STRESS MODULATION OF THE DEGREE OF SPIN POLARIZATION ON BULK SEMICONDUCTORS

THESIS BY
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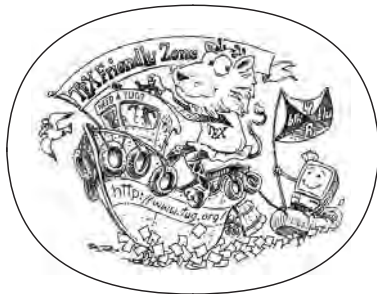

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Juan Cuauhtémoc Salazar González: *Stress Modulation of the Degree of Spin Polarization on Bulk Semiconductors*, Master in Sciences (Optics), © December 11, 2008

Dedicated to all the people that have decided
to be with me along this years at CIO.

To those who have done that in the distance,
like my parents Rosario Gonzalez and Juan Salazar,
my brothers Xóchitl, Francisco and Xicoténcatl,
and my aunt and uncle Teresa and Raúl Gonzalez.

Specially to my girlfriend Saray who has had
the confidence to share with me her family,
and the patience to have a long-distance relationship.

ABSTRACT

The thesis work presented here is part of the research I performed under the supervision of Dr. Bernardo Mendoza during my Master in Science studies at Centro de Investigaciones en Óptica, A.C. (León, México). Its main objectives are (1) to investigate the well known fact that the optical electron spin-injection on bulk semiconductors is affected by the application of strain, and (2) to explore the possibility of modulate such phenomenon by either compressive or expansive strains.

To address this project, a simple and effective method to compute the spin injection as a function of strain (actually, of a related quantity) is proposed, considering both compressive and expansive strains.

For this purpose, the approach of density functional theory (DFT) was taken, employing pseudopotential band structures based on the local density approximation (LDA). The computational tools employed were a computer cluster and almost solely *free software* programs. At the end it is shown that the application of stress can effectively modulate, and even enhance, the optical spin-injection on bulk semiconductors.

RESUMEN

El trabajo de tesis aquí presentado forma parte de las labores de investigacion que realicé bajo la supervisión del Dr. Bernardo Mendoza, durante mis estudios de Maestría en Ciencias en el Centro de Investigaciones en Óptica, A.C. (Léon, México). Sus objetivos principales son (1) investigar el hecho conocido de que la inyección de espín electrónico es afectada por la aplicación de esfuerzos, así como (2) explorar la posibilidad de modular este fenómeno ya sea mediante esfuerzos de compresión o expansión.

Para abordar este proyecto, se implementó un método sencillo y efectivo de calcular la inyección de espín como función del esfuerzo aplicado (en realidad, de una cantidad relacionada con él), tanto en compresión como expansión.

Para este propósito se empleo el formalismo de la Teoría Funcional de la Densidad (DFT) y estructuras de bandas pseudo-potenciales basadas en la aproximación local de la densidad (LDA). Las herramientas computacionales empleadas fueron un *cluster* de cómputo y en forma casi exclusiva programas de *software libre* . Al final se muestra cómo la aplicación de un esfuerzo puede efectivamente modular, e incluso mejorar, la inyección óptica de espín en semiconductores de bulto.

PUBLICATIONS

This thesis is strongly based on the ideas and techniques appeared previously in the following publications:

REFERENCE [1]. F. Nastos, J. Rioux, M. Strimas-Mackey, Bernardo S. Mendoza, and J. E. Sipe. Full band structure LDA and $\mathbf{k} \cdot \mathbf{p}$ calculations of optical spin-injection. *Phys.Rev. B*, 76, 2007.

REFERENCE [2]. B.S. Mendoza, F. Nastos, N. Arzate and J.E. Sipe. *Phys.Rev. B*, 74, 075318 - 2006.

Indeed, the work presented here can be thought as an extension of Reference [1].

Modern man is a mass–man; highly socialized, but very lonely.
He is alienated from others, and confronted with a dilemma:
afraid of close contact with another, and equally afraid to be alone.
It is the function of trivial conversation to answer the question:
How do I remain alone without being lonely?.

— Erich Fromm [3]
The Art of Being.

ACKNOWLEDGMENTS

El hombre moderno es un hombre de las masas;
sumamente socializado, pero muy solitario.
Está alienado por otros, y confrontado con un dilema:
temeroso de tener contacto cercano con otro,
e igualmente temeroso de estar solo.
La función de la conversación trivial [banal]
es entonces la encargda de responder a esta pregunta:
¿Cómo me mantengo a solas sin ser un solitario?

— Erich Fromm [3]
The Art of Being.

AGRADECIMIENTOS

Deseo agradecer a todas aquellas personas que se han sacrificado por mí. Esta tesis de maestría no representa el trabajo de sólo dos años, sino que es algo que comenzó mucho tiempo atrás en el regazo de mis padres y de mis tíos.

Deseo agradecer en forma muy especial a mi asesor, el Dr. Bernardo Mendoza Santoyo, por todo el apoyo que me ha brindado. Tanto por aquella estancia de verano de licenciatura en el año 2002, así como por todos sus consejos que en varias ocasiones fueron mas allá del ámbito académico. Él es para mí ejemplo de trabajo arduo, astucia y visión.

Quiero expresar mi franca gratitud a dos de las más cercanas amistades que gané durante este tiempo: a mi compañera de clase, Araceli Guerrero, por su sincera amistad e invaluable apoyo, así como al estudiante doctoral José Luis Cabellos, quien no sólo ha compartido conmigo su avidez para hacer funcionar los programas, sino también su sincera y graciosa compañía. Por sus invaluables sugerencias, a los revisores de esta tesis, Dr. Norberto Arzate Plata y Dr. Raul Vázquez Nava. En general, a todos los miembros del Grupo de Superficies Ópticas del CIO, y al resto de mis compañeros de clase: Diana, Yenysey, Guillermo y al singular Jorge. Al Dr. Norberto Arzate, al Dr. Rafael Espinosa Luna y a Maximiliano por las facilidades otorgadas para mi hospedaje. Todos ustedes han contribuido a incrementar lo que he adquirido aquí en León.

De manera muy especial, a todo el Departamento de Formación Académica por el apoyo otorgado; muy en particular por la ayuda para asistir (1) a cursos y estancias de especialización, como ABINIT-2008, la Segunda Escuela Mexicana en Computación Cuántica e Información Cuántica (gracias Dr. Venegas-Andraca por su apoyo logístico; gracias Dr. Macro Lanzagorta por sus consejos), (2) a la estancia de verano

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LIST OF ACRONYMS

Future appearance of the following acronyms
are hyperlinked to this page.

ABINIT   Software to compute *ab-initio* ('from first principles')
properties of atoms, nuclei, and solids.

BASH   Bourne-Again SHell. Bash is the shell in the GNU operating
system. A shell is a command language interpreter.

BZ   Brillouin Zone

CIO   Centro de Investigaciones en Óptica, A.C.

CONACYT   Consejo Nacional de Ciencia y Tecnología

CONCYTEG   Consejo de Ciencia y Tecnología del Estado de Guanajuato

DARPA   U.S. Defense Advanced Research Projects Agency

DFT   Density Functional Theory

DSP   Degree of Spin Polarization

EDSR   Electric Dipole Induced Spin Resonance

GNU   Gnu is Not Unix [Recursive acronym]

GMR   Giant Magneto Resistance Device

JDOS   Joint Density Of States

LATM   Linearized Analytic Tetrahedron Method

LDA   Local Density Approximation

NMR   Nuclear Magnetic Resonance

RF   Radio Frequency

SCF   Self-Consistent Field [method]

SEP   Secretaria de Educación Pública

SPINS   Spins IN Semiconductors

TINIBA   ABINIT written backwards. A set of bash shells to compute
optical properties of materials. See Section A.2 and Ref. [4].

LIST OF MNEMONICS

Future appearance of the following programming mnemonics are hyperlinked to this page. They refer to variables or parameters in the computer programs, either ABINIT or TINIBA. They are used from Section 4.3 onward (page 41).

acell	scAle CELL
cband	Conduction BANDs
ecut	Energy CUToff
nband	Number of BANDs (valence plus conduction).
nkpt	Number of k−PoinTs
rprim	Real PRIMitive vectors

Part I

BACKGROUND

INTRODUCTION

Elegir es anunciar y renunciar.

(To choose is to announce and to renounce)

— Enrique Rojas
Spanish Humanist

1.1 MOTIVATION AND OVERVIEW

One of the most important tendencies of technology is miniaturization, to the point that in the late part of last century the term *nanotechnology* was coined to refer to devices around or below 100 nm in size. As this miniaturization continues, technologists and scientists are faced with new opportunities and awkward challenges. Essentially the tinier they become, the more scientists are faced with quantum phenomena, like quantum tunneling, spin effects, and entangled states, to mention some of the most popular. Such issues represent current areas of research for the design, control, and operation of devices at such dimensions.

Most of the technology in use over the past century was strongly based on the study, design, and use of devices based on the conduction of electricity in a vacuum, a gas, or a semiconductor medium. Such devices are called *electronic* and the conduction of such electricity constitutes an electric current [1], that is, a flow of charge carriers, which may be electrons, holes, or ions. At present, another dominant device-technology arises from the integration of electronics with an ancient and older technology, namely with optics; it is called *optoelectronics*.

As mentioned above, quantum phenomena that may have interesting applications to technology are *spin effects*. Spin is an intrinsic property of elementary particles and nuclei and represents another degree of freedom for them. Bohr's theory of the atom predicts that lines in the spectra of alkali metals [2] should be single, but in fact, they consists of doublets. Pauli suggested that each electron could exist in two states

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[1] In the International System of Units (www.bipm.org/en/si/) the electric current is measured in Amperes, abbreviated as 'A'; one Ampere is equivalent to the flow of 10^{18} electrons per second.

[2] Alkali metals are chemical elements in group I of the periodic table (except hydrogen): lithium, sodium, potassium, rubidium, caesium, and francium. These elements all have one electron in their outermost shell, so the energetically preferred state of achieving a filled electron shell is to lose one electron to form a singly charged positive ion, i.e. a cation. Alkali metals have the lowest ionization potentials in their respective periods, as removing the single electron from the outermost shell gives them the stable inert gas

with the same orbital motion. Uhlenbeck and Goudsmit interpreted these states as due to the spin of the electron about an axis; thus the electron is assumed to have an intrinsic angular momentum in addition to any angular momentum due to its orbital motion. Moreover, in the presence of an external magnetic field the angular momentum vector of the electron precesses[3] around the field direction. In such precession not all orientations of the vector to the field direction are allowed: there is a quantization so the component of the angular momentum along the direction is restricted to certain values. This phenomenon is called *space quantization*.

As seen, this quantity was originally coined in relation to *rotation of particles* around their own axis, although the concept *'rotation of a particle'* does not make sense, the quantum spin follows the same mathematical structure of quantized angular momenta, but with some peculiarities, such as non-integer quantum units of spin.

Quantum spin properties play a fundamental role in the basic theory of physics, for instance,

- Spin is a fundamental constituent of the Pauli's Principle of Exclusion, being the spin one of the four quantum numbers.

- Ultra high sensitive spectroscopic tools are based on spin effects to study spin-orbit and hyperfine interactions, pairing symmetries of high temperature superconductors and parity violation of high energy physics.

- Imaging techniques based on the manipulation of nuclear spins have played a crucial role in chemical spectroscopy and medical imaging. For instance, Nuclear Magnetic Resonance (NMR) techniques use radio frequency (RF) signals to control spins.

Initial research in spin-physics

Perhaps the first reported experiment on spin-physics is that of Wood and Ellett, where in 1923 they investigated the variations in the polarization of the fluorescence of mercury vapor excited by polarized light. With their work they discovered the depolarization of luminiscence by transverse magnetic fields, know as the Hanle effect. About 25 years later, in the 1950s, Brossel and Kastler carried out intensive research in optical polarization and electric control of atomic angular moments. Almost in the 1970s, Lampel executed experiments on the optical spin orientation of electrons in semiconductors.

Hanle effect

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configuration. Their second ionization potentials are very high, as removing an electron from a species having a noble gas configuration is very difficult.

3 Precession: If a body is spinning about an axis OC, where O is a fixed point and C is rotating round an axis OZ fixed outside the body, the body is said to be precessing around OZ, which is called the precession axis [5].

From spin-physics to spin-technology

Devices that exploit the spin degree of freedom of electrons, holes, and nuclei are called *spintronics* and were first massively investigated around 1996 by the U.S. Defense Advanced Research Projects Agency (DARPA) in an initiative called *Magnetic Materials and Sensors*, aimed to develop such devices through spin transport electronics. This initiative was soon extended to include a broader kind of spin-based devices and was then called *Spins IN Semiconductors* (SPINS). The term *spintronics* was then coined by S.A. Wolf et al. (see Ref. [6]), one of the principal researchers of the initiative.

According to Das Sarma on Ref. [7], spintronic devices have some important key advantages compared with conventional electronic devices, notably

NATURAL BINARY LOGIC. As electrons can have spin $+1/2$ or $-1/2$, they led naturally to a binary logic of ones and zeroes. These values correspond to parallel and anti-parallel alignment with respect to an applied magnetic field.

EASY MANIPULATION. Experiments have shown that spin systems are easily manipulated by external applied magnetic or optical fields (see Najmaie et al. on Ref. [8] and Bhat et al. on Ref. [9]).

LONG COHERENCE. Coherence or relaxation time refers to the time spin direction tends to remain after external control is removed and spins start to decay to random directions, mainly due to spin-orbit coupling and momentum scattering; this is called *spin relaxation*. Spin coherence has been showed to be longer than those of electric charges, because electric coherence tends to be destroyed by scattering and collisional effects with defects, impurities, and other charges (see Section 1.4).

1.2 SPIN POLARIZATION

Ferromagnets are solid materials that, due to their large positive susceptibility, are magnetizable by weak magnetic fields. Typical ferromagnetic materials are iron, cobalt, nickel, and alloys containing them as well. Depending on the material, ferromagnets can retain their magnetization even after the magnetic field is removed[4].

The permanent spin polarization in ferromagnets is called *equilibrium* carrier spin polarization, nevertheless, according to Igor Žutić et al.

Equilibrium spin polarization

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4 Ferromagnetic magnetization is due to *the growth* of ferromagnetic domains, which are regions of crystalline matter with volumes ranging from 10^{-12} to $10^{-8}\mathrm{m}^3$; such domains contain atoms whose magnetic moments are aligned in the *same* direction; therefore ferromagnetic domains posses magnetic axis and moment. In an unmagnetized ferromagnet the domains are polarized at random, but if a weak magnetic field is applied,

*non-equilibrium spin
polarization*

on Ref. [10], it is not enough for spintronic applications, which rely on current flow and/or coherent manipulation of *non-equilibrium* spin polarization. The latter is created with the aid of a spin pumping source. Usually, the spin injection rate is controlled by optical, electrical, or resonant techniques. The basic principles of operation are:

OPTICAL SPIN-ORIENTATION. Apart from electrons, nuclei, and ions, photons also possess intrinsic angular momentum, i.e. spin, which is quantized to two values, $S = \pm\hbar$, corresponding to a spin direction parallel or anti-parallel to their momentum vector. Because a linear photon has an equal probability of exhibiting parallel or anti-parallel spin-orientation, it can be thought as composed of a right-circularly and a left-circularly photon, both with 1/2 probability.[5] When a photon is absorbed it transfers its linear momentum to the medium and if the photon is circular-polarized, it transfers angular momentum, exerting a torque on the medium.

*This
thesis*

Optical orientation of spins refers to the spin-polarization by the absorption of circular polarized light, for instance, by transference of angular momenta from circular-polarized photons to electrons. The work presented in this thesis lies in this type of spin polarization.

ELECTRICAL SPIN-ORIENTATION. Magnetism is the result of the motion of electrons when the circulatory current created by the angular momentum of an electron moving in its orbit produces a magnetic moment known as Bohr Magneton,[6] $\mu_{Bohr} = \hbar e/2m_e$, where e is the elementary charge, $\hbar$ is the reduced Planck constant, and m_e is the electron rest mass.
Electrical spin-orientation refers to the spin-polarization of a sample by the transport (injection) of spin-oriented electrons. Such electrons from a magnetic electrode bonded to the sample; the transport is induced by the application of an electric current.

RESONANT SPIN-ORIENTATION. Nuclear spin is the vector sum of its constituent particle spins, protons and neutrons. Therefore, nuclei also possess a magnetic moment, which in the presence of an external magnetic field, precesses about the applied field direction.

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the domains whose axis point along or close to the direction of the applied field grow at the expense of their neighbors. In a limiting case, the domain growth tends to the size of the specimen.

5 A beam of light is said to be circularly polarized if its electric vector undergoes uniform rotation in the xy plane, being z the direction of propagation. Circularly polarized photons are considered right- of left-handed depending if they have positive or negative angular momentum along the direction of propagation. The convention for the correspondence between right/left and positive/negative varies in the literature (see Yariv and Yeh on Ref. [11], p. 21).

6 $\mu_{Bohr} \approx 5.8 \times 10^{-5}$ eV/T $\approx 927.4 \times 10^{-26}$ J/T.

The orientation of the nuclear magnetic moment is discretized and each of these directions corresponds to different nuclear energies, whose difference depends on the applied field. The nucleus can make transitions from one state to another with the emission or absorption of electromagnetic radiation according to a selection rule. Actually, NMR is based on the adsorption of RF radiation ($1 - -100$ MHz): a strong variable magnetic field about 2 Teslas is applied to the sample, and then a RF field is applied at right angles and a coil detector is wounded around the sample. As the strong magnetic field is varied, the spacing of the energies varies, and at certain value of the magnetic field, this spacing is such that RF radiation is strongly absorbed; this resonance produces a signal in the detector coil. The nuclear magnetic moments can be determined from the resonance spectrum, plotting the coil signal versus the applied magnetic field.

A spin-orientation technique called Electric Dipole Induced Spin Resonance (EDSR) exists, where electric RF fields give rise to internal fields coupling to the spin. Choosing an adequate configuration of the electric RF fields and a static magnetic field defining a quantization axis for the spin, arbitrary spin rotations can be realized.

According to Duckheim and Loss on Ref. [12] and Golovach et al. on Ref. [13], EDSR has the advantage that it can be integrated in gated nanostructures.

1.3 SPIN MEASUREMENT

With the current capabilities it is possible, although awkwardly, to measure spin the direction of a single electron via its (small) magnetic moment, i.e. its Bohr Magneton μ_B —for spin polarizable systems, spin measurement involves an ensemble average of spins. Actually spin measurement in devices is more related the sense of effects caused by spin population accumulation in the sample than with the measurement of individual spins. A typical measurement process involves:

INJECTION OF A SPIN POPULATION. A *non-equilibrium* spin population could be created by a number of means, like *interband* absorption of circularly polarized light (one of the most efficient methods) or spin transport from a ferromagnet.

