QUARMEN
Erasmus Mundus Joint Master
QUANTUM SCIENCE & TECHNOLOGY

Semester 2: University of Porto

Contents

Plan of Studies ... 2

Curricular Units ... 3

Introduction to quantum information ... 3

High Performance Computing in Quantum Matter ... 6

Quantum Matter ... 8

Computational Complexity ... 10

Sensing and Signal Analysis ... 12

Topics in Theoretical Physics ... 14

Internship Projects ... 16

Experimental Optical analogues for the simulation two-dimensional quantum fluids ... 16

Tuning properties of novel quantum 2D materials ... 18

Manipulating phonons at the nanoscale level ... 20

Interaction-free quantum imaging and computation ... 22

Excitonic instability and exciton condensation in 2D materials with nontrivial electronic topology ... 24

Ab-initio modeling of carbon-based minerals ... 26

Exploring novel electronic devices based on topological insulators grown by molecular beam epitaxy ... 28

Decreasing the sign problem with the sampling of sets ... 29

Plan of Studies

Compulsory

Code	Name	Contact hours	ECTS
FIS4047	Introduction to quantum information	42 TP	6
FIS4046	High Performance Computing in Quantum Matter	42 TP	6
FIS4044	Quantum Matterials	42 TP	6
	Portuguese Language Course		3
	Internship (*)		3

Options (1 option to choose)

Code	Name	Contact hours	ECTS
F4036	Topics in Theoretical Physics	42 TP	6
CC4011	Computational Complexity	42 TP	6
	Sensing and Signal Analysis	42 TP	6

(*) Examples of Internship projects are detailed below and some take place at Iberian Nanotechnology laboratory in Braga (50 Km from Porto, with regular trains connections)

Introduction to quantum information

Code FIS4047

Teaching components (total hours in semester)

T	TP	PL	Total Contact hours	ECTS	Total hours of student work
	42		42	6	162

Lecturers

Ariel Ricardo Negrão da Silva Guerreiro (asguerre@fc.up.pt)
Duarte Manuel Nogueira Magano (duarte.magano@fc.up.pt)

Goals

The main objectives of this curricular unit are:

- Development of a mind map of quantum information theory, its interconnection with other science disciplines and applications in quantum technologies; and
- Understanding the concepts, models and fundamental knowledge of this theory and acquiring skills in its operationalization and extension, leading to the progressive autonomy of students in understanding the specialized scientific literature and in the study of more advanced disciplines, promoting the ability to develop research and development activities in this area.

- From this derive several other objectives, namely:
  - To promote the connection of knowledge and principles of the Quantum Theory of Information with those of other areas of Science and Physics Engineering, its framing in an integrated view of Physics and Modern Sciences and their technological applications.;
  - To know the general structure of the quantum theory of information, of consubstantiation in physical systems, with particular emphasis on its fundamental principles and laws;
  - To operationalize the mathematical formulation and calculation methods in Quantum Information Theory;
  - To be able to establish a relationship between the conceptual and formal models of the theory of Quantum Information Theory and research work in the area, albeit at an elementary level.
  - Develop scientific intuition and critical thinking;
  - To provide the knowledge base and competences necessary for students to be able to continue their studies in more advanced areas of knowledge.

In addition to the technical and scientific aspects, this curricular unit should also contribute to increasing the culture of students in Physics, Engineering and Science.

In addition to these general objectives, it is intended that, for students to pass this curricular unit, they must meet the following minimum learning goals:

- to know the fundamentals, techniques and most relevant results of the Quantum Theory of Information;
- to be able to use the theoretical and formal technical tools of this discipline in problem solving and model building;
- to be able to identify the limitations and validity domains of the models;
- to be able to identify and understand the most relevant current applications and research topics in Quantum Information Theory.

Learning Outcomes and Skills

Development of a mind map of quantum information theory, its interconnection with other science disciplines and applications in quantum technologies; and

Understanding the concepts, models and fundamental knowledge of this theory and acquiring skills in its operationalization and extension, leading to the progressive autonomy of students in understanding the specialized scientific literature and in the study of more advanced disciplines, promoting the ability to develop research and development activities in this area.

