Dawson, C. T. Foxon, and K. J. Moore, "Determination of valence-band effective-mass anisotropy in gaas quantum wells by optical spectroscopy," *Phys. Rev. B*, vol. 38, pp. 4314–4317, Aug 1988. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.38.4314> (Cited on pages 21 and 23.)
- [93] S. Adachi, *Properties of semiconductor alloys: group-IV, III-V and II-VI semiconductors*. John Wiley & Sons, 2009, vol. 28. (Cited on pages 21 and 23.)
- [94] L. C. Lew Yan Voon and M. Willatzen, *Heterostructures: Basic Formalism*. Berlin, Heidelberg: Springer Berlin Heidelberg, 2009, pp. 273–362. (Cited on page 21.)
- [95] O. Donmez, F. Nutku, A. Erol, C. M. Arikan, and Y. Ergun, "A study of photomodulated reflectance on staircase-like, n-doped gaas/al_xga_{1-x}as quantum well structures," *Nanoscale Research Letters*, vol. 7, no. 1, p. 622, 2012. (Cited on pages 21 and 23.)
- [96] D. Zhou and B. F. Usher, "Deviation of the AlGaAs lattice constant from Vegard's law," *Journal of Physics D: Applied Physics*, vol. 34, no. 10, pp. 1461–1465, May 2001, publisher: IOP Publishing. [Online]. Available: <https://doi.org/10.1088/0022-3727/34/10/304> (Cited on page 21.)
- [97] S. Birner, T. Zibold, T. Andlauer, T. Kubis, M. Sabathil, A. Trellakis, and P. Vogl, "nextnano: General purpose 3-d simulations," *IEEE Transactions on Electron Devices*, vol. 54, no. 9, pp. 2137–2142, 2007. (Cited on page 22.)
- [98] Y. Takahashi, Y. Kato, S. S. Kano, S. Fukatsu, Y. Shiraki, and R. Ito, "The effect of electric field on the excitonic states in coupled quantum well structures," *Journal of Applied Physics*, vol. 76, no. 4, pp. 2299–2305, 1994. (Cited on page 23.)
- [99] R. L. Greene, K. K. Bajaj, and D. E. Phelps, "Energy levels of wannier excitons in GaAs – ga_{1-x}al_xAs quantum-well structures," *Phys. Rev. B*, vol. 29, pp. 1807–1812, Feb 1984. (Cited on page 23.)
- [100] K. Sivalertporn, "Effect of barrier width on the exciton states in coupled quantum wells in an applied electric field," *Physics Letters A*, vol. 380, no. 22, pp. 1990–1994, 2016. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0375960116300664> (Cited on page 25.)
- [101] N. S. Averkiev, L. E. Golub, A. S. Gurevich, V. P. Evtikhiev, V. P. Kochereshko, A. V. Platonov, A. S. Shkolnik, and Y. P. Efimov, "Spin-relaxation anisotropy in asymmetrical (001) al_xga_{1-x}As quantum wells from hanle-effect measurements: Relative strengths of rashba and dresselhaus spin-orbit coupling," *Phys. Rev. B*, vol. 74, p. 033305, Jul 2006. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.74.033305> (Cited on page 25.)

- [102] L. V. Kotova, A. V. Platonov, V. N. Kats, V. P. Kochereshko, S. V. Sorokin, S. V. Ivanov, and L. E. Golub, “Optical activity of quantum wells,” *Phys. Rev. B*, vol. 94, p. 165309, Oct 2016. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.94.165309> (Cited on page 25.)
- [103] C. Schönhuber, M. P. Walser, G. Salis, C. Reichl, W. Wegscheider, T. Korn, and C. Schüller, “Inelastic light-scattering from spin-density excitations in the regime of the persistent spin helix in a gaas-algaas quantum well,” *Phys. Rev. B*, vol. 89, p. 085406, Feb 2014. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.89.085406> (Cited on page 25.)
- [104] P. Tronc, “Spin phenomena in asymmetrical [001] GaAs/Al_xGa_{1-x}As quantum wells,” *Semiconductor Science and Technology*, vol. 27, no. 5, p. 055016, apr 2012. [Online]. Available: <https://doi.org/10.1088/0268-1242/27/5/055016> (Cited on page 25.)
- [105] X.-L. Ye, Y. H. Chen, J. Z. Wang, Z. G. Wang, and Z. Yang, “Determination of the values of hole-mixing coefficients due to interface and electric field in gaas/al_xga_{1-x}As superlattices,” *Phys. Rev. B*, vol. 63, p. 115317, Mar 2001. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.63.115317> (Cited on pages 26 and 27.)
- [106] O. Krebs, D. Rondi, J. L. Gentner, L. Goldstein, and P. Voisin, “Inversion asymmetry in heterostructures of zinc-blende semiconductors: Interface and external potential versus bulk effects,” *Phys. Rev. Lett.*, vol. 80, pp. 5770–5773, Jun 1998. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.80.5770> (Cited on page 27.)
- [107] X. Ye, Y. H. Chen, J. Z. Wang, B. Xu, Z. G. Wang, and Z. Yang, “In-plane optical anisotropy of symmetric and asymmetric (001) gaas/al(ga)as superlattices and quantum wells,” *Journal of Applied Physics*, vol. 90, no. 3, pp. 1266–1270, 2001. [Online]. Available: <https://doi.org/10.1063/1.1383018> (Cited on page 27.)