LUMINESCENCE ANALYSIS. Electronic spin can be measured by analyzing the luminescence generated by the recombination process of spin polarized electrons with holes, provided that the electronic spin relaxation time is not very short compared with the recombination time.

Apart from luminescence, other schemes for spin detection have been proposed. For instance, one of them is based on Pauli's Principle, which reduces the measurement of spin polarization to a charge or current measurement, requiring a single-charge electrometer (already available) and a switchable spin-filter tunnel barrier (see Spintronic Devices on Section 1.5, page 9). As mentioned by Awshalom et al. on page 253 of Ref. [14], optical measurements are also possible via the Faraday Rotation effect.

1.4   SPIN RELAXATION

Single Spin Relaxation

As commented above, the spin-coherence, or spin relaxation time, refers to the time the spin direction tends to remain after external control is removed, causing spins to decay to random directions. Electronic spin-coherence results long in metals and semiconductors (about a nanosecond), what makes these materials a promising framework for spin-based devices and applications, like spin-encoded information (see Section 1.5 on page 9). This decaying can be understood as a result of spin-orbit coupling, that is, spin precession around time-varying magnetic fields. Because those magnetic fields vary randomly, after a short time the spin is precessing around a completely different direction.

The genesis of such random fields is varied, ranging from interactions of electron-spins with nuclei-spins, momentum scattering, and the so called Elliot-Yafet, Dyakonov-Perel, and Bir-Aronov-Pikus mechanisms.

Spin decoherence is for single (few) spins

The single (or few) spin relaxation time is more often called *spin decoherence*, to distinguish it from spin ensemble relaxation. It is important for applications in spin-based quantum-computing (see Section 1.5 on page 9), where it is believed that individual spins should last for about 10^5 gate operations.

Ensemble Spin Relaxation

As mentioned by Igor Žutić et al. on Ref. [10], spin relaxation of a spin ensemble is typically described through two parameters,

Thermal equilibrium

SPIN RELAXATION TIME (T_1, Longitudinal time, or spin-lattice time). Is the time it takes for the longitudinal magnetization to reach equilibrium, or equivalently, the time in which thermal equilibrium is reached between the spin population and the lattice, by means of phonon transference.

Phase coherence

SPIN DEPHASING TIME (T_2, Transverse time, or decoherence time). The spin ensemble is initially precessing in phase about the longi-

tudinal field, but due to spatial and temporal fluctuations of the precessing frequencies an ensemble of transverse electron spins loses their phase. T_1 is the time such loss takes to occur.

These parameters came from the phenomenological Bloch-Torrey equations for magnetization dynamics. But if a microscopic expression for T_1 and T_2 is desired, a density-matrix formulation of the magnetization dynamics is usually performed and then compared with the Bloch equations to obtain T_1 and T_2.

As pointed out by Igor Žutić et al. in Ref. [10], it is customary that, for either small magnetic fields or when no matter the experimental set up, both times T_1 and T_2 are referred as a single symbol τ_s. Moreover, T_1 is more often used in theoretical calculations whereas experiments tend to measure T_2.

1.5 SPINTRONIC DEVICES

Semiconductor spintronics could be the base for a new generation of devices that combine standard microelectronics with spin effects, but first, in order to be able to write and extract information of such devices, one must have the capability to create a spin population, transport it across the device (through different materials), manipulate it, and detect it. Unfortunately, not all of these operations have been performed, and in some cases, there isn't a complete theoretical understanding of the details, and much research remains to be done. Current open problems on spin physics and spin technology are, for example,

- Enhancement of spin polarization on conventional and novel materials, *This thesis*

- Detection of spin coherence on nano-devices, like quantum dots and quantum wells,

- Enhancement of electron spin lifetimes,

- Transport of spin polarized carriers (electrons, holes, nuclei, and ions),

- All-electrical and all-optical spin control,

- Fast spin-polarization switching.

Nevertheless, many devices have been proposed, and it is believed that they will possess singular advantages compared to conventional electronic devices, like non-volatility, high speed data processing, less power consumption, increased integration densities, and increased phase control of coherence on length and time scales larger than in conventional electronics. Some remarkable proposals include:

GMR DEVICE. The Giant Magneto Resistance (GMR) structure device consists of alternating ferromagnetic and nonmagnetic metal layers (ferromagnetic materials are permanently magnetic). In this structure, the electric resistance through the layers has abrupt variations, depending on the relative magnetization orientation of the ferromagnetic layers, which is controlled by a magnetic field parallel to the layers: for parallel relative magnetizations the resistance is small, but for anti-parallel ones it is very large. The abrupt change in resistance is used as a high sensitive detector of variable magnetic fields, and is used for instance in the read/write heads of current magnetic storage devices.

SPIN-LED. In the Spin Light-Emitting-Diode the recombination of spin-polarized carriers results in the emission of right or left circularly polarized light in the direction normal to the surface. Through polarization analysis of the resulting radiation it is possible to get quantitative measurements of the spin injection efficiency, so that this device has served more as a test bed instrument than a commercial product, mostly because its low-temperature and high-magnetic field requirements.

FIELD-EFFECT SPIN TRANSISTOR. In 1989, Datta and Das proposed the first spintronic device. Its structure made of indium-aluminium-arsenide and indium-gallium-arsenide provides a channel for electron transport between two ferromagnetic electrodes. One of them acts as an *emitter electrode* and the other as a *collector electrode*, in analogy to the source and drain in a conventional electronic field-effect transistor. The operation is as follows: the emitter sends electrons with their spins oriented along the direction of the electrodes magnetization, while the collector (with the same *Spin filter* electrode magnetization) acts as a *spin filter*, accepting electrons that have the same spin. A *gate electrode* applies a field that causes the electron spins to precess, thus acting as a modulator of the *Datta-Das* electronic current that can pass the spin filter. This proposal is *device* known as the Datta-Das device, but it is yet to be realized because of the technical difficulties concerning clean spin control and injection from ferromagnetic sources. See Refs. [15] and [10].

ALL-METAL SPIN TRANSISTOR. It was proposed by Johnson (Ref. [16]) and consists of a 3-layered structure: a nonmagnetic metallic layer sandwiched between 2 ferromagnetic layers, being similar in *Spin-Switch* structure and function to the GMR device. In this device the non-*Spin-Valve* metallic layer acts as the *base*, one of the ferromagnetic layers as the *collector* and the other as the *emitter*; a battery is included in the *control circuit* (emitter-base) and the *direction* of the current in the *control circuit* (base-collector) is switched by changing the

magnetization of the collector layer. This device acts as a spin valve or a switch, that is, it neither amplifies the current nor the voltage. See Ref. [16].

SPINTRONIC SOLAR CELLS. This proposal by Das Sarma plans to direct circular polarized solar light, coming from a filter, to a PN semiconductor junction of type III-V. This will create spin polarized electron-hole pairs in the *depletion layer*[7], but because of the semiconductor type, the spin polarization will only be retained by electrons. The internal electric field in the depletion zone will cause that the holes move through the P side and the electrons to the N side. If this junction is connected to a circuit, then a spin polarized current will flow. See Ref. [7]

SPIN-BASED QUANTUM COMPUTERS. There are many proposals for quantum computing, and the Spin-Based Quantum Computer is one of them. Nevertheless, all these are long term projects because of tough technical difficulties, like coherence control. The spin-based proposal aims to use the natural property of spin-up or spin-down of electrons as the new binary units of processing, called *qubits*, which will be not restricted to represent just zeroes or ones, but an arbitrary superposition of them. Basically, to perform a computation, an initial state is imposed on the spins, and then they is allowed to evolve through a process of entanglement, which is a quantum property of correlation between spins, even though they are spatially separated.

David P. Di Vicenzo, an IBM's researcher, states that to realize a quantum computer [spintronic or not] a set of 5+2 requirements must be fulfilled (see Ref. [17]), namely

5+2 Quantum Computing Requirements

1. A scalable physical system with well characterized qubits,

2. The ability to initialize the state of the qubits to a simple fiducial [reference] state, such as $|000\cdots 0>$,

3. Long relevant coherence times, much longer than the gate operation time,

4. A universal set of quantum gates,

5. A qubit specific measurement capability,

6. The ability to interconnect stationary and flying qubits, and

7. The ability to faithfully transmit flying qubits between specified locations.

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7 The depletion layer is formed from a conducting region by removal of all free charge carriers, leaving none to carry a current. It is formed, for example, in the interface of a N–P junction.

The first five requirements are meant to serve for *quantum computation* (prime factoring and code-breaking crypto-systems are two ambitious problems aimed to be solved with it) and the last two requirements are needed to connect quantum computation to *quantum information processing* (at present, there are commercial cryptographic systems based on quantum cryptography) and some other operations require both quantum computation and quantum information (like the computation with input data dotted through many parties).

Because quantum computation requires a long coherence and fine control of quantum states, nuclear and electronic spins can function as qubits. Some particular proposals for spin-based quantum computers include:

QUANTUM DOTS. In this scheme the spin of a *single* electron trapped in a *quantum dot* is used as qubit, then an array of quantum dots is allowed to interact to form an entanglement of qubits. The individual electrons are manipulated with magnetic fields, and this is precisely one of the difficulties of this scheme: the individual manipulation of electrons. Another issue is the trapping of a single electron in a quantum dot, but recently it has been shown that an odd number of electrons trapped in a quantum dot could serve as a qubit (instead of only one). The problem of the disturbance caused on neighbor qubits by the magnetic field is planned to be eliminated with *quantum error correction* techniques.

PHOSPHORUS NUCLEI ON SILICON. This scheme was proposed by Kane (See Ref. [18]), where phosphorus atoms doped in a silicon substrate act as qubits. Each phosphorus nucleus transmits its spin to its electrons, which serve for single qubit operations. Two-qubit like operations are performed with electron-nucleus and electron-electron interactions.

In brief

Spintronic devices represent a great promise of improvement in current technology, and hundreds of scientists and engineers work around the world to solve the respective theoretical and practical drawbacks.

1.6 OBJECTIVES AND OVERVIEW OF THIS THESIS

The thesis work presented here is part of the research I performed under the supervision of Dr. Bernardo Mendoza during my Master in Science studies at Centro de Investigaciones en Óptica, A.C. (León, México).

Its main objectives are (1) to investigate the well known fact that the optical electron spin-injection on bulk semiconductors is affected by the application of stress, and (2) to explore the possibility of modulate such phenomenon by either compressive or expansive stresses. For that matter, a simple and effective method to compute the spin injection as a function of stresses (or a related quantity) is proposed, considering both compressive and expansive stresses.

To address this project, first in this Chapter 1 a review of the broad field of spintronics has been given, including some remarkable proposals for spin-devices. Then in Chapter 2 the basic theory of electronic spin is presented, and is followed in Chapter 3 by a description of the framework used to quantify the spin injection on bulk semiconductors. In the last third of the presentation, Chapter 4, expressions of the preceding chapters are evaluated, taking the approach of density functional theory (DFT) and employing pseudopotential band structures based on the local density approximation (LDA). For this purpose almost solely, *free* software programs were used.

At the end of the chapter, the main objective of this thesis demonstrated, i.e. the fact that in principle, the tuning of the spin-injection and its enhancement are possible by means the application of stresses. Finally, in Chapter 6 a review of the results and the corresponding conclusions are presented.

ELECTRONIC SPIN

2.1 BASIC DEMONSTRATION OF SPIN EXISTENCE

The first and most basic demonstration of the spin existence was performed in Germany (1921) by Gerlach and Stern. Actually they showed (see Ref. [19]) the existence of the electron's magnetic moment due to its spin. Basically, the experimental set up is as follows: paramagnetic silver atoms contained in a furnace heated at high temperature are permitted to escape through a small opening. After propagating in straight line in the vacuum, a collimating slit selects those atoms whose velocity is parallel to a particular direction. The emerging collimated beam then traverses the gap of an electromagnet and then condenses on a plate.

Stern-Gerlach Experiment

The classic theory predicted a deflection of the beam, but instead they observed an split of the beam into two beams, which were deflected in opposite directions. This showed that atoms had different magnetic properties. When the two beams impact in the plate they form two spots, whose width is due to the dispersion of the velocities and the width of the slit.

This experiment proved that only certain permitted orientations were allowed, i.e. the angular momentum is quantized.

Other experimental evidences of spin existence are:

FINE STRUCTURE OF ATOMIC SPECTRA. When atomic spectra is observed in detail, each spectral line is actually composed of a finite number of lines, i.e. there are groups of atomic levels very closely spaced.

THE ANOMALOUS ZEEMAN EFFECT. In the *normal* Zeeman effect the atomic spectra of an atom splits into several lines when a magnetic external field is present. The Schrödinger theory predicts that such splitting must result in an odd number of spectral lines, but experimental evidence showed that spectral lines of atoms with *odd* atomic number Z (the number of protons, which uniquely identifies a chemical element) were split into an *even* number of sub-levels.

HALF-INTEGRAL ANGULAR MOMENTA. This problem is closely related to the Stern-Gerlach experiment, which suggests that half-integral values of the quantum number j exist, but it is in conflict

with the fact that the orbital angular momentum ℓ can only be integral

MAGNETIC PROPERTIES. Many substances, like metallic ferromagnets such as iron, cobalt, and nickel, are magnetizable with an external magnetic field, and retain its magnetization after the field has been removed. This phenomena can only be explained with the concept of ferromagnetic *domains* and *spin* (see footnote 4 on page 5).

2.2   SPIN INCLUSION INTO THE QUANTUM THEORY

Schrödinger Equation

The time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V\right)\psi \tag{2.1}$$

describes quantumly the motion of an electron that is under the influence of a potential. Here the electron is a particle that possesses three degrees of freedom, corresponding to the x, y, and z coordinates, therefore its wave function has dependence only as $\psi(x, y, z)$. In Equation 2.1 $i\hbar\partial/\partial t$ is the energy operator $\widehat{E}$, $-\hbar^2/2m\boldsymbol{\nabla}^2$ is the kinetic energy operator $\widehat{T}$, and $\widehat{V}$ is the potential operator. With the Schrödinger approach to quantum mechanics it is possible to study *exactly* only the Hydrogen atom, which only possesses two particles: a proton and an electron. More complex atoms, like Helium (a 3-body problem) and the rest (many-body problems) require to make *mathematical* simplifications in order to obtain analytical solutions. Such simplified solutions which nevertheless explain adequately many observed quantum phenomena, are inadequate in many studies, like the fine details in atomic spectra (spectral lines that seem to be one, but are actually two or more closely spaced).

Because removing the preceding mathematical simplifications make it impossible to solve analytically the Schrödinger equation, it became imperative to review the physical assumptions done in such theory, in order to explain a number of inconsistencies (like those mentioned in Section 2.1). For example, among the most important missing effects in the Schrödinger formulation were relativistic kinematics (mass, time, and length variations due to velocity) and magnetic effects (the orbital electron around the nucleus represents a varying electric current, which induces magnetism).

Relativistic effects were first included by simple substitution of the relativistic energy in the Schrödinger theory (de la Peña, p. 834 of Ref. [20]),

$$E^2 = m^2c^4 + c^2p^2 \tag{2.2}$$

leading to the Klein-Gordon equation; which for the free particle $(V = 0)$ it takes the form

$$\left(\boldsymbol{\nabla}^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\psi - \frac{m^2c^2}{\hbar^2}\psi = 0. \tag{2.3}$$

Although this formulation includes relativistic effects, it nevertheless requires the spin property to be included by hand; moreover, it also presents some inconsistencies in the particle density (caused by the second order temporal derivative), and solutions with negative energies as well.

To circumvent these problems, in 1930 Paul Dirac proposed to linearize the relativistic energy expression in Equation 2.2, i.e. to find a linear relationship between $\widehat{E}$ and $\widehat{p}$, whose square satisfied the relativistic energy equation. This linearization did not remove the problem of negative energies, which now Dirac interpreted as energies of anti-particles.[1] Dirac's equation for the free particle has the form

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-i\hbar c\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + mc^2\beta\right)\Psi, \tag{2.4}$$

where $\boldsymbol{\alpha}$ and β are 4×4 matrices that must be chosen to fulfill the relativity laws. Therefore, Dirac's equation gives a relativistic quantum mechanical description of the electron and leads naturally to a new characteristic of the electron, its spin.

2.3 PAULI'S DESCRIPTION OF SPIN

In between the discovery of the electron spin and the introduction of Dirac's equation, Pauli proposed to incorporate the spin characteristic into the Schrödinger theory by introducing a number of supplementary non-relativistic postulates, offering an electron theory much simpler than Dirac's theory, but which nevertheless provides excellent agreement with experimental evidence (see Cohen-Tannoudji et al., on p. 968 of Ref. [21]).

In academic texts, Pauli's equation may be usually written in two forms (de la Peña, Ref. [20]):

$$i\hbar\frac{\partial\Psi}{\partial t} = \frac{\boldsymbol{P}^2}{2m}\Psi + \left(V - \widehat{V}_{\text{coupling}}\right)\Psi, \tag{2.5a}$$

$$i\hbar\frac{\partial\Psi}{\partial t} = \widehat{H}_0\Psi + \frac{\mu_0}{\hbar}\boldsymbol{B}\cdot\left(\widehat{\boldsymbol{L}} + 2\widehat{S}\right)\Psi, \tag{2.5b}$$

---

[1] Two years before this proposal, D. Anderson found for the first time the anti-electron, most commonly known as positron.

where the interaction/coupling term between the external magnetic moment B and the intrinsic magnetic moment $\widehat{\mu}$ (associated to spin) is given by

$$\widehat{V}_{coupling} = -\widehat{\mu} \cdot B = \mu_0 \, \widehat{\sigma} \cdot B = \frac{e\hbar}{2mc} \, \widehat{\sigma} \cdot B, \tag{2.6}$$

with μ_0 as the Bohr's magneton $\mu_{Bohr} = \hbar e/2m_e$ and $\widehat{\sigma}$ as the Pauli's matrices (see Equation 3.66 on page 35).

The Hamiltonian $H_0 = P^2/2m$ in Equation 2.5 is written in terms of the electron's *Canonical Momentum* p_{can} due to its motion and due to the influence of an external magnetic field

$$p_{can} = P_{kinetic} + \frac{e}{c} A, \tag{2.7}$$

where $P_{kinetic} = mv$ is the *mechanical/kinetic momentum* and A is the magnetic vector potential.

