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

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ABBREVIATIONS

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

LIST OF CODES AND PACKAGES

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

ASE The Atomic Simulation Environment (ASE) is a set of tools and Python modules for setting up, manipulating, running, visualizing and analyzing atomistic simulations. [1]

SOLCORE A multi-scale, Python-based library for modelling solar cells and semiconductor materials [2]

Aestimo One-dimensional (1D) self-consistent Schrödinger-Poisson solver for semiconductor heterostructures [3]

VESTA 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies. [4]

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. [5]

SYMBOLS

X⁻ Negative Trion

X⁺ Positive Trion

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

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PHYSICAL MODEL

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

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SEMICONDUCTORS are alloy of materials with pare structural characteristics, it's the alloys which can generates an amazing quantum process that is quantum confinement. But, all of them couldn't possibly be achieved with 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 previous 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 in 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 [6]. 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 [7,8]. 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 [7].

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 [7,9,10]. It is important to remark which the heterostructure to will study is composed by $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ semiconductors, then we started with the GaAs crystal to propound the symmetry role in the CQWs. Then, already raised the starting point, remember that the crystal solid can be defined as an arrangement of atoms in strictly periodic arrays [11,12], from here arises two concepts: basis and lattice, where that last is

the set of mathematical points to which the basis is attached [11]. 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) [11].

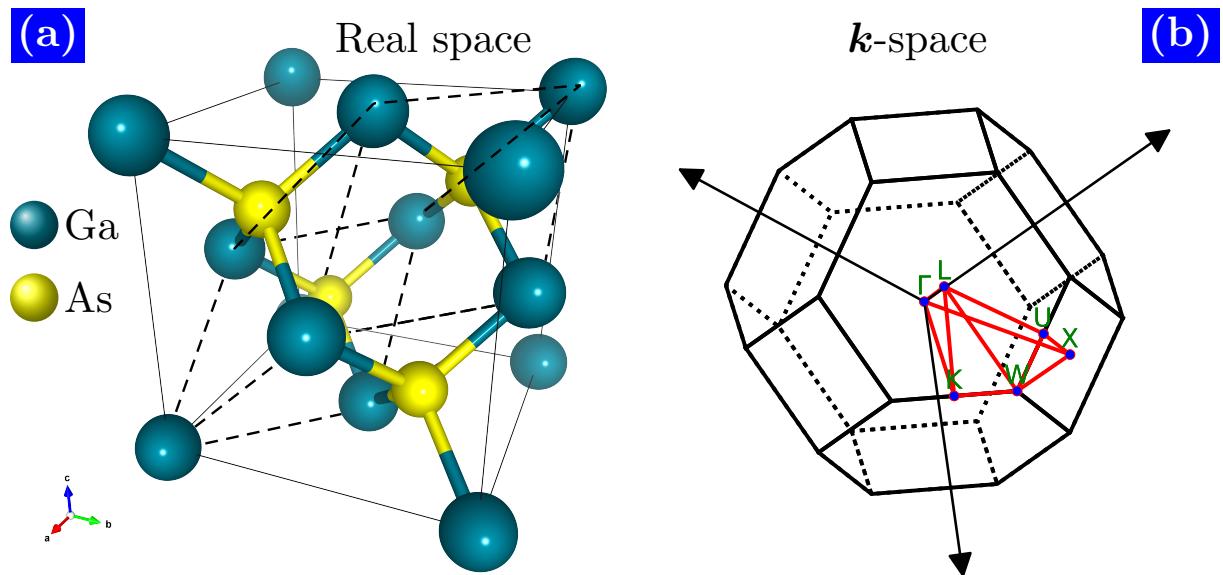


Figure 1.1: (a) GaAs crystal structure in “real space”, this region is known as *unit cell*, into that with dashed line is denoted the primitive cell. This lattice is well-defined by the vectors \mathbf{a} , \mathbf{b} and \mathbf{c} , these vectors are defined as the basis vectors. In (b) is schematized 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” [13]. 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 [11, 14]. 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 [13]. 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" [13] 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 [7, 15]. 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 [16]. Then taken into account this, and the vectors \mathbf{a} , \mathbf{b} and \mathbf{c} in reciprocal space can describe the total unit cell [7, 16].

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} [7]*. 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 [17] 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 [18–21]*. 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 [22].

Thus the band structure as a whole exhibits the symmetry characterized by the crystal [22]. 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 [23–25], in this case, the basis functions it's forming linear combinations of atomic orbitals (LCAO) to specific symmetry group [18].

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 [18, 22]. 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 [26], 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} [22]

1.2Symmetry breaking in Semiconductor Structures

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 [18]. 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.

1.3General revision of numerical methods

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

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

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

1.3.1Finite Difference Method

1.4Structural Parameters

1.5Anisotropy model in CQWs

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