Therefore, for an electron that is influenced by an external magnetic field, the kinetic momentum operator is written as

$$\widehat{P}_{kinetic} = \widehat{p}_{can} - \frac{e}{c} A. \tag{2.8}$$

In Equation 2.5b, L is the orbital angular momentum, s is the intrinsic (spin) angular momentum, and $J = L + S$ is the total angular momentum.

2.4 PAULI'S POSTULATES

As axiomatically pointed out by Cohen-Tannoudji et al. in Ref. [21], the Pauli's postulates that lead to the preceding Equation 2.5 are:

1. The spin operator S is an angular momentum. Therefore, its three components are observables which cyclically satisfy the commutation relations

   $$[S_x, S_y] = i\hbar S_z. \tag{2.9}$$

2. The spin operators act in a new space, the *spin state space* $\mathcal{E}_s$, where S^2 and S_z constitute a *complete set of commuting observables* (CSCO).

3. The state space $\mathcal{E}$ of the particle being considered is the tensor product of the orbital state space $\mathcal{E}_r$ and the spin state space $\mathcal{E}_s$:

   $$\mathcal{E} = \mathcal{E}_r \otimes \mathcal{E}_s. \tag{2.10}$$

   Consequently, all spin observables commute with all orbital observables.

4. The electron is a spin-$\frac{1}{2}$ particle ($s = \frac{1}{2}$) and its intrinsic magnetic moment is given by

$$M_S = 2\frac{\mu_B}{\hbar}S. \tag{2.11}$$

Therefore, the electronic spin state space $\mathcal{E}_s$ is two dimensional.

In brief

Before the 1920's quantum theory could not explain a number of experimental evidences. Then researchers realized that it was required to include a new quantum property associated to the electron's spin around itself. Such quantity, known as quantum spin, was included *ad hoc* into Schrödinger theory with the adoption of the Pauli's Principles, and lately it was shown that spin arose from a more complete description given by Dirac, where relativistic effects were taken into consideration.

Part II

THEORY

DSP: THE DEGREE OF SPIN POLARIZATION

3.1 INTRODUCTION

The purpose of this chapter is to show the key steps to derive an expression to quantify the degree of spin polarization (DSP) in bulk semiconductors. This polarization is carried out by absorption of circular polarized light, which causes electrons (1) to be promoted from the valence to the conduction band[1] and (2) to be optically oriented by the transference of angular momentum from photons to the electrons; the orientation of the electron spin is parallel or anti-parallel to the beam. The presentation of this chapter follows Nastos et al. as in Ref. [1].

The computation of the band structure, required to describe the optical spin injection, is made within the density functional theory (DFT, see Refs. [22] and [23]). These band structure calculations are restricted to the local density approximation (LDA), which is an approximation to the exchange-correlation energy functional in the DFT. The external perturbation is taken to come from a laser beam, and the Hamiltonian for the perturbation is written as

$$H_{ext} = -er^a E^a(t), \tag{3.1}$$

where e is the electric charge, r is the position operator, $E(t)$ is the electric field of the applied beam. The Roman superscripts indicate Cartesian coordinates, that, when repeated as in Equation 3.1, mean that the coordinates are to be summed over. The intraband matrix elements that describe the change of state along the same band do not take part in the quantification of the spin polarization, therefore they are isolated from the interband matrix elements. The latter describe electron's change of states that include transition between different bands.

3.2 DENSITY-MATRIX EQUATION OF MOTION

The spin polarization can be quantified through the *spin injection rate*, which in turn can be computed by a Fermi golden rule derivation.

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1 ISOLATED ATOMS possess what are known as *quantum states*, each of them characterized by a set of quantum numbers and an energy level. For an isolated atom the energy levels are *discrete*. The atom's electrons always tend to be at the lowest energy level, one electron per quantum state. For a CONDENSATE OF ATOMS, like a crystal, each state of each atom becomes a state of the crystal, and the energies become spread over certain continuous bands. That results in the formation of allowed and forbidden bands.

Nevertheless, such approach is not suitable to take into account the excited coherences that emerge in noncentrosymmetric semiconductors (i.e., those lacking of inversion symmetry), where the conduction bands are spin-split by amounts smaller than the laser width, causing the laser beam to excite a coherent superposition of two conduction bands.

A more rigorous approach is to use a density-matrix single-particle description, where atoms are assumed to have only one electron, procedure that permits to include excited coherences consistently.

The equation of motion is

$$\frac{d}{dt}\rho_{mn}(\mathbf{k};t) = -i\widehat{\omega}_{mn}(\mathbf{k})\rho_{mn}(\mathbf{k};t)$$
$$-\frac{i}{\hbar}\left(\left[H^{ext}(t),\rho(\mathbf{k};t)\right]\right)_{mn}, \tag{3.2}$$

where the commutator matrix elements are

$$\left(\left[H^{ext}(t),\rho(\mathbf{k};t)\right]\right)_{mn} = \sum_p H^{ext}_{mp}(t)\,\rho_{pn}(\mathbf{k};t)$$
$$-\sum_p H^{ext}_{mp}(t)\,\rho_{pn}(\mathbf{k};t), \tag{3.3}$$

and loss and dephasing are taken into account in

$$\widehat{\omega}_{mn}(\mathbf{k}) = \omega_{mn} - i\Gamma_{mn}, \tag{3.4}$$

with Γ_{mn} being positive and small, and

$$\omega_{mn} \equiv \omega_c(\mathbf{k}) - \omega_v(\mathbf{k}). \tag{3.5}$$

Equation 3.3 can be solved assuming the presence of excited coherences, that is, the simultaneous excitation of two close bands, c and c′, by the energy width of the laser beam (see Figure 1).

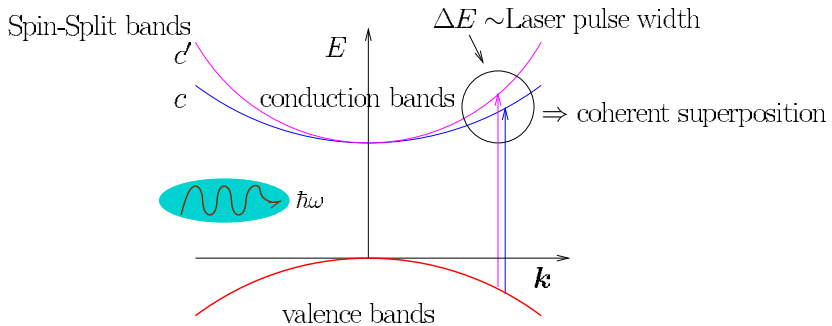Figure 1: (color online). Coherence arise from simultaneous excitation of two close conduction bands, c and c′, by the finite energy width of the laser beam.

3.3 MULTI-SCALE SOLUTION OF THE EQUATION OF MOTION

Multiple-scale analysis is a general perturbation framework that is useful in systems characterized by different time scales (see Kevorkian and Cole on Ref. [24]). For the problem at hand, Equation 3.2, the method allows the separation of the pulse time, the carrier cycle, and the dephasing and loss times. The interest is in the response to a continuous wave field of the form

$$\boldsymbol{E}(t) = \boldsymbol{E}_{\text{env}}(t)e^{-i\omega t} + \boldsymbol{E}^{\star}_{\text{env}}(t)e^{i\omega t} \tag{3.6}$$

where the amplitude $\boldsymbol{E}_{\text{env}}(t)$ is called the *slowly varying envelope function*. To implement the multiple scales treatment a new variable is defined

$$\tau = \omega t \tag{3.7}$$

and then the preceding equations are re-defined in terms of τ:

$$\frac{d}{d\tau}\rho_{mn}(\tau) = -i\frac{\widehat{\omega}_{mn}(\boldsymbol{k})}{\omega}\rho_{mn}(\tau) - \frac{i}{\hbar\omega}\left([H^{\text{ext}}(\tau), \rho(\tau)]\right)_{mn}, \tag{3.8}$$

$$H_{\text{ext}}(\tau) = -e\, r^{a}E^{a}(\tau), \tag{3.9}$$

$$\boldsymbol{E}(\tau) = \boldsymbol{E}_{\text{env}}(\tau)e^{-i\omega\tau} + \boldsymbol{E}^{\star}_{\text{env}}(\tau)e^{i\omega\tau}. \tag{3.10}$$

Since the intraband matrix elements of r^{a}_{mn} do not contribute to the spin injection in the conduction band, they are neglected from the beginning. To introduce the different time scales, the preceding functions are explicitly written in terms of two new variables: τ_0 and τ

$$\tau_0 = \tau \quad \text{and} \tag{3.11a}$$

$$\tau_1 = \eta\tau \quad \text{with} \quad \eta \ll 1, \tag{3.11b}$$

That is, τ_0 describes faster phenomena than τ_1. Notice that the functions depending on these new variables vary significantly only as τ and τ_0 range over unity; therefore the *slowly varying envelope function* is written as

$$\boldsymbol{E}(\tau) = \boldsymbol{E}_{\text{env}}(\tau_1)e^{-i\omega\tau_0} + \boldsymbol{E}^{\star}_{\text{env}}(\tau_1)e^{i\omega\tau_0}. \tag{3.12}$$

As pointed out above, multiple scale analysis is a perturbative method and the solution to Equation 3.8 is proposed as

$$\rho_{mn}(\tau) = \sum_{u=-\infty}^{\infty} e^{-iu\tau_0}\rho_{mn;u}(\tau), \tag{3.13}$$

where the u's are integers. Inserting Equation 3.13 into Equation 3.8, we write the equation of motion as,

$$
\begin{aligned}
\frac{d}{d\tau}\rho_{mn;u}(\tau) \;=\; & -i\left(\frac{\widehat{\omega}_{mn}}{\omega} - u\right)\rho_{mn;u}(\tau) \\
& + i\eta\Big[\, \sigma_{mp}(\tau_1)\quad \rho_{pn;(u-1)}(\tau) \\
& \qquad + \overline{\sigma}_{mp}(\tau_1)\quad \rho_{pn;(u+1)}(\tau) \\
& \qquad - \rho_{mp;(u-1)}(\tau)\quad \sigma_{pn}(\tau_1) \\
& \qquad - \rho_{mp;(u+1)}(\tau)\quad \overline{\sigma}_{pn}(\tau_1)\Big]
\end{aligned}
\tag{3.14}
$$

where the σ terms, which are dimensionless, are defined as

$$
\eta\sigma_{mp}(\tau_1) \;\equiv\; \frac{er^a_{mp}E^a(\tau_1)}{\hbar\omega} \quad\text{and}
\tag{3.15a}
$$

$$
\eta\overline{\sigma}_{mp}(\tau_1) \;\equiv\; \frac{er^a_{mp}E^{a\star}(\tau_1)}{\hbar\omega}.
\tag{3.15b}
$$

Now a perturbative solution in powers of ρ of Equation 3.14 is proposed,

$$
\rho_{mn;u}(\tau) = \rho^{(0)}_{mn;u}(\tau_1) + \eta\rho^{(1)}_{mn;u}(\tau_1) + \eta^2\rho^{(2)}_{mn;u}(\tau_1) + \cdots
\tag{3.16}
$$

Defining

$$
\left(\frac{\widehat{\omega}_{mn}}{\omega} - u\right) \to C_{mn;u} = C^{(0)}_{mn;u} + \eta C^{(1)}_{mn;u}
\tag{3.17}
$$

and assuming that due to damping, for a given (mnu) both $C^{(0)}_{mn;u}$ and $C^{(1)}_{mn;u}$ will not be nonzero, that is, only one survives for a given (mnu). (see Figure 2).

Now a set of equations can be constructed from Equation 3.14, one for each power of η, if

$$
\frac{\partial}{\partial\tau} = \frac{\partial}{\partial\tau_0} + \eta\frac{\partial}{\partial\tau_1} + \cdots
\tag{3.18}
$$

The proposed solution in Equation 3.16 sets all time dependence at the τ_1−level (slow time), therefore, from now the sub-index '1' is dropped. For further simplicity, all time dependence is left out. With these conventions

$$
\text{for}\,\eta^0: \quad C^{(0)}_{mn;u}\rho^{(0)}_{mn;u} = 0,
\tag{3.19}
$$

$$
\text{for}\,\eta^{i+1}: \quad \frac{\partial}{\partial\tau}\rho^{(i)}_{mn;u} = -iC^{(0)}_{mn;u}\rho^{(i+1)}_{mn;u} - iC^{(1)}_{mn;u}\rho^{(i)}_{mn;u}
$$

$$
+iD^{(i)}_{mn;u},
\tag{3.20}
$$

where

$$
\begin{aligned}
D^{(i)}_{mn;u} &= \sum_p \left(\sigma_{mp} \rho^{(i)}_{pn;(u-1)} + \overline{\sigma}_{mp} \rho^{(i)}_{pn;(u+1)} \right) \\
&\quad - \sum_p \left(\rho^{(i)}_{mp;(u-1)} \sigma_{pn} + \rho^{(i)}_{mp;(u+1)} \overline{\sigma}_{pn} \right).
\end{aligned} \tag{3.21}
$$

Now we separate the terms for which $C^{(0)}_{mn;u} = 0$ from those for which $C^{(0)}_{mn;u} \neq 0$ (called *allowed* and *forbidden* terms, respectively. See Figure 2).

$$
\rho^{(i)}_{mn;u} =
\begin{cases}
\alpha^{(i)}_{mn;u} & \text{if} \quad C^{(0)}_{mn;u} = 0 \quad \text{allowed} \\
\\
\beta^{(i)}_{mn;u} & \text{if} \quad C^{(0)}_{mn;u} \neq 0 \quad \text{forbidden}
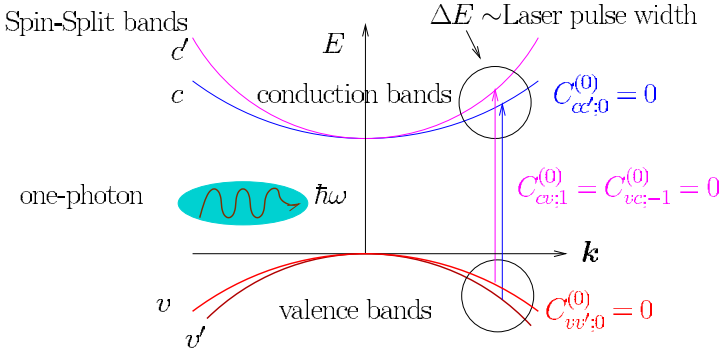\end{cases} \tag{3.22}
$$

Figure 2: (color online) Diagrammatic representation of the *allowed* and the *forbidden* terms of Equation 3.22. It is assumed that due to damping, for a given (mnu) both $C^{(0)}_{mn;u}$ and $C^{(1)}_{mn;u}$ will not be nonzero, that is, only one survives for a given (mnu)

From Equation 3.19

$$
\beta^{(0)}_{mn;u} = 0, \tag{3.23}
$$

that is, the only components $\rho^{(0)}_{mn;u}$ that survive are the allowed terms. The $i = 0$ term of Equation 3.20 with $u = 0$ gives

$$
\frac{\partial}{\partial \tau} \alpha^{(0)}_{mn;u} = -iC^{(1)}_{mn;u} \alpha^{(0)}_{mn;u} + i a_{mn;u} A^{(0)}_{mn;u} \tag{3.24}
$$

$$
\beta^{(1)}_{mn;u} = \frac{b_{mn;u} A^{(0)}_{mn;u}}{C^{(0)}_{mn;u}} \tag{3.25}
$$

where

$$A_{mn;u}^{(i)} = \sum_P \left(\sigma_{mp} \alpha_{pn;(u-1)}^{(i)} + \overline{\sigma}_{mp} \alpha_{pn;(u+1)}^{(i)} \right)$$

$$- \sum_P \left(\alpha_{mp;(u-1)}^{(i)} \sigma_{pn} + \alpha_{mp;(u+1)}^{(i)} \overline{\sigma}_{pn} \right) \qquad (3.26)$$

and

$$a_{mn;u} = 1 \quad \text{and} \quad b_{mn;u} = 0 \quad \text{if} \quad C_{mn;u}^{(0)} = 0,$$

$$a_{mn;u} = 0 \quad \text{and} \quad b_{mn;u} = 1 \quad \text{if} \quad C_{mn;u}^{(0)} \neq 0.$$

For the problem at hand, there are two sets of levels for the (mn) pairs: the conduction bands (cc') and the valence bands (vv'). As bands of the same kind (conduction or valence) are supposed to be close to each other

$$C_{cc';0}^{(0)} = 0 \quad \text{and} \quad C_{cc';-1}^{(0)} = 0, \qquad (3.27a)$$

and as in this problem only one-photon processes are considered

$$C_{cv;1}^{(0)} = 0 \quad \text{and} \quad C_{vc;-1}^{(0)} = 0. \qquad (3.27b)$$

The rest of the $C_{mn;u}^{(0)}$ are nonzero; therefore,

$$\alpha_{cv;1}^{(0)}, \quad \alpha_{vc;-1}^{(0)}, \quad \alpha_{cc';0}^{(0)}, \quad \text{and} \quad \alpha_{vv';0}^{(0)} \neq 0. \qquad (3.27c)$$

Collecting terms from Equation 3.24 and dropping the superscript (0)

$$i\frac{\partial \alpha_{cv;1}}{\partial \tau} = C_{cv;1}^{(1)} \alpha_{vc;1} - \sum_{v'} \sigma_{cv'} \alpha_{v'v;0} + \sum_{c'} \alpha_{cc';0} \sigma_{c'v}, \qquad (3.28a)$$

$$i\frac{\partial \alpha_{vc;-1}}{\partial \tau} = C_{vc;-1}^{(1)} \alpha_{vc;-1} - \sum_{c'} \overline{\sigma}_{vc'} \alpha_{c'c;0} + \sum_{v'} \alpha_{vv';0} \overline{\sigma}_{v'c}, \qquad (3.28b)$$

$$i\frac{\partial \alpha_{cc';0}}{\partial \tau} = C_{cc';0}^{(1)} \alpha_{cc';0} - \sum_{v} \left(\sigma_{cv} \alpha_{vc';-1} - \alpha_{cv;1} \overline{\sigma}_{vc'} \right), \qquad (3.28c)$$

$$i\frac{\partial \alpha_{vv';0}}{\partial \tau} = C_{vv';0}^{(1)} \alpha_{vv';0} - \sum_{c} \left(\overline{\sigma}_{vc} \alpha_{cv';1} - \alpha_{vc;-1} \sigma_{cv'} \right). \qquad (3.28d)$$

These equations are said to derive full excitation and saturation of the upper levels.

3.3.1 *Perturbative Solution*

Equations 3.28 can be solved by a perturbative approach. For instance, by setting

$$\alpha_{vv';0} \approx \delta_{vv'}, \qquad (3.29)$$

throughout the time integration of Equation 3.28d and solving approximately Equations (3.28a), (3.28b), and (3.28c) for $\alpha_{cv;1}$, $\alpha_{vc;-1}$, and $\alpha_{cc';0}$. Such a process gives

$$i\frac{\partial \alpha_{cv;1}}{\partial \tau} \approx C_{cv;1}^{(1)}\alpha_{vc;1} - \sigma_{cv} \qquad \text{and} \tag{3.30}$$

$$i\frac{\partial \alpha_{vc;-1}}{\partial \tau} \approx C_{vc;-1}^{(1)}\alpha_{vc;-1} + \overline{\sigma}_{vc}. \tag{3.31}$$

The last equation has the form

$$\frac{dy}{dx} + p(x)y = q(x), \tag{3.32}$$

which is a linear equation whose solution can be obtained by the application of an integrating factor μ, as follows

$$y = \mu^{-1}(x)\int dx'\mu(x')q(x') + c, \quad \text{with} \quad \mu(x) = e^{\int dx'p(x')}. \tag{3.33}$$

Now, assuming that τ is much longer than the damping and dephasing times and that $\boldsymbol{E}_{\text{env}}$ is nearly constant, one gets

$$\begin{aligned}
\alpha_{cv;1} &= e^{-iC_{cv;1}^{(1)}\tau}\int_0^\tau d\tau'\,[i\sigma_{cv}(\tau')]\,e^{iC_{cv;1}^{(1)}\tau'} \\
&\approx \frac{\sigma_{cv}}{C_{cv;1}^{(1)}}(1 - e^{-iC_{cv;1}^{(1)}\tau}) \\
&\approx \frac{\sigma_{cv}}{C_{cv;1}^{(1)}} \quad \text{for} \quad \tau \gg 1.
\end{aligned} \tag{3.34}$$

Similarly

$$\alpha_{vc;-1} \approx -\frac{\overline{\sigma}_{vc}}{C_{vc;-1}^{(1)}} \quad \text{for} \quad \tau \gg 1. \tag{3.35}$$

Substituting Equation 3.34 and Equation 3.35 into Equation 3.28c one gets

$$\frac{\partial \alpha_{cc';0}}{\partial \tau} = -iC_{cc';0}^{(1)}\alpha_{cc';0} + \frac{1}{i}\sum_v \left(\frac{\sigma_{cv}\overline{\sigma}_{vc'}}{C_{vc';-1}^{(1)}} + \frac{\sigma_{cv}\overline{\sigma}_{vc'}}{C_{cv;1}^{(1)}}\right), \tag{3.36}$$

where

$$C_{cv;1}^{(1)} = -\frac{1}{\eta\omega}(\omega - \omega_{cv} + i\gamma_{cv}) \qquad \text{and} \tag{3.37a}$$

$$C_{vc';-1}^{(1)} = \frac{1}{\eta\omega}(\omega - \omega_{c'v} - i\gamma_{vc'}). \tag{3.37b}$$

The time dependence can be inserted back with the substitution

$$\frac{\partial}{\partial \tau_1} \rightarrow \frac{1}{\eta\omega}\frac{\partial}{\partial t}, \tag{3.38}$$

and the variable of interest, the density matrix, is placed instead of α,

$$\alpha_{cc';0} \to \rho_{cc'}, \tag{3.39}$$

and the loss and dephasing implied in γ are expressed clearly as being small by writing γ as a small number ϵ,

$$\gamma \to \epsilon. \tag{3.40}$$

All these considerations give

$$
\begin{aligned}
\frac{\partial \rho_{cc'}}{\partial t} &= -i\left(\omega_{cc'} - i\epsilon\right)\rho_{cc'} - \frac{e^2 E^a(\omega) E^{b\star}(\omega)}{i\hbar^2} \\
&\quad \times \sum_v r^a_{cv} r^b_{vc'} \left(\frac{1}{\omega - \omega_{c'v} - i\epsilon} - \frac{1}{\omega - \omega_{cv} + i\epsilon}\right).
\end{aligned} \tag{3.41}
$$

It remains to solve Equation 3.42 for $\rho_{cc'}$.

$$
\begin{aligned}
\frac{\partial \rho_{cc'}}{\partial t} &= -i\left(\omega_{cc'} - i\epsilon\right)\rho_{cc'} + \frac{e^2 E^a(\omega) E^{b\star}(\omega)}{i\hbar^2} \\
&\quad \times \sum_v r^a_{cv} r^b_{vc'} \left(\frac{1}{\omega - \omega_{c'v} - i\epsilon} - \frac{1}{\omega - \omega_{cv} + i\epsilon}\right).
\end{aligned} \tag{3.42}
$$

In order to proceed further, we take $\epsilon \to 0$ in the first term, and then we change the density matrix operator to the so called *interaction representation*, which requires the following replacement

$$\widehat{\rho} \longrightarrow \widetilde{\widehat{\rho}} = e^{iH_0 t/\hbar}\,\widehat{\rho}\,e^{-iH_0 t/\hbar}, \tag{3.43}$$

with H_0 the ground state Hamiltonian. The matrix elements are now,

$$
\begin{aligned}
\langle c\mathbf{k}|\,\widetilde{\widehat{\rho}}\,|c'\mathbf{k}\rangle &= \langle c\mathbf{k}|\,e^{iH_0 t/\hbar}\widehat{\rho}e^{-iH_0 t/\hbar}\,|c'\mathbf{k}\rangle \\
&= e^{i\omega_c t}\langle c\mathbf{k}|\,\widehat{\rho}\,|c'\mathbf{k}\rangle\,e^{-i\omega_{c'} t} \\
\widetilde{\rho}_{cc'}(\mathbf{k}) &= e^{i\omega_{cc'} t}\rho_{cc'}(\mathbf{k}),
\end{aligned} \tag{3.44}
$$

where we used $H_0|n\mathbf{k}\rangle = \hbar\omega_n(\mathbf{k})|n\mathbf{k}\rangle$ with $\hbar\omega_n(\mathbf{k})$ the energy of the electronic band n at point $\mathbf{k}$, and $|n\mathbf{k}\rangle$ the Bloch state. The reciprocal lattice vector $\mathbf{k}$ is restricted to the irreducible part of the first Brillouin zone. From Eq. (3.44) the time derivative of $\widetilde{\rho}_{cc'}(\mathbf{k})$ is given by

$$
\begin{aligned}
\frac{d\widetilde{\rho}_{cc'}(\mathbf{k})}{dt} &= \left(i\omega_{cc'}\rho_{cc'}(\mathbf{k}) + \frac{\partial \rho_{cc'}(\mathbf{k})}{\partial t}\right)e^{i\omega_{cc'} t} \\
&= \frac{e^2 E^a(\omega) E^{b\star}(\omega)}{i\hbar^2}e^{i\omega_{cc'} t} \\
&\quad \times \sum_v r^a_{cv} r^b_{vc'} \left(\frac{1}{\omega - \omega_{c'v} - i\epsilon} - \frac{1}{\omega - \omega_{cv} + i\epsilon}\right),
\end{aligned} \tag{3.45}
$$

where we used Eq. (3.42), and the $\epsilon \to 0$ still needs to be taken.

Within the density matrix formalism, the expectation value of an observable $\mathcal{O}$ is given by

$$\mathcal{O} = \text{Tr}(\widehat{\rho}\widehat{\mathcal{O}}), \tag{3.46}$$

where Tr denotes the trace, given by the sum over the diagonal matrix elements, and $\widehat{\mathcal{O}}$ is the quantum mechanical operator associated to the observable $\mathcal{O}$. Then,

$$
\begin{aligned}
\mathcal{O} &= \int \frac{d^3k}{8\pi^3} \sum_c \langle c\mathbf{k}|\widehat{\rho}\widehat{\mathcal{O}})|c\mathbf{k}\rangle = \int \frac{d^3k}{8\pi^3} \sum_{cc'} \langle c\mathbf{k}|\widehat{\rho}|c'\mathbf{k}\rangle\langle c'\mathbf{k}|\widehat{\mathcal{O}})|c\mathbf{k}\rangle \\
&= \int \frac{d^3k}{8\pi^3} \sum_{cc'} \rho_{cc'}(\mathbf{k})\mathcal{O}_{c'c}(\mathbf{k}),
\end{aligned}
\tag{3.47}
$$

where we used the closure relationship $\sum_c |c\mathbf{k}\rangle\langle c\mathbf{k}| = 1$. In the interaction picture, $\widetilde{\mathcal{O}}_{c'c} = \langle c'\mathbf{k}|\, e^{iH_0 t/\hbar}\, \widehat{\mathcal{O}}\, e^{-iH_0 t/\hbar}\, |c\mathbf{k}\rangle = \mathcal{O}_{c'c} e^{-i\omega_{cc'} t}$ and thus we can also write

$$\mathcal{O} = \int \frac{d^3k}{8\pi^3} \sum_{cc'} \widetilde{\rho}_{cc'}(\mathbf{k})\widetilde{\mathcal{O}}_{c'c}(\mathbf{k}), \tag{3.48}$$

and so, we can calculate the expectation value using $\widehat{\rho}$ and $\widehat{\mathcal{O}}$ in either the standard Schrödinger representation or the interaction representation. From the previous equation, the rate of change of $\mathcal{O}$ is given by

$$
\begin{aligned}
\frac{d\mathcal{O}}{dt} &= \int \frac{d^3k}{8\pi^3} \sum_{cc'} \frac{d\widetilde{\rho}_{cc'}(\mathbf{k})}{dt} \widetilde{\mathcal{O}}_{c'c}(\mathbf{k}) \\
&= \frac{e^2}{i\hbar^2} \int \frac{d^3k}{8\pi^3} \sum_{vcc'} \widehat{\mathcal{O}}_{c'c} r^a_{cv} r^b_{vc'} \left(\frac{1}{\omega - \omega_{c'v} - i\epsilon} - \frac{1}{\omega - \omega_{cv} + i\epsilon} \right) \\
&\quad E^a(\omega)E^{b\star}(\omega),
\end{aligned}
\tag{3.49}
$$

where we used Eq. (3.45), and we notice that the $e^{i\omega_{cc'} t}$ and $e^{-i\omega_{cc'} t}$ factor cancel each other.

3.4 DEGREE OF SPIN POLARIZATION

can be used to compute the *spin-injection rate* $\dot{\mathcal{S}} \equiv d\mathcal{S}/dt$ with

$$\widehat{\mathcal{O}} \to \widehat{\mathcal{S}}^a = \frac{\hbar}{2}\widehat{\sigma}^a \tag{3.50}$$

where $\widehat{\sigma}^a$ are the Pauli Matrices

$$\widehat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \widehat{\sigma}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \widehat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.51}$$

that are operators in spinor space, therefore,

$$\frac{d}{dt}\mathcal{S}^a = \frac{e^2}{i\hbar^2}\int\frac{d^3k}{8\pi^3}\sum_{vcc'}\hat{\mathcal{S}}^a_{c'c}r^b_{cv}r^c_{vc'}$$

$$\left(\frac{1}{\omega-\omega_{c'v}-i\epsilon} - \frac{1}{\omega-\omega_{cv}+i\epsilon}\right)$$

$$E^b(\omega)E^{c\star}(\omega). \tag{3.52}$$

Using the so called time-reversal invariance, as described by Lax on Ref. [25] and Najmaie et al. on Ref. [8], by which

$$\omega_m(-\mathbf{k}) = \omega(\mathbf{k}), \tag{3.53a}$$

$$r^a_{mn}(-\mathbf{k}) = r^a_{nm}(\mathbf{k}), \quad \text{and} \tag{3.53b}$$

$$\mathcal{S}^a_{mn}(-\mathbf{k}) = -\mathcal{S}^a_{nm}(\mathbf{k}), \tag{3.53c}$$

we can add the $\mathbf{k}$ and $-\mathbf{k}$ contributions to the integral in Eq. (3.54) to obtain

$$\frac{d\mathcal{S}^a}{dt} = \frac{e^2}{i\hbar^2}\int_{\mathbf{k}>0}\frac{d^3k}{8\pi^3}\sum_{vcc'}\left[\left(\mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'}\right)\Big|_{\mathbf{k}} + \left(\mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'}\right)\Big|_{-\mathbf{k}}\right]$$

$$\times\left(\frac{1}{\omega-\omega_{c'v}-i\epsilon} - \frac{1}{\omega-\omega_{cv}+i\epsilon}\right)E^b E^{c\star}$$

$$= \frac{e^2}{i\hbar^2}\int_{\mathbf{k}>0}\frac{d^3k}{8\pi^3}\sum_{vcc'}\left[\left(\mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'}\right)\Big|_{\mathbf{k}} - \left(\hat{\mathcal{S}}^a_{cc'}r^b_{vc}r^c_{c'v}\right)\Big|_{\mathbf{k}}\right]$$

$$\times\left(\frac{1}{\omega-\omega_{c'v}-i\epsilon} - \frac{1}{\omega-\omega_{cv}+i\epsilon}\right)E^b E^{c\star}$$

$$= \frac{e^2}{i\hbar^2}\frac{1}{2}\int\frac{d^3k}{8\pi^3}\sum_{vcc'}\left[\left(\mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'}\right) - \left(\hat{\mathcal{S}}^a_{c'c}r^b_{cv}r^c_{vc'}\right)^\star\right]$$

$$\times\left(\frac{1}{\omega-\omega_{c'v}-i\epsilon} - \frac{1}{\omega-\omega_{cv}+i\epsilon}\right)E^b E^{c\star}$$

$$= \frac{e^2}{\hbar^2}\int\frac{d^3k}{8\pi^3}\sum_{vcc'}\operatorname{Im}\left[\mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'}\right]$$

$$\times\left(\frac{1}{\omega-\omega_{c'v}-i\epsilon} - \frac{1}{\omega-\omega_{cv}+i\epsilon}\right)E^b E^{c\star}, \tag{3.54}$$

where in going from the second to the third equal sign, we use the fact that for any Hermitian operator $\mathcal{O}_{mn}(\mathbf{k}) = \mathcal{O}^*_{nm}(\mathbf{k})$, and that the one half comes from the unrestricted integration over all values of $\mathbf{k}$ and not only $\mathbf{k} > 0$. Aided by the identity

$$\lim_{\epsilon\to0}\frac{1}{\omega-\omega_{cv}-i\epsilon} = \mathcal{P}\left(\omega-\omega_{cv}\right) + i\pi\,\delta\left(\omega-\omega_{cv}\right), \tag{3.55}$$

where $\mathcal{P}$ means the *principal part*, Eq. (3.54) can be written as

$$
\begin{aligned}
\frac{d\mathcal{S}^a}{dt} &= \frac{e^2}{\hbar^2} \int \frac{d^3k}{8\pi^3} \sum_{vcc'} \mathrm{Im}\left[\mathcal{S}^a_{c'c} r^b_{cv} r^c_{vc'}\right] \left\{ \mathcal{P}\left(\frac{1}{\omega - \omega_{c'v}} - \frac{1}{\omega - \omega_{cv}}\right) \right. \\
&\quad \left. + i\pi\left[\delta(\omega - \omega_{c'v}) + \delta(\omega - \omega_{cv})\right] \right\} E^b E^{c\star} \\
&= \frac{e^2}{\hbar^2} \int \frac{d^3k}{8\pi^3} \sum_{vcc'} \mathrm{Im}\left[\mathcal{S}^a_{c'c} r^b_{cv} r^c_{vc'}\right] \left\{ \mathcal{P}\left(\frac{\omega_{c'c}}{(\omega - \omega_{c'v})(\omega - \omega_{cv})}\right) \right. \\
&\quad \left. + i\pi\left[\delta(\omega - \omega_{c'v}) + \delta(\omega - \omega_{cv})\right] \right\} E^b E^{c\star}
\end{aligned}
$$

$$
\begin{aligned}
\frac{d\mathcal{S}^a}{dt} &\simeq \frac{i\pi e^2}{\hbar^2} \int \frac{d^3k}{8\pi^3} \sum_{vcc'}{}' \mathrm{Im}\left(\mathcal{S}^a_{c'c} r^b_{cv} r^c_{vc'}\right) \\
&\quad \left[\delta(\omega - \omega_{c'v}) + \delta(\omega - \omega_{cv})\right] E^b E^{c\star},
\end{aligned}
\tag{3.56}
$$

since the term that goes with the principal part is of the order of $\omega_{cc'}$ which is very small as the states c and c' are quasi degenerate. Indeed, the primed sigma symbol $\sum'$ means that the sum is to be performed on pairs cc' of quasi-degenerate conduction bands. It seems that in Equation 3.63 there are two resonant frequencies, one at $\omega = \omega_{cv}(\mathbf{k})$ and other at $\omega = \omega_{c'v}(\mathbf{k})$, but actually there is only one. This can be shown if one changes $c \rightleftharpoons c'$ in the second δ function, then

$$
\begin{aligned}
\frac{d\mathcal{S}^a}{dt} &= \frac{i\pi e^2}{\hbar^2} \int \frac{d^3k}{8\pi^3} \sum_{vcc'}{}' \left(\mathrm{Im}\left[\mathcal{S}^a_{c'c} r^b_{cv} r^c_{vc'}\right] + \mathrm{Im}\left[\mathcal{S}^a_{cc'} r^b_{c'v} r^c_{vc}\right]\right) \\
&\quad \delta(\omega - \omega_{cv}) E^b E^{c\star},
\end{aligned}
\tag{3.57}
$$

where it is clear that the only resonant frequency is at $\omega = \omega_{cv}(\mathbf{k})$. Moreover, the coherence of the $v \to c$ and $v \to c'$ processes is given by the addition of the two imaginary $\mathrm{Im}()$ terms that are proportional to the probability of such transitions. Compactly time rate of $\mathcal{S}^a$ is written as,

$$
\frac{d\mathcal{S}^a}{dt} = \tilde{\zeta}^{abc} E^b(\omega) E^{c\star}(\omega),
\tag{3.58}
$$

where

$$
\begin{aligned}
\tilde{\zeta}^{abc} &= \frac{i\pi e^2}{\hbar^2} \int \frac{d^3k}{8\pi^3} \sum_{vcc'}{}' \left(\mathrm{Im}\left[\mathcal{S}^a_{c'c} r^b_{cv} r^c_{vc'}\right] + \mathrm{Im}\left[\mathcal{S}^a_{cc'} r^b_{c'v} r^c_{vc}\right]\right) \\
&\quad \delta(\omega - \omega_{cv}),
\end{aligned}
\tag{3.59}
$$

is denoted as the *spin-injection 3th rank pseudo-tensor component* [2], which, in the argot of nonlinear optics, plays a similar role than the 2th order

---

[2] In simple terms, a pseudo-tensor is an object that transforms like a tensor under a proper rotation, but changes sign under an improper rotation. That is, a pseudo-tensor is a transformation that can be expressed as an inversion followed by a proper rotation.

susceptibility χ^{abc}. We see that ζ^{abc} is purely imaginary and that $\zeta^{abc} = -\zeta^{acb}$, since

$$
\begin{aligned}
2i&\left(\text{Im}\left[\mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'}\right] + \text{Im}\left[\mathcal{S}^a_{cc'}r^b_{c'v}r^c_{vc}\right]\right)\\
&= \mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'} - \left(\mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'}\right)^*\\
&\quad + \mathcal{S}^a_{cc'}r^b_{c'v}r^c_{vc} - \left(\mathcal{S}^a_{cc'}r^b_{c'v}r^c_{vc}\right)^*\\
&= \mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'} - \mathcal{S}^a_{cc'}r^b_{vc}r^c_{c'v} + \mathcal{S}^a_{cc'}r^b_{c'v}r^c_{vc} - \mathcal{S}^a_{c'c}r^b_{vc'}r^c_{cv}\\
&= -\mathcal{S}^a_{cc'}r^b_{vc}r^c_{c'v} + \mathcal{S}^a_{cc'}r^b_{c'v}r^c_{vc} - \mathcal{S}^a_{c'c}r^b_{vc'}r^c_{cv} + \mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'}\\
&= -2i\left(\text{Im}\left[\mathcal{S}^a_{cc'}r^b_{vc}r^c_{c'v}\right] + \text{Im}\left[\mathcal{S}^a_{c'c}r^b_{vc'}r^c_{cv}\right]\right)\\
&= -2i\left(\text{Im}\left[\mathcal{S}^a_{c'c}r^c_{cv}r^b_{vc'}\right] + \text{Im}\left[\mathcal{S}^a_{cc'}r^c_{c'v}r^b_{vc}\right]\right).
\end{aligned}
\tag{3.60}
$$

Now, from Equation 3.70 we have that

$$
\begin{aligned}
\frac{d\mathcal{S}^a}{dt} &= \widetilde{\zeta}^{abc}E^bE^{c*} + \widetilde{\zeta}^{acb}E^cE^{b*} &&\text{no sum over} b \neq c\\
&= \widetilde{\zeta}^{abc}E^bE^{c*} - \widetilde{\zeta}^{abc}E^cE^{b*} &&\text{no sum over} b \neq c\\
&= \widetilde{\zeta}^{abc}\left(E^bE^{c*} - E^cE^{b*}\right) &&\text{no sum over} b \neq c\\
&= -2i\widetilde{\zeta}^{abc}\,\text{Im}\left[E^{b*}E^c\right] &&\text{no sum over} b \neq c.
\end{aligned}
\tag{3.61}
$$

Writing $\widetilde{\zeta}^{abc} = i\zeta^{abc}$, we finally obtain, as we must,

$$
\frac{d\mathcal{S}^a}{dt} = 2\zeta^{abc}\text{Im}[E^{b*}E^c],
\tag{3.62}
$$

as a real quantity, with

$$
\begin{aligned}
\zeta^{abc} &= \frac{\pi e^2}{\hbar^2}\int\frac{d^3k}{8\pi^3}\sum_{vcc'}{}'\left(\text{Im}\left[\mathcal{S}^a_{c'c}r^b_{cv}r^c_{vc'}\right] + \text{Im}\left[\mathcal{S}^a_{cc'}r^b_{c'v}r^c_{vc}\right]\right)\\
&\quad \delta(\omega - \omega_{cv}),
\end{aligned}
\tag{3.63}
$$

For the purposes of this work, bands that are separated from each other by less than 30 meV are considered as quasi-degenerate, which is approximately both the laser pulse energy and the room temperature energy (see Figure 1).

3.5   DEGREE OF SPIN POLARIZATION

Equation 3.42 can be used to compute the *spin-injection rate* $\dot{\mathcal{S}} \equiv d\mathcal{S}/dt$ with

$$
\dot{\mathcal{S}} = \text{Tr}\left(\dot{\rho}\,\widehat{\mathcal{S}}\right) \quad \text{or} \quad \dot{\mathcal{S}}^a = \text{Tr}\left(\dot{\rho}\,\widehat{\mathcal{S}}^a\right),
\tag{3.64}
$$

where

$$\widehat{\mathcal{S}} = \frac{\hbar}{2}\boldsymbol{\sigma} \quad \text{or} \quad \widehat{\mathcal{S}}^a = \frac{\hbar}{2}\sigma^a \tag{3.65}$$

and σ^a are the Pauli Matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.66}$$

Aided by the identity

$$\frac{1}{\omega - \omega_{cv} - i\epsilon} = \mathcal{P}\left(\omega - \omega_{cv}\right) + i\pi\,\delta\left(\omega - \omega_{cv}\right), \tag{3.67}$$

where $\mathcal{P}$ means the *principal part*, the spin injection rate can be found combining the preceding equations, giving

$$\begin{aligned} \frac{d}{dt}\mathcal{S}^a &= \frac{\pi e^2}{\hbar^2}\Big\{ \sum_{cc'v}{}' \int \frac{d^3 k}{8\pi^3} \mathcal{S}^a_{c'c}(\mathbf{k})\, r^b_{vc'}(\mathbf{k})\, r^c_{cv}(\mathbf{k}) \\ &\quad \left[\delta\left(\omega_{cv}(\mathbf{k}) - \omega\right) + \delta\left(\omega_{c'v}(\mathbf{k}) - \omega\right)\right] \Big\} \\ &\quad E^b(-\omega)\, E^c(\omega). \end{aligned} \tag{3.68}$$

The primed sigma symbol $\sum'$ means that the sum is to be performed on pairs cc' of quasi-degenerate conduction bands. It seems that in Equation 3.68 there are two resonant frequencies, one at $\omega = \omega_{cv}(\mathbf{k})$ and other at $\omega = \omega_{c'v}(\mathbf{k})$, but actually there is only one. This can be shown if one changes $c \rightleftharpoons c'$ in the second δ function, then

$$\begin{aligned} \frac{d}{dt}\mathcal{S}^a &= \frac{\pi e^2}{\hbar^2}\Big\{ \sum_{cc'v\mathbf{k}} \left[\mathcal{S}^a_{cc'}(\mathbf{k})r^b_{cv}(\mathbf{k})r^c_{vc'}(\mathbf{k}) + \mathcal{S}^a_{c'c}(\mathbf{k})r^b_{c'v}(\mathbf{k})r^c_{vc}(\mathbf{k})\right] \\ &\quad \delta(\omega - \omega_{cv}(\mathbf{k})) \Big\}\, E^b(-\omega)\, E^c(\omega), \end{aligned} \tag{3.69}$$

where it is clear that the only resonant frequency is at $\omega = \omega_{cv}(\mathbf{k})$. The $(-\omega)$ argument refers to the complex conjugate of the field in the frequency domain. The term in curly braces is a 3th rank pseudo-tensor[3], and is denoted as the *spin-injection pseudo-tensor component* ζ^{abc}, which, in the argot of nonlinear optics, plays a similar role than the 2th order susceptibility χ^{abc}. Compactly $\dot{\mathbf{S}}$ is written as,

$$\frac{d}{dt}\mathcal{S}^a = \zeta^{abc}E^b(-\omega)\, E^c(\omega) \tag{3.70}$$

$$\zeta^{abc}(\omega) = \frac{\pi e^2}{\hbar^2} \sum_{cc'v\mathbf{k}} \left[\mathcal{S}^a_{cc'}(\mathbf{k})r^b_{cv}(\mathbf{k})r^c_{vc'}(\mathbf{k}) + \mathcal{S}^a_{c'c}(\mathbf{k})r^b_{c'v}(\mathbf{k})r^c_{vc}(\mathbf{k})\right] \\ \delta(\omega - \omega_{cv}(\mathbf{k})). \tag{3.71}$$

---

3 In simple terms, a pseudo-tensor is an object that transforms like a tensor under a proper rotation, but changes sign under an improper rotation. That is, a pseudo-tensor is a transformation that can be expressed as an inversion followed by a proper rotation.

For the purposes of this work, bands that are separated from each other by less than 30 meV are considered as quasi-degenerate, which is approximately both the laser pulse energy and the room temperature energy (see Figure 1).

The *spin injection rate* $\dot{S}$ and *spin-injection pseudo-tensor component* ζ^{abc} describe the *total* spin injected to the conduction band. Albeit by themselves, they don't describe clearly if large values of them correspond to the injection of few electrons with high alignment to the beam direction, or just many electrons poorly spin polarized. For this reason it is necessary to describe the spin polarization as an average of the electron spin, i.e., as the rate of the spin injection rate $\dot{S}$ respect to the [total] *carrier injection rate* $\dot{n}$, i.e.

$$\text{DSP}^a = \frac{2}{\hbar} \frac{\dot{S}^a}{\dot{n}} \tag{3.72}$$

The DSP is measured along the light propagation vector, specified by the Roman superscript a. Either a multiple scale analysis or a Fermi Golden Rule derivation gives for the carrier injection rate, $\dot{n} \equiv dn/dt$,

$$
\begin{aligned}
\dot{n} &= \frac{2\pi e^2}{\hbar^2} \int \sum_{cv} \frac{d^3k}{8\pi^3}\, r_{vc}^a(\mathbf{k})\, r_{cv}^b(\mathbf{k})\, \delta[\omega_{cv}(\mathbf{k}) - \omega] \\
&\quad \times E^a(-\omega)\, E^b(\omega)
\end{aligned} \tag{3.73}
$$

where the same connotation as in Equation 3.70 applies for the $(-\omega)$ argument. The term in curly braces is identified as the *carrier-injection tensor component* ξ^{ab}, that is,

$$\dot{n} = \xi^{ab}\, E^a(-\omega)\, E^b(\omega) \tag{3.74}$$

$$\xi^{ab} = \frac{2\pi e^2}{\hbar^2} \int \sum_{cv} \frac{d^3k}{8\pi^3}\, r_{vc}^a(\mathbf{k})\, r_{cv}^b(\mathbf{k})\, \delta[\omega_{cv}(\mathbf{k}) - \omega]. \tag{3.75}$$

In brief

Equations (3.70) to (3.75) represent the main results of this chapter. In Part II, Chapter 4, they are evaluated to compute the DSP of two bulk semiconductors, gallium arsenide and silicon, firstly under normal conditions, and then for the cases that compressive and expansive stress are applied. It is shown that DSP can be enhanced by the application of stress.

STRESS MODULATION OF DSP ON BULK SEMICONDUCTORS

4.1 OBJECTIVES

As pointed out in Chapter 1, Section 1.6, the aim of this thesis is to show that the Degree of Spin Polarization (DSP) in bulk semiconductors can be modulated, and even enhanced, by the application of compressive or expansive stress.

4.2 COMPUTATIONAL APPROACH

In Chapter 3 it was shown that the DSP in a cold and clean bulk semiconductor[1] is described by

$$\text{DSP}^a \quad = \quad \frac{2}{\hbar} \frac{\dot{S}^a}{\dot{n}}, \tag{4.1a}$$

$$\dot{S}^a \quad = \quad \zeta^{abc}(\omega)\, E^b(-\omega)\, E^c(\omega), \tag{4.1b}$$

$$\dot{n} \quad = \quad \xi^{ab}\, E^a(-\omega)\, E^b(\omega), \tag{4.1c}$$

$$\zeta^{abc}(\omega) \quad = \quad \frac{\pi e^2}{\hbar^2} \sum_{cc'vk} \left[S^a_{cc'}(\mathbf{k}) r^b_{cv}(\mathbf{k}) r^c_{vc'}(\mathbf{k}) + S^a_{c'c}(\mathbf{k}) r^b_{c'v}(\mathbf{k}) r^c_{vc}(\mathbf{k}) \right]$$
$$\delta(\omega - \omega_{cv}(\mathbf{k})), \tag{4.1d}$$

$$\xi^{ab} \quad = \quad \frac{2\pi e^2}{\hbar^2} \int \sum_{cv} \frac{d^3k}{8\pi^3}\, r^a_{vc}(\mathbf{k})\, r^b_{cv}(\mathbf{k})\, \delta[\omega_{cv}(\mathbf{k}) - \omega]. \tag{4.1e}$$

$$\omega_{mn} \quad \equiv \quad \omega_c(\mathbf{k}) - \omega_v(\mathbf{k}). \tag{4.1f}$$

As mentioned on Section 3.5, the DSP is measured along the light propagation vector, specified by the Roman superscript z. The frequencies of interest for the present work are optical frequencies, i.e. those in the energy range $\hbar\omega$ from 0.5 to 4.5 eV (ν in 120–1,090 THz). The first thing to do to evaluate expressions (4.1) is to obtain the position and spin matrix elements, $r^a_{cv}(\mathbf{k})$ and $S^a_{mn}(\mathbf{k})$ respectively,

$$S^a_{cm}(\mathbf{k})\, \delta(\mathbf{k} - \mathbf{k}') \quad = \quad \langle c\mathbf{k} | \hat{S}^a | m\mathbf{k}' \rangle, \tag{4.2a}$$

$$r^a_{cv}(\mathbf{k}) \quad = \quad \frac{v^a_{cv}(\mathbf{k})}{i\,\omega_{cv}(\mathbf{k})}, \tag{4.2b}$$

$$v^a_{cv}(\mathbf{k})\, \delta(\mathbf{k} - \mathbf{k}') \quad = \quad \langle c\mathbf{k} | \hat{v}^a | v\mathbf{k}' \rangle. \tag{4.2c}$$

---

1 A cold semiconductor has all its electrons in the valence band.

4.2.1   *First-principles band structure computation*

The computation of the band structure from first-principles is used to evaluate the set of equations 4.1. In general, first-principles band structure computations enable to find the total energy of a system as a function of atomic positions only. Specifically it was employed the density-functional theory (DFT) within the local density approximation (LDA) as well as pseudo-potentials.

The density-functional theory

DFT

The DFT, attributed to Hohenberg and Kohn (1964) (Ref. [26]), is a strict formulation of the general many-body problem in which the basic idea is that the dependence on the external potential $V(r)$ is replaced by a dependence on the density distribution of charge $n(r)$. The key idea behind the DFT is that *the total energy of a system*

- is a *unique* functional of the density-charge $n(r)$, and that

- the functional is minimal for the correct density.

DFT *requires two approximations*

Nevertheless, the direct application of DFT requires to approximate both the kinetic and the exchange-correlation energies, giving poor agreement with experiments.

KINETIC ENERGY APPROXIMATION: A year later, in 1965, Kohn and Sham (Ref. [27]), instead of approximating the contribution of the kinetic energy, proposed to introduce a conceptual auxiliary non-interacting system that reproduces the charge density of the interacting system. There, the ground state of the non-interacting system is given by a set of Schrödinger-like equations, the Kohn-Sham equations, that are to be solved self-consistently.

Non-interacting system

Kohn-Sham equations

Concept of Self-consistency

The self-consistent field method (SCF) (see the review by Blinder on Ref. [28]) has its origins in the Hartre-Fock model of the atom. SCF method implies to solve a set of equations, one equation for each particle (the electrons, in this thesis), taking into account the influence of all other $N-1$ particles, by means of a *mean-field* that represents such $N-1$ particles. The equations are solved numerically, generally by iterative fixed-point algorithms (see the review by Payne et al. on Ref. [29]).

EXCHANGE-CORRELATION APPROXIMATION: The remaining approximation, that to the energy from the exchange-correlation interactions between electrons, is done via *exchange-correlation functionals*. A number of such functionals exists, but the one employed in this thesis is the *local-density approximation* (LDA). In this approximation, the contribution to the exchange-correlation energy from a

LDA

point in space r_i is taken as that from a uniform electron-gas at some appropriate density for that point in space r_i.

Further reading on DFT

The subject of first-principles computations is rich and complex. General references to the DFT include that of Jones and Gunnarsson on Ref. [23] and the succinct and short review by Argaman on Ref. [22]. An tiny but effective description of first-principles electronic structure calculations is given in Sec. III-V of Ref. [30] by A. Mujica et al. A general reference for electronic structure theory is the book by Martin, Ref. [31]. Actual numerical techniques are given by Payne et al. on Ref. [29]; also useful is the online tutorial of the ABINIT Software at www.abinit.org. A succinct review of the self-consistency field (SCF) method is given by Blinder on Ref. [28].

4.2.2 *Computational implementation: The Abinit Software*

The first-principles band structure computation is implemented with the aid of the *free* software ABINIT[2] developed by Gonze et al. (Ref. [32]). This program computes, from *ab-initio* principles, material properties such as the total energy, charge density, and electronic structure of systems made of electrons and nuclei, using pseudo-potentials and planewave basis within the DFT formalism, as well as excited states by the Time-Dependent-DFT or within Many-Body Perturbation Theory.

In this way, the DSP for a given semiconductor structure can be systematically computed, provided that one knows essential parameters of the material, like the unitary cell geometry, the number of atoms in the unitary cell, the primitive translation vectors defining the crystal, etc. Such values are fed to ABINIT to compute the spin and position matrix elements (Equation 4.2a and Equation 4.2b).

In the examples worked out in this thesis (see Section 5.2 and Section 5.3), the pseudopotential calculations were done as described by Nastos et al. on Ref. [1].The momentum matrix elements were calculated as described by Mendoza et al. on Ref. [2]. *This thesis*

Because LDA band structure computations underestimate the band gap of insulators (see Jones and Gunnarsson on Ref. [23]), a *scissors-correction* was applied. It consists of a rigidly upward shift in energy of all conduction bands by an amount that corrects the LDA estimation.

4.2.3 *Integration on the Brillouin Zone*

Once the position and spin matrix elements, $r_{cv}^a(\mathbf{k})$ and $S_{mn}^a(\mathbf{k})$, have been computed, the *spin-injection pseudo-tensor components* $\zeta^{abc}(\omega)$

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2 Visit www.abinit.org.

(Equation 4.1d) and the *carrier-injection tensor components* ξ^{ab} (Equation 4.1e) remain to be determined. To do so, one takes advantage of the fact that both equations have the form

$$G(\omega) = \sum_{cv} G_{cv}(\omega) \qquad (4.3)$$

with

$$G_{cv}(\omega) = \int \frac{d^3k}{8\pi^3} \, g_{cv}(\mathbf{k})\delta\left[\omega - \omega_{cv}(\mathbf{k})\right]. \qquad (4.4)$$

This sort of integral is known as *Joint-Density of States Integrals* (JDOS-
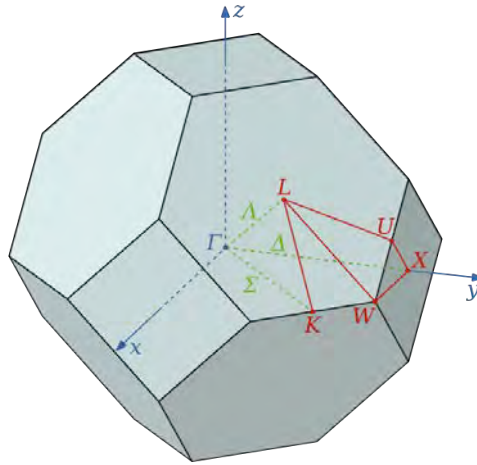
Figure 3: (color online) The first Brillouin Zone (BZ) is a uniquely defined primitive cell of the reciprocal lattice in the frequency domain. The image shows the high symmetry lines and points. The former definition and the image were taken from http://en.wikipedia.org; they are licensed to be used under the Gnu Public License.

JDOS Integrals

Integrals), where the δ function effectively reduces the 3-dimensional integral over the Brillouin Zone (BZ, see Figure 3) to a 2-dimensional integral on the surface given by

$$\omega_{cv}(\mathbf{k}) = \omega \qquad \text{(Integration Surface, within the BZ).} \qquad (4.5)$$

These JDOS-Integrals can be evaluated by simple sampling on $\mathbf{k}$, nevertheless, because of the usual complexity of both the crystal semiconductors and the constant-energy surface-integrals, is preferable to calculate them by the so-called linearized analytic tetrahedron method (LATM).

The LATM Integration Method

The evaluation of JDOS's by the LATM requires to perform the following steps (refer to Equation 4.3 and Equation 4.4):

1. Break up the BZ volume into tetrahedra (triangular pyramids having four plane triangular faces). This is called the tetrahedral grid.

2. Evaluate and store the integrand factor $g_{cv}(\mathbf{k})$ and the energy eigenvalues $\hbar\omega_m(\mathbf{k})$ at every tetrahedron vertex,

3. For each energy ω, identify inside each tetrahedron the constant-energy surface $\omega_{cv}(\mathbf{k}) = \omega$ (defined by the δ function). By the knowledge of the energy at each vertex (step 2), find by linear interpolation the energies within the tetrahedra.

4. Evaluate analytically the surface integral in Equation 4.4. Use linear interpolation of the integrand $g_{cv}(\mathbf{k})$ over the tetrahedron.

5. Finally, sum over the contributions of all tetrahedra to get $G_{cv}(\omega)$.

Linear Analytic Tetrahedral Method of Integration

People in Surface Optics Group at CIO, in collaboration with Nastos et al. (authors of Ref. [1]), have developed a FORTRAN subroutine to implement the LATM.

4.3 CONVERGENCE ANALYSIS

On band structure computations, apart from the model itself (DFT, GW[3], etc.), there are some parameters that must be properly set, to a minimum or a maximum, in order to obtain good concordance between the computed signals and the experimental evidence. To find out the most adequate value, one must run at least several calculations at various values of them till one obtains [almost] the same response. This is called convergence analysis.

Convergence Analysis

For the problem at hand in this thesis, there are three of those parameters that significantly influence the results. They three must be set to a *minimal* value to get converged results (if they are set to a higher value the results are *almost* exactly the same, but the computational time increases largely). They are[4]:

> NOTE: Words written in the typewriter font refer to variables or parameters in the computer programs, either ABINIT or TINIBA.

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3 GW calculations use a set of self-consistent equations for the one-electron Green's function to compute the self-energy of many-body systems. The approximation was first proposed by L. Hedin. See L. Hedin, Phys. Rev. 139, **A** 796 (1965).

4 See the ABINIT's documentation at www.abinit.org.

NUMBER OF *k*-POINTS (nkpt). The number of k−points (number of $\boldsymbol{k}$ vectors) influences on the sampling of the BZ (see Figure 3 on p.).

NUMBER OF CONDUCTION BANDS (cband). The number of conduction bands plus the number of valence bands, gives the total number of bands (nband), occupied or possibly unoccupied. For all them the wave-functions should be computed along with eigenvalues.

This thesis

The semiconductors studied on this thesis, silicon and gallium arsenide, have both four valence bands.

ENERGY CUTOFF (ecut). Is a real parameter used for the kinetic energy cutoff. It controls the number of plane-waves at a given k−point by:

$$\frac{1}{2} \left[2\pi |\boldsymbol{k} + \boldsymbol{G}_{\mathrm{max}}| \right]^2 = \mathrm{ecut} \tag{4.6}$$

1 Hartree is roughly 27.21 eV

All plane-waves inside this basis-sphere (centered at k) are included in the basis. This parameter has a huge effect on the quality of a calculation; basically the larger ecut, the better convergence of the calculation. The units of ecut are units of energy; in ABINIT it is typically given in Hartrees (Ha), the energy unit in the Atomic Unit System[5] (roughly 1 Ha $\approx$ 27.21 eV), but it can be given in other energy units.

4.4   STRESS-INDUCED VOLUMETRIC CHANGE

This thesis

As mentioned in Section 1.6 (page), the main objective of this thesis is to investigate the possibility for the modulation of the optical electron spin-injection on bulk semiconductors, by the application of stresses, either compressive or expansive.

4.4.1   *Experimental realization*

As pointed out in the review by A. Mujica et al. on Ref. [30] the techniques of high-pressure physics are highly developed. The employed devices mostly based on the diamond anvil cell (DAC), see Figure 4, which has the important characteristic that applies very static high-pressures well above 100 GPa. The basic idea behind it is the same of all high-pressure devices: the application of a force to a small surface.

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5 There are 'two' Atomic Unit Systems, one of them measures energy in Hartree units and the other in Rydberg units. In both of them, the numerical values of the following six physical constants are all unity by definition: the electron's mass and charge; the Hydrogen's Bohr radius and its absolute value of the electric potential energy in the ground state; the Planck's constant h, and Coulomb's constant k.

Figure 4: Schematic depiction of a diamond anvil cell (DAC), which is the basis of almost all high-pressure devices (the gasket is commonly a metallic foil). Because diamond is transparent on a wide energy range, DACs are adequate to study the sample via its radiation-matter properties (sketch reproduced from Ref. [30]).

In a DAC, the sample is placed between two diamonds, and the sample is normally immersed in a fluid contained in a *pressure chamber* into which the sample is placed. The chamber is normally filled with a fluid, in order to ensure quasi-hydrostatic and homogeneous conditions. Typical fluids in use are methanol-ethanol, silicon oils, N_2, Ar, and He. Special care must be taken because the fluid could undergo phase changes or produce complex diffraction patterns. To diminish this effects one can use cryogenic techniques.

The fact that diamond is transparent on frequencies that go from the near ultraviolet (~ 5.5 eV) to the infrared (~ 10 meV), including also a window at hard X-rays energy (>10 keV), makes this device so attractive for the use of radiation to study the sample under such high-pressures.

Expansion experiments are mostly based on thermal expansions.

4.4.2 *Range of volumetric change*

The application of large forces on a material can cause a *structural phase transition* in the material, that is, a sudden change in the arrangement of its atoms. Such phase transition can be caused by a continuous or discontinuous change; the important phenom is that a change in the crystal symmetry occurs. Moreover, the phase transition may be reversible or irreversible. Then a natural question arises: what are the adequate bounds of the volumetric compression (expansion) in order to avoid phase and structure changes?

At a first look to the bibliography of High Pressure Physics, I found out about Prof. Stefan Turneaure, from Washington State University.

phase transition

What is the range of acceptable volumetric change?
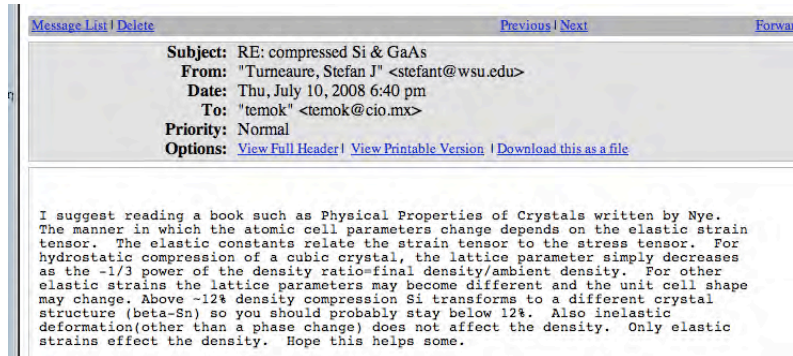
Figure 5: (color online) Prof. Turneaure's e-mail(Researcher at Washington University). In his missive, he suggests me to stay below 12% of volumetric change compression for bulk silicon. In agreement with mi advisor, Dr. Bernardo Mendoza, the computations on this thesis for both crystals were restricted to ±10% of volumetric change.

He is author of many publications on the subject, one of them closely related to such bounds (Ref. [33]). Afterwards, I interchanged a couple of e-mails with him to get an advice. He kindly explained to me that (see Figure 5 on page 44) silicon suffers a structure change to β-Sn when it undergoes about 12% of density compression. As a general approach, and in agreement with my advisor, Dr. Bernardo Mendoza, the computations on this thesis for both crystals were restricted to ±10% of volumetric change.

This thesis

4.4.3 *Numerical Implementation*

To address that, the ratio of the volumetric change due to an applied stress was used as the independent-input-variable, that is, the volume variations quantify the amount of compression or expansion at the crystal structures studied in this thesis, bulk silicon and bulk gallium arsenide (see Section 5.2 and Section 5.3).

Independent input variable

Once the independent variable was defined, the next issue was how to indicate the ABINIT program to compute the spin and position matrix elements, $r_{cv}^a(\mathbf{k})$ and $\mathcal{S}_{mn}^a(\mathbf{k})$ (Equation 4.2a and Equation 4.2b), for a crystal structure that has suffered a volumetric change. The answer lies in two fundamental concepts used in the study of crystalline structures (see pages 64 and 65 of Ashcroft and Mermin's textbook, Ref. [34]):

Key operational question

THE BRAVAIS LATTICE (3D) Are all points with position vectors $\mathbf{R}$ of the form

$$\mathbf{R} = n_1 \mathbf{a_1} + n_2 \mathbf{a_2} + n_3 \mathbf{a_3} \tag{4.7}$$

where n_1, n_2, and n_3 range through all integral values, and a_1, a_2, and a_3 are any three non-coplanar vectors, called PRIMITIVE VECTORS, that are said to generate or span the lattice[6].

PRIMITIVE (UNIT) CELL A volume in space that, when translated through all the vectors in a Bravais lattice, just fills out all the space without either overlapping itself or leaving voids. A primitive (unit) cell *must* contain precisely one lattice point. For a given set of primitive vectors, the corresponding primitive (unit) cell is the set of all points r of the form

$$r = x_1 \, a_1 + x_2 \, a_2 + x_3 \, a_3 \qquad x_i \in (0, 1) \tag{4.8}$$

As both concepts rely on the primitive vectors:

> A variation in length of the primitive vectors induces a variation of both, the Bravais lattice and the unit cell.

Key idea

To induce such variation in ABINIT implies to vary the ABINIT's acell parameter, which stands for scAle CELL. It is a real triad acell(1,2,3) given in Bohr units[7] that acts as a length parameter . Essentially it gives the length scales that, when applied to the *dimensionless* Real space PRIMitive translation vectors (rprim, a 3×3 unity matrix), gives the *dimensional* primitive vectors (rprimd),

Key action

Concrete action

$$\text{rprimd}(i, j) = \text{rprim}(i, j) \times \text{acell}(j) \qquad \text{for} \quad i, j = 1, 2, 3$$
$$(\text{i.e. } x, y, z). \tag{4.9}$$

In brief

The modulation of DSP via the application of either compressive or expansive stresses is obtained by setting the independent-variable as an hypothetical change in volume due to the application of the stress. To avoid phase and structural changes in the crystal, those variations are restricted to be in the $\pm 10\%$ range.

Then ABINIT is instructed to compute the spin and matrix elements for a number of hypothetical volumetric variations. This is accomplished by varying the ABINIT's acell parameter in the mentioned range.

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6 Alternatively, the Bravais lattice is an infinite array of discrete points arranged in such manner that seem *absolutely* the same from whichever point the lattice is observed.

7 [Atomic Units] One Bohr is roughly 0.53 Angstroms or 53×10^{-3} nm.

Part III

RESULTS AND CONCLUSIONS

5

EXAMPLES OF DSP MODULATION

5.1 OBJECTIVES

The fact that the DSP response can be modulated by the application of either compressive or expansive stresses was already known.

In Chapter 4, a simple method to achieve such modulation was proposed, and in this chapter it is applied to study two important crystal semiconductors: bulk silicon and bulk gallium arsenide.

5.2 EXAMPLE 1. BULK SILICON STUDY

5.2.1 *The Silicon Semiconductor*

Silicon is the crystal semiconductor that is the most prominent component in electronic devices. Its outstanding characteristics are: steady electric behaviour, wide abundant, and it is easily grown in furnaces. Some outstanding facts about silicon are:

Atomic Number	14
Electron configuration	$3s^2\ 3p^2$
Electrons per shell	2, 8, 4
Crystal structure	Diamond cubic

Silicon versus Gallium Arsenide

ABUNDANT. Silicon is abundant and cheap to process.

SILICON DIOXIDE Silicon dioxide can easily be incorporated onto silicon circuits, and such layers are adherent to the underlying Si. GaAs does not form a stable adherent insulating layer.

HIGH HOLE MOBILITY. This high mobility allows the fabrication of higher-speed P-channel-FET's (field effect transistors), which are required for CMOS logic. Consequently, they consume less power.

5.2.2 *Convergence Process*

As explained in Section 4.3, page 41, before any attempt to perform a band structure computation via the DFT formalism, one *must* find out the most suitable values for three parameters, such that he DSP signal

For Silicon

49

is converged. Namely: the number of k−points (nkpt), the value of the energy cutoff (ecut), and the number of conduction bands (cband).

STEP 1. Convergence on the number of k−points. To work out the convergence process on nkpt, the DSP signal was computed for about 15 values of them, with *low* and fixed values of ecut and cband (6 Ha and 2 bands, respectively).

18,424
k−*points*

The Figure 6 on page 50 contains the most significant results, and the small inset in it has the two-to-last nkpt tested values. Because of the small magnitude of ecut and cband, the obtained signal resembles more a set of bonded lines than a smooth signal. One can conclude from the figure that, increasing the nkpt value beyond 18,424 k−points (see the inset) leaves the signal almost unchanged. Therefore the value of 18,424 k−points is taken as the convergence value.
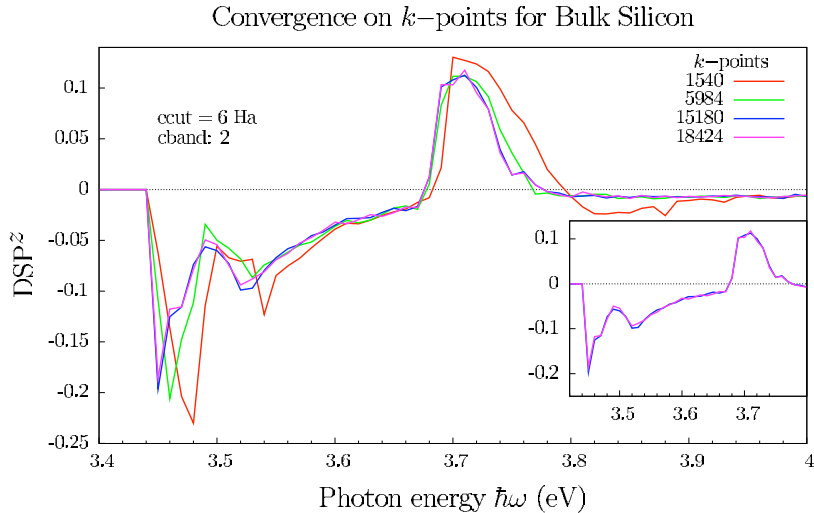
Figure 6: (color online) Convergence of the DSP signal as a function of the number of k−points for bulk silicon. Used an increasing number of k−points with *low* and fixed values of energy cutoff (ecut) and conduction bands (cband). The inset contains only the last two signals, and shows that acceptable convergence is reached at 18,424 k−points.

STEP 2. Convergence on Energy Cutoff. With the converged nkpt value of STEP 1, and a fixed and low value of cband (2 bands), the DSP response is computed for a set of 10 different energy cutoff values.

30
Hartrees

The Figure 7 on page 51 shows the most notable DSP responses as a function of the photon energy and the inset in it displays the two highest signals in ecut. From it, one concludes that a further

increase of ecut above 30 Hartrees leaves the DSP signal almost unchanged.
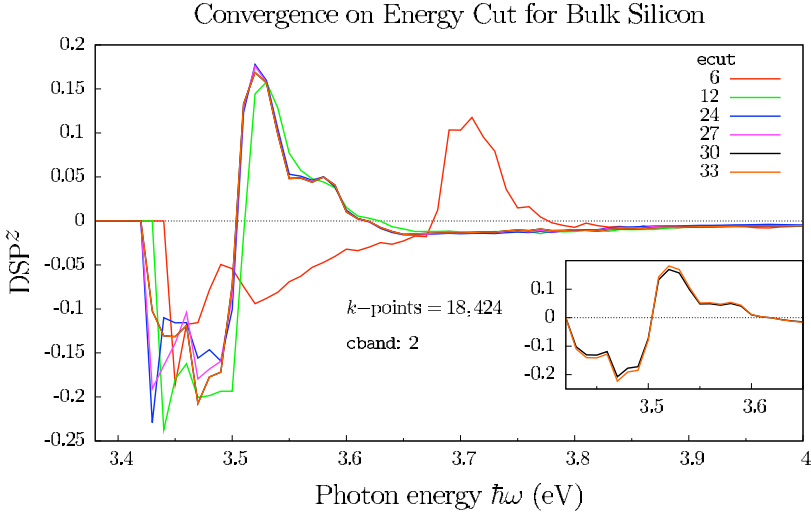
Figure 7: (color online) Convergence of the DSP signal as a function of the energy cutoff for bulk silicon. Used increasing values of energy cutoff (ecut) with a *low* and fixed value of conduction bands (cband) and $18,424$ k−points (converged value, see Figure 6 on p. 50). The inset contains only the last two signals, and shows that acceptable convergence is reached at 30 Hartrees.
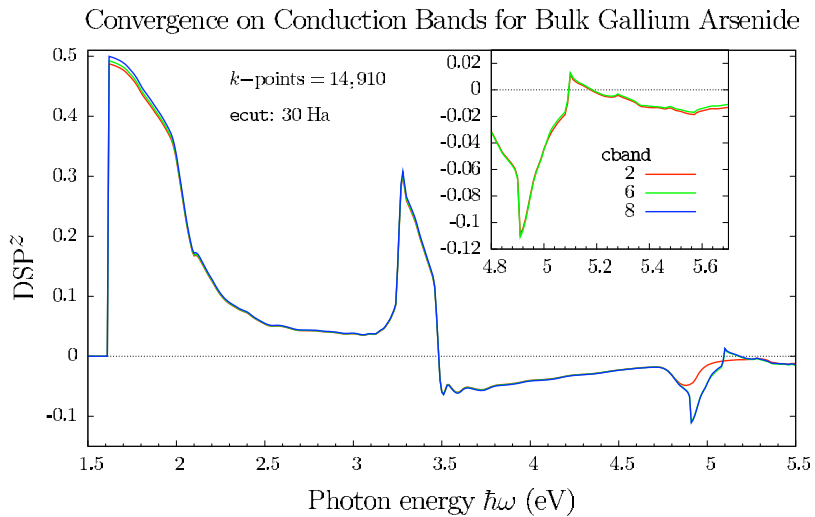
STEP 3. Convergence on the number of conduction bands. In the last step of the convergence process one takes the converged values of the preceding steps and computes the DSP for a number of conduction bands.

The Figure 8 on page 52 shows the most significant DSP responses and the inset in it presents the two highest signals in cband. From it, one concludes that further increase of cband above 8 conduction bands leaves almost unchanged the DSP signal.

In brief

The DSP signal for bulk silicon is well converged for the following set of values: nkpt ∼ 18 000, ecut = 30 Ha, and cband = 8 bands.

5.2.3 *Stress Modulation of DSP*

In this section the DSP response is computed for different values of volumetric changes, induced by expansive or compressive stresses, as explained in Section 4.4. For this purpose the values of nkpt, ecut, and

8
bands
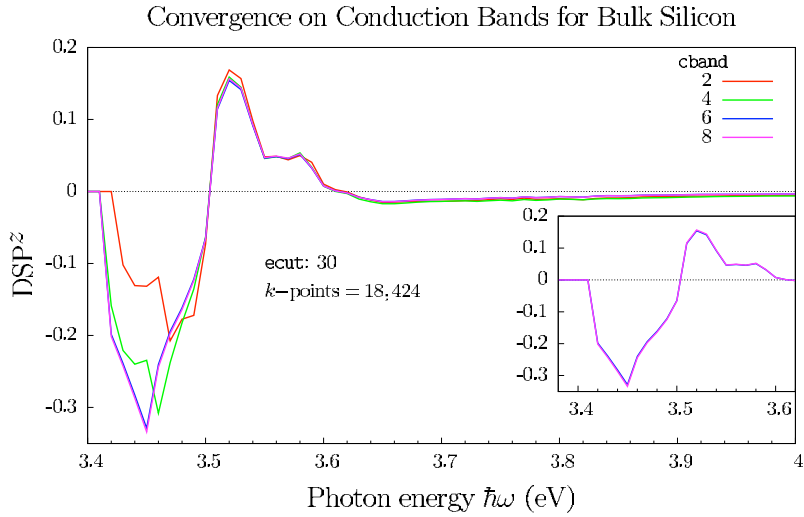
Figure 8: (color online) Convergence of the DSP signal as a function of the number of conduction bands on silicon. Used increasing values of conduction bands (cband) with $18,424$ k−points and 30 Hartrees of energy cutoff (ecut), which are the converged values (see Figure 6 on p. 55 and Figure 7 on p. 51). The inset contains only the last two signals, and shows that excellent convergence is reached at 8 conduction bands.

cband adequate for the convergence of the DSP signal were used. The Figure 9 on page 53 displays the obtained results. In it one can realize that, qualitatively,

- Compressive stress shortens and shifts the DSP signal to higher energies.

- Expansive stress augments and shifts the DSP signal to lower energies.

- The overall signal *does* change: the downward peak at compressed states changes polarity and splits in two upward peaks as the bulk silicon undergoes a volumetric expansion from -8% to $+8\%$.
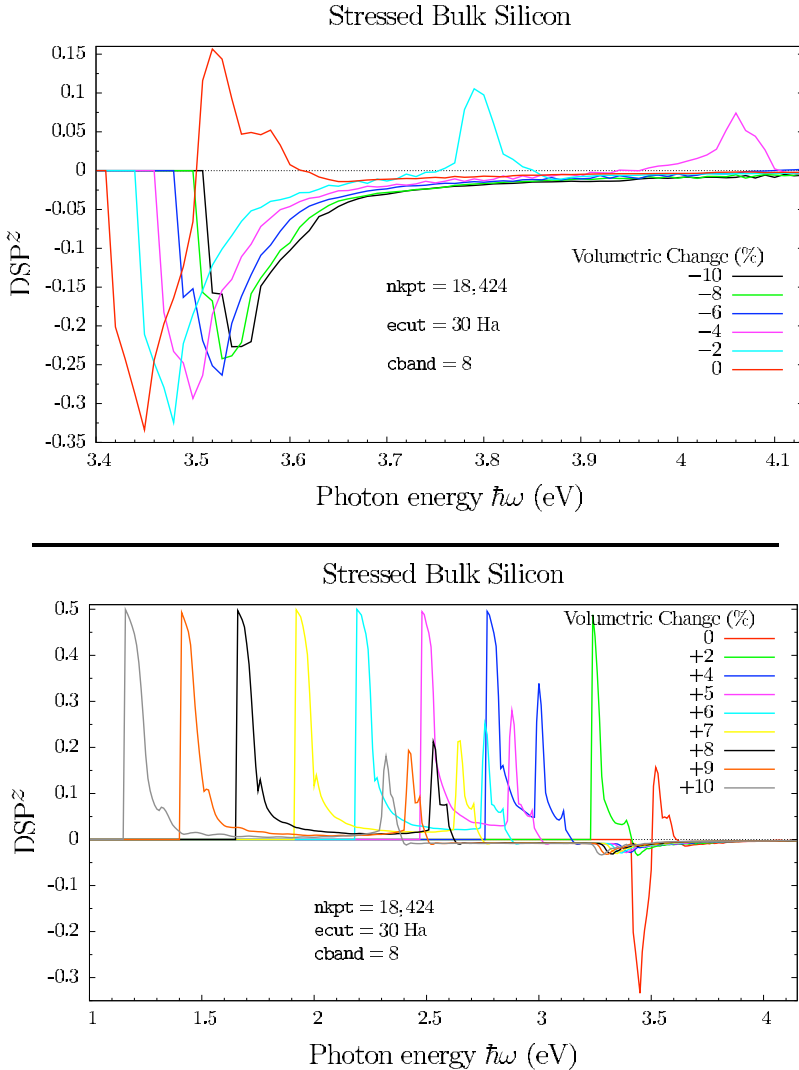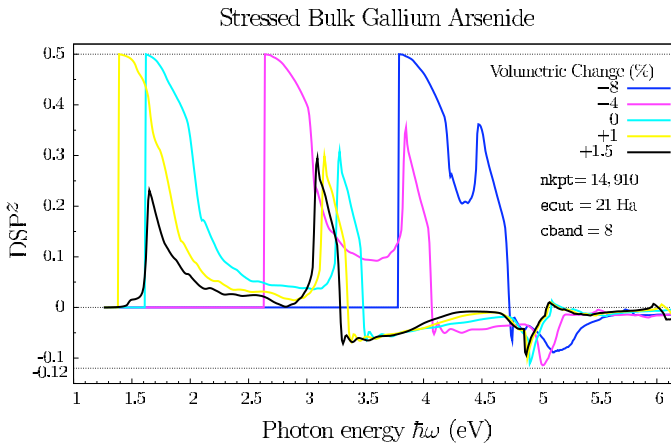
Figure 9: (color online) Stress modulation of the DSP on silicon. Computed with 18,424 k–points, 8 conduction bands (cband), and an energy cutoff (ecut) of 30 Hartrees (values for DSP convergence, see Figure 6, Figure 7, and Figure 8 on pages 50, 51, and 52, respectively).

The upper (lower) figure shows the DSP signals for compressive (expansive) stresses. Both figures display that, qualitatively, compressive (expansive) stress effectively modulates the DSP signal on energy operation, and that the overall signal *does* change. Notably, the downward peak at all compressive stresses (all signals in the upper plot, and the unstressed (0%) signal in the lower plot), changes its polarity and splits into two upward peaks as the sample undergoes a volumetric expansion.

5.3   EXAMPLE 2. BULK GALLIUM ARSENIDE STUDY

5.3.1   *The Bulk Gallium Semiconductor*

The gallium arsenide (GaAs) is a semiconductor that has a Zinc Blende crystal structure. It is composed by two elements, gallium and arsenic and is mainly used to make semiconductor devices, like electronic circuits, solar cells, diodes, etc.

Gallium is a byproduct of the smelting of other metals, notably aluminum and zinc, and it is rarer than gold. Arsenic is not rare, but it is poisonous.

Electrons per shell 2, 8, 4
Crystal structure   Zinc Blende

GaAs versus Silicon

GaAs has several characteristics that makes it excel silicon on *some* applications. The most notables are (Ref. [5]):

DIRECT GAP. GaAs is a direct gap semiconductor, what makes it most suited for manufacturing *optoelectronic devices*, like detectors devices. Actually, its absorptivity is so high that it requires a cell only a few microns thick to absorb sunlight.

DRIFT MOBILITY. GaAs has a better *drift mobility*, allowing it to be used in high speed logic circuit.

MICROWAVE OPERATION. GaAs can be operated on microwave frequencies, and silicon not. Therefore GaAs is suited for Gunn and Impatt Diodes, receivers for satellite broadcasting and radars.

IONIZING RESISTANCE. Compared with silicon, GaAs has a large resistivity to ionization, which is composed by subatomic particles or waves that are energetic enough to detach (ionize) electrons from atoms or molecules[1].

5.3.2   *Convergence Process and DSP Modulation*

The gallium arsenide was studied with the same *modus operandi* than the bulk silicon, and here only the results are given. Apart from the computed DSP signals on this thesis, an experimental plot of the DSP

---

1 Ionizing ability depends on the energy of the impinging individual particles or waves, and not on their number (refer to the photoelectric effect elsewhere). Examples of ionizing radiation are α and β radiation, as well as photonic in the short wavelength end (ultraviolet, x-rays, and gamma rays).

dynamics is shown on Figure 13. It was reported by Bhat et al. on Ref. [9]. The figure shows, as they point, *the dynamics of the DSP of electrons after one–photon (closed squares) and two-photon (open circles) excitation.*

Finally, on Figure 15, the modulation of DSP is presented. Notably, the figure only shows the DSP signal till a volumetric expansion of +1.5%, because it was not possible to obtain signals at further expansions. Apparently the implemented scheme of computation (DFT, LDA, acell variation, etc) envisions that the band gap of GaAs becomes null for volumetric expansions onward $\approx$ 2%.
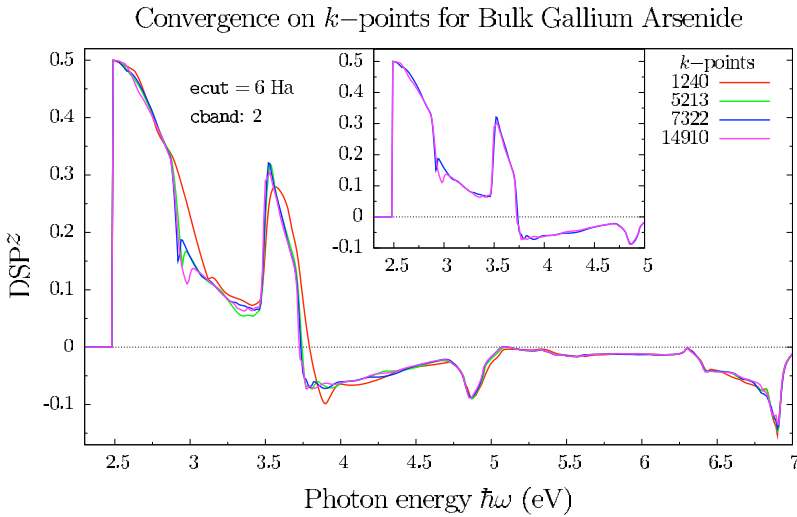
Figure 10: (color online) Convergence of the DSP signal as a function of the number of k−points. Used an increasing number of k−points with *low* and fixed values of energy cutoff (ecut) and conduction bands (cband). The inset contains only the two last signals, and shows that acceptable convergence is reached at 14,910 k−points. See the comment on the body text about the window at 3 eV (inset).
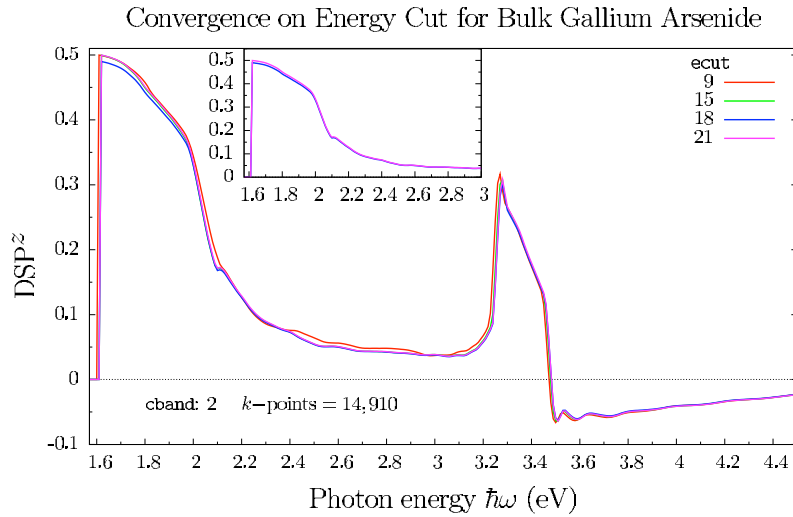
Figure 11: (color online) Convergence of the DSP signal as a function of the energy cutoff on GaAs. Used increasing values of energy cutoff (ecut) with a *low* and fixed value of conduction bands (cband) and 14,910 k−points (converged value, see Figure 10 on p. 55). The inset contains only the last two signals, and shows that acceptable convergence is reached at 21 Hartrees.

Figure 12: (color online) Convergence of the DSP signal as a function of the number of conduction bands on GaAs. Used increasing numbers of conduction bands (cband) with 14,910 k−points and 21 Hartrees of energy cutoff (ecut), which are the converged values (see Figure 10 on p. 55 and Figure 11 on p. 56). The inset contains only the last two signals, and shows that excellent convergence is reached at 8 conduction bands.
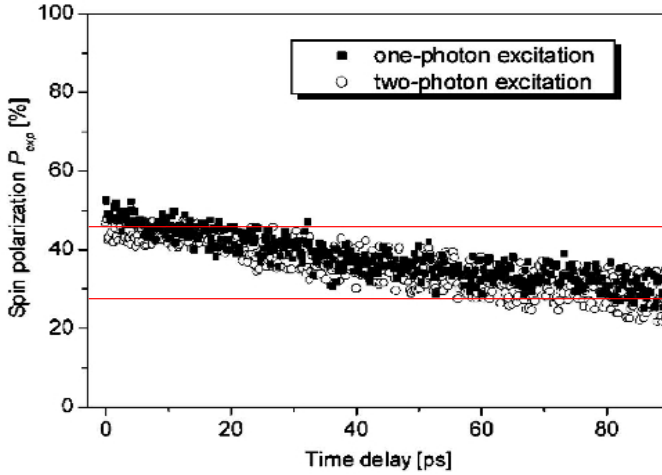
Figure 13: Experimental measurement of the DSP on bulk GaAs, as reported by Bhat et al. on Ref. [9]. The figure shows, as they point, *the dynamics of the DSP of electrons after one–photon (closed squares) and two-photon (open circles) excitation.* Notice that the DSP signal decays from 48% to 28% in about 90 seconds. Considering the decay remains linear, the DSP signal would fall to zero in about 225×10^{-12} seconds. Compare with the computed signal in this thesis, Figure 15.

Figure 14: (color online) Stress modulation of DSP on GaAs. Computed with $14,910$ k−points, 8 conduction bands (cband), and an energy cutoff (ecut) of 21 Hartrees (values of convergence, see Figure 10, Figure 11, and Figure 12). Qualitatively, the DSP signal is compacted (enlarged) and shifted to higher (lower) energies by compressive (expansive) stresses. Moreover, stress does *not* change significantly the DSP peak values. Expansive stress causing volumetric changes greater than 1.5% could not be computed, see the body text for an explanation.

6

SUMMARY AND CONCLUSIONS

> *All endeavor calls for the ability to tramp the last mile,*
> *shape the last plan, endure the last hours toil.*
> *The fight to the finish spirit is the one characteristic*
> *we must possess if we are to face the future as finishers.*
>
> —Henry David Thoreau
> American Philosopher and Activist

6.1 SUMMARY

The thesis work presented here is part of the research I performed under the supervision of Dr. Bernardo Mendoza during my Master in Science studies at Centro de Investigaciones en Óptica, A.C. (León, México). Its main objectives are (1) to investigate the well known fact that the optical electron spin-injection on bulk semiconductors is affected by the application of stresses, and (2) to explore the possibility of modulate such phenomenon by either compressive or expansive stresses. For that matter, a simple and effective method to compute the spin injection as a function of stress (or a related quantity) was proposed, considering both compressive and expansive stresses.

The scheme is to consider that the applied stress induces a hypothetical variation of the bulk sample and consider that variation as the independent variable. Then the whole sample volume can be thought as a stack of primitive unit cells rooted at the Bravais lattice points. The primitive unit cell depends on the primitive translational vectors (rprimd) through Equation 4.7 and Equation 4.8. In turn, rprimd depends on the ABINIT's scAle CELL parameter (acell) and the primitive unit vectors (rprim) via Equation 4.9. Therefore, the volumetric variation of the sample due to the applied stress can effectively be indicated through a variation in acell.

After that, the spin and position matrix elements required to evaluate the DSP expressions (Equations 4.2 on page 37) are computed for each variation of the acell parameter, employing a band structure calculation within the DFT with LDA pseudo-potentials.

6.2   CONCLUSIONS

IN GENERAL

- Optical spin injection can be optimized, in magnitude and energy-operation, by applying either expansive or compressive stresses.

- Material properties in crystalline semiconductors (like the band structure, the linear and nonlinear susceptibilities, the DSP, etc.) can be calculated for strained samples by computing such properties with the ABINIT software and varying the program's acell parameter to simulate an hypothetical volumetric change due to the stress.

FOR BULK SILICON   (Left plot of Figure 15)

- It is more spin-polarizable at expansive stress (DSP peak ∼ 50 %) than at compressive stress (DSP peak ∼ −20 %) or unstressed state (DSP peak∼ −30%).

FOR BULK GALLIUM ARSENIDE   (Right plot of Figure 15)

- It is roughly equally spin-polarizable at compressive, expansive, or unstressed states (DSP peak ∼ 50 %), but the application of expansive stress can shift the range of operation to a more suitable energy (in the experimental sense).
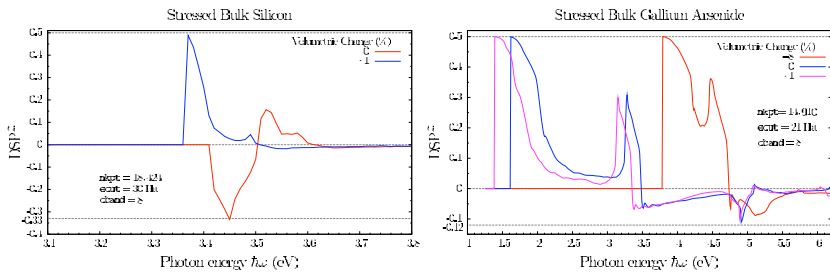
Figure 15: (color online) Some particular results of the DSP modulation by applied stress. The complete set appear at full scale on pages 53 and 57 (Figure 9 and Figure 14)

Part IV

APPENDIX

COMPUTATIONAL TOOLS

A.1 "FREE SOFTWARE, FREE SOCIETY"

> *Free software is a matter*
> *of the users' freedom to run,*
> *copy, distribute, study, change*
> *and improve the software.*
>
> — Richard M. Stallman [35]

The free software movement was started in 1983 by computer scientist Richard M. Stallman, when he launched a project called GNU (www.gnu.org), which stands for "GNU is Not UNIX", to provide a replacement for the UNIX operating system —a replacement that would respect the freedoms of those using it. Then in 1985, Stallman started the Free Software Foundation (www.fsf.org), a nonprofit organization with the mission of advocating and educating on behalf of computer users around the world [...]

To use free software is to make a political and ethical choice asserting the right to learn, and share what we learn with others. Free software has become the foundation of a learning society where we share our knowledge in a way that others can build upon and enjoy.[1]

· · ·

The computational tools employed at the Optics Surface Group

http://aida.cio.mx/

at Centro de Investigaciones en Óptica, A.C. use almost exclusively free(ware) software, being the only exception the use of the Apple's OSX. Apart of the advantage of being costless, free(ware) software gives us the opportunity to adapt and develop our own tools, like the TINIBA shells, detailed in Section A.2.

For instance, the present thesis employed the ABINIT software to compute the band structure calculations, together with a set of FORTRAN modules. Both of them are controlled by a set of BASH scripts (TINIBA). The figures were produced with GNUPLOT and XFIG, and the thesis document was typeset with the classicthesis style. The edition process was done on *the* EMACS editor.

---

1 Taken from http://www.fsf.org/about/what-is-free-software.

A.2   TINIBA: A SET OF BASH SCRIPTS

> *We have seen that computer programming is an art,*
> *because it applies accumulated knowledge to the world,*
> *because it requires skill and ingenuity, and especially*
> *because it produces objects of beauty.*
>
> — Donald E. Knuth [36]

TINIBA is a computer software that some members of the Surface Optics Group at CIO have developed. Its purpose is to perform parallel computations of semiconductor properties, like the electronic structure and the linear and non-linear responses in surface and bulk semiconductors. TINIBA is composed by a number of modules written in BASH, the standard shell program (command interpreter) of the GNU/Linux operative system, i.e. TINIBA is not a compiled program, but one that is interpreted line-by-line.

Interpreted programs have the advantage that they are easy to develop and maintain and that they are slow to perform numerical and string computations. Nevertheless TINIBA shells delegate all numerical computations to FORTRAN subroutines that the group has developed in collaboration with Nastos et al., authors of Ref. [1].

Therefore, TINIBA shells have the best of two worlds: speed and facility for maintenance and development. In Figure 16 a simplified TINIBA's flow diagram is displayed, and in Section A.2.1 a verbose description of it is given.

A.2.1   *The* TINIBA *Modules*

Next the main steps of a standard computation are described. The names in square brackets and typewriter font refer to the name of the bash modules that perform the action.

A. Set up the configuration-file according to the physical properties of the semiconductor (setUpAbinit_<foo>.in), and give the coordinates of the location of each atom in the unit cell [<foo>.xyz].

B. Generate a list of k−points [rklist.sh].

C. Perform a *weighted* distribution of the k−points generated on item B over all execution cores. The weight is done according to the speed of each processor, for example, [2]. The objective is that each execution core works out a subset of the k−points [arrangeMachines.pl].

---

2 Roughly, 1 Quad = 2 Itanium = 4 Xeon
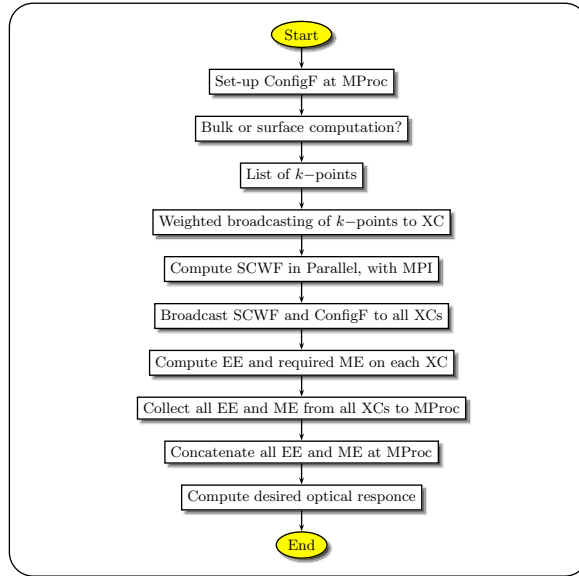
Nomenclature (in order of appearance)

ConfigF	CONFIGuration Files, according to physical properties.
MProc	Master PROCessor
XC	eXecution Core
SCWF	Self Consistent Wave Function
MPI	Message Passing Interface standard for parallel computation
EE	Eigen-Energies
ME	Matrix Elements

Figure 16: TINIBA. Home-made Bash-scripts to compute optical responses in semiconductors.

D. Broadcast of the configuration-files (item A) and the subset of the list of k−points (item C) [copySCF2nodes.sh].

E. In a single processor, presumably on the master, perform a self-consistent computation of the wave-function [runSCFxeon.sh, runSCFitan.sh, or runSCFquad.sh, depending on the architecture of the selected processors, Xeon, Itanium, or Quad]. The self-consistent files are then broadcasted to all the processors [copySCF2nodes.sh].

F. Compute the eigenenergies and momentum matrix elements on each execution core[3]. The output files of each execution core correspond to the result of a subset of the total number of k−points [runBulk.sh].

---

3 Xeon, Itanium, and Quad processors have 2, 2, and 8 execution cores each one, respectively.

G. The output files of item F are copied to the master processor and concatenated (linked together in series) in the correct order, according to the list of k−points [concatena.pl].

H. Optionally, an optical response might be calculated. For example, the first and second order susceptibilities, the spin carrier injection, etc. [response.sh].

A.3 MEDUSA: THE COMPUTING CLUSTER

The Optics Surface Group (http://aida.cio.mx/) at Centro de Investigaciones en Óptica, A.C. owns a computing cluster called MEDUSA. It is composed of several Intel processors of three kinds: Xeon, Itanium, and Quad Core. Each processor has its own hard disk and RAM memory (see Figure 18).
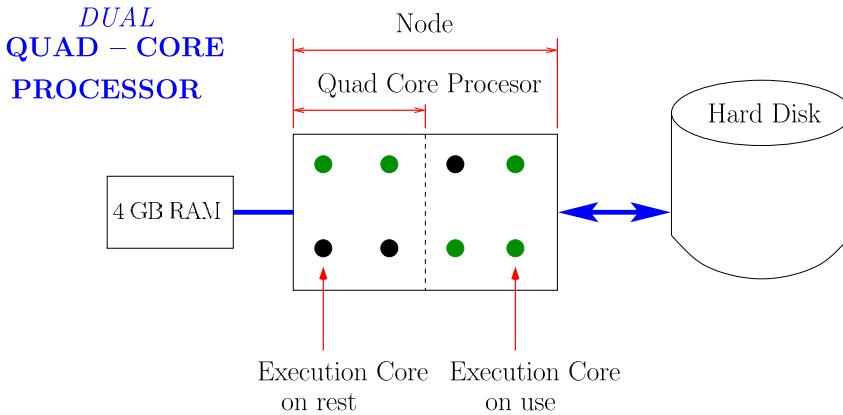
Figure 17: Schematic representation of a Medusa's Quad processor.

Each processor has a different number of execution cores. For instance, the Dual Quad-Core Processors (see Figure 17) have two processors, each of them with four execution cores, summing then eight execution cores 'per Quad'. The Xeon and Itanium processors are 'single processors' with two execution cores. Considering these three brands, Medusa has a total of 152 execution cores (see Figure 18 for a breakdown of facts).
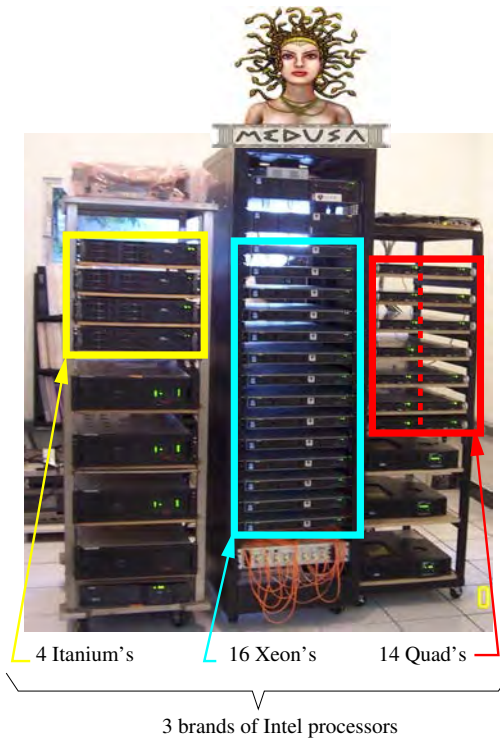
The cluster
34 computers (nodes)

per Quad: 2 nodes, per node:4−cores
per Itanium: 1 node, per node 2−core
per Xeon: 1 node, per node 2−core

8 Itanium cores
32 Xeon cores
112 Quad cores

Round numbers:
152 execution cores
170 GB of RAM
5,720 GB of HDisk

Software tools:
GNU/Linux CentOS
MPIch & openMP
LAPACK & ScaLAPACk
Fortran, Bash, Perl, Python
Abinit, **Tiniba (home−made)**

4 Itanium's   16 Xeon's   14 Quad's

3 brands of Intel processors

Edited with XFIG
a 'free' drawing tool
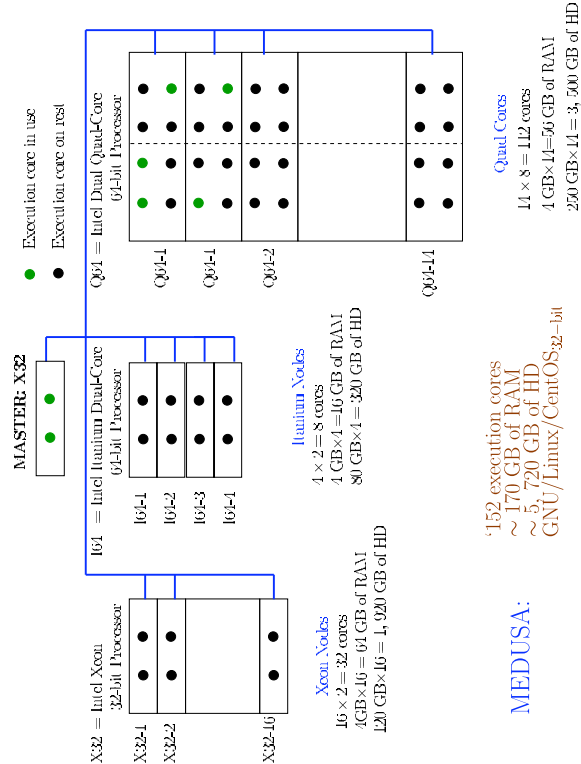
Figure 18: Medusa: The group's cluster computer.

A.4   PERFORMANCE OF THE COPY AND ABINIS PROCESSES

The computation of the self consistent wave-function and the band structure (eigen-energies for each $k-$point) require much less time to be completed than the the computation of the matrix elements for the position, momentum, and spin. Therefore, these computations are done in parallel, with some selected (by hand) set of cores performing a part of the computation.

TINIBA calculates the matrix elements in such a manner that each 'execution core' has its own self-consistent wave-function (SCWF) to do its job, i.e. it requires to replicate this function as many times as execution cores we decide to use.

For typical surface calculations, like surface responses, the SCWF's size can be as large as 2 Giga Bytes, therefore, the replication needs significant machine resources. For each replica: split the function into manipulable small files, transport the small files thoughtout the buss, concatenate all the small files to recover the original. Then naturally a question arose: Could we cut down resources if each core shares a single SCWF per node?

To address this question, a typical surface computation of matrix elements was done, employing a SCWF of 1.2 GB on a single QUAD processor (see Figure 17 on page 67). As commented above, such kind of processor possesses 8 execution cores. Two scenarios were studied:

SINGLE COPY CASE.   (standard procedure) All the selected execution cores share a single SCWF.

MULTI COPY CASE.   All the selected execution cores possess their own SCWF.

Then two experiments were performed, a Copy Experiment and a Matrix Elements Computation Experiment. Each of them starting with only one execution core, both experiments were carried out 8 times for each case, increasing in one the number of employed execution cores each time. The results appear on page 70, Table 1 and Figure 19.

The conclusions from these experiments are:

COPY EXPERIMENT.   It is faster to broadcast single copies than multi-copies, which is natural. The importance of this experiment relies on the quantification of the time differences. The biggest difference is at 8 execution cores (with 8 $k-$points), with a difference of about 15 minutes.

MATRIX ELEMENTS EXPERIMENT.   It is faster to compute the matrix elements with a multi-copy scheme than with the single-copy scheme. The time difference is about 410 min (6.8 hours).

Cores &	Copy Experiment		Matrix Elements Experiment	
k−points	Single-Copy	Multi-Copy	Single-Copy	Multi-Copy
1	3.8	5.3	225.4	143.3
2	3.7	5.5	153.3	152.6
3	3.7	7.9	448.0	452.2
4	3.7	9.8	515.1	508.4
5	3.7	12.3	870.8	687.7
6	5.9	13.8	1367.9	947.0
7	5.3	17.3	1659.2	1383.1
8	6.0	20.0	2310.4	1900.1

Table 1: Single- and Multi- Copy Benchmarking. Required times, in minutes, to complete the copy and matrix elements experiments. The number of execution cores is equal to the number of sampled k−points.

Horizontal axis: ♯kpts (with ♯kpts = ♯cores)
SCWF=Self Consistent Wave Function [1.2 GB]
Machine: quad07
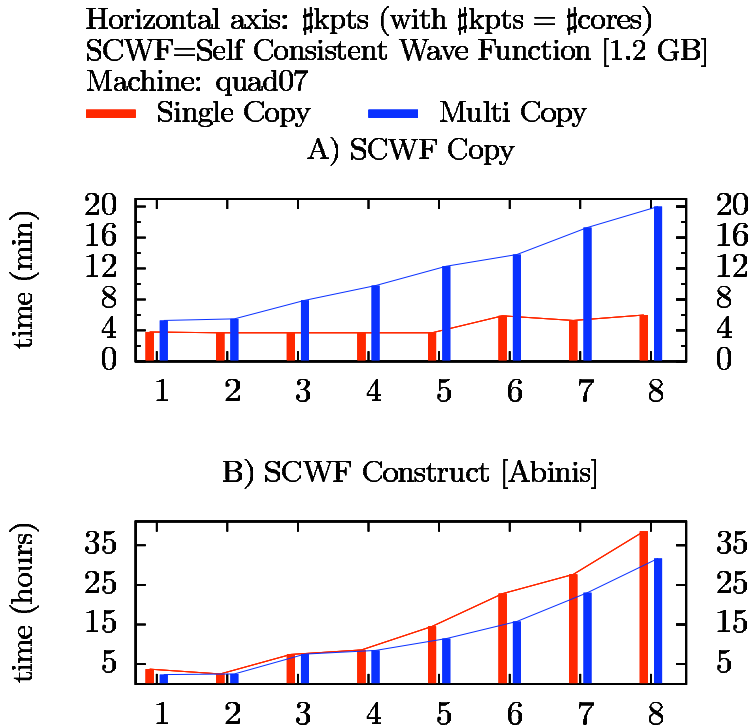
Figure 19: Performance of the Copy and Abinis Processes.

POSTER PRESENTATION

The results of this thesis were presented on October 21, 2008 at the "*LI Congreso Nacional de Física*" (60th National Congress of Physics) held at Zacatecas, México. The poster session was the 2MA02.

Figure 20: Poster at the National Congress of Physics, Zacatecas, México.

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INDEX

Except by the use of the OSX operative system, all the computational tasks performed in this thesis employed solely ***Free Software***[1]. This includes the typesetting (LATEX with CLASSICTHESIS style[2]), the figures (GNUPLOT and XFIG), the computations (BASH intepreter, FORTRAN compilers, and ABINIT software) and the cluster's operative system (CENTos). The edition was done on *the* EMACS editor[3].

Cuauhtémoc

December, 2008.
Léon, MÉXICO.

Final Version as of February 13, 2009 at 18:03.

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1 See *Free Software, Free Society: Selected Essays of Richard M. Stallman*, Ref. [35].

2 By André Miede, http://www.miede.de, who states that CLASSICTHESIS style "was typeset with LATEX 2ε using Hermann Zapf's *Palatino* and *Euler* type faces (Type 1 PostScript fonts *URW Palladio L* and *FPL* were used). The listings are typeset in *Bera Mono*, originally developed by Bitstream, Inc. as "Bitstream Vera". (Type 1 PostScript fonts were made available by Malte Rosenau and Ulrich Dirr.)

The typographic style was inspired by Bringhurst's genius as presented in *The Elements of Typographic Style* [37]. It is available for LATEX via CTAN as classicthesis ."

3 Emacs originally was an acronym for Editor MACroS. The first Emacs was a set of macros written in 1976 at MIT by Richard Stallman for the editor TECO (Text Editor and COrrector). The current version of Emacs, GNU Emacs, was originally written in 1984. GNU Emacs is an highly extensible and customizable text editor. Visit www.gnu.org/software/emacs/.