Subject Matter

1. Introduction to Quiskit.
2. Introduction to information theory.
Historical view. Statistical description of the information. Entropy and information measurements. Theory of estimation and inference. Fisher information and Cramer-Rao limit.
3. Mathematical structure of quantum theory.
Elementary quantum theory. Multiparty systems and quantum sets (density operator, separability, nonlocality, entanglement and heat). Quantum dynamics and open systems (quantum operations, noise and decoherence). Measure and indeterminacy (projection and not demolition measures, P.O.V.M. and Q.S.T.)
4. Information in quantum registers.
Theorems “no-go”, “no-cloning”, “no-broadcast” and “no-deleting”. Entanglement as a resource (Bell states and inequalities, entanglement and information measures).
5. Second-generation quantum technologies.
Communications, computing, simulation and quantum sensors (teleportation, QKD, dense coding, quantum algorithms, error correction, quantum sensing protocol).

Main Bibliography

Michael A. Nielsen; Quantum computation and quantum information. ISBN: 0-521-63503-9
Vlatko Vedral; Introduction to quantum information science. ISBN: 0-19-921570-7
Gregg Jaeger; Quantum information. ISBN: 0-387-35725-4
Dieter, ed. lit. Heiss; Fundamentals of quantum information. ISBN: 3-540-43367-8
Dirk Bouwmeester; The physics of quantum information. ISBN: 3-540-66778-4

Teaching Methods and Learning Activities

The curricular unit Introduction to Quantum Information is an optional curricular unit that is integrated in the 1st or 2nd year of the Master in Physics and Master Quarmen course. Therefore, their attendance presupposes knowledge of Linear Algebra and General Mathematics, as well as basic knowledge of Quantum Mechanics, Electromagnetism and Electrodynamics, which are subjects covered at the level of a first cycle of studies in Engineering Physics, Physics, Mathematics, and Computer Science.

Description of assessment

Pratical project: 100%

A student-centered methodology is chosen, in which the chapters of the recommended bibliography for prior study are previously identified, accompanied by activities that aim to focus the student on the relevant concepts, models and knowledge, leading to their operationalization and the development of skills previously explained. Contact hours consist of classes that combine exposition, discussion and application of the contents prepared in the previous study. These are supplemented with problems and individual solving exercises that cover the topics and methods studied, having varying levels of difficulty. Mostly, its resolution resorts to methodologies based on the Quiskit platform, introduced in the first classes and whose usage skills are developed throughout the school period, along with the remaining contents.

The assessment consists of:
1. Solving proposed problems (50%)
2. Final practical work (50%)

Final practical work is carried out at home with consultation and over a period of 24 hours and seeks to assess students' ability to combine the knowledge of the various chapters, carrying out some research on the topic and being able to use simulation or numerical calculation tools, in order to build a small model that describes a situation or solves a problem or problems.

Observations

Any situation not foreseen in this discipline regulation must be communicated to the teacher during the first two weeks of classes or, if this situation arises from events that occurred later, should be communicated to the teacher until one week after the facts that support it.

The Jury of the unit is
Ariel Guerreiro
Vítor Pereira
Eduardo Castro

High Performance Computing in Quantum Matter

Code: FIS4046

Teaching components (total hours in semester)

T	TP	PL	Total Contact hours	ECTS	Total Hours
	42		42	6	

Lecturers

João Manuel Viana Parente Lopes (jlopes@fc.up.pt)

Goals

Learn the main concepts of parallel programming and be exposed to advanced quantum computing algorithms.

Learning Outcomes and Skills

Being able to interpret a problem, translate it into numerical methods, choose the parallelization approach, implement using parallelization techniques and manage the processes in an HPC infrastructure.

Pre-requisites

Knowledge of Quantum Mechanics, Statistical Physics, Solid State Physics, numerical methods, and C (or C++) programming.

Subject Matter

Key ideas of HPC and parallelization architectures. Introduction to OpenMP.
Domain decomposition. Spectral methods and exact diagonalization methods.
Introduction to MPI. Introduction to CUDA.
Study of electronic transport problems, with and without disorder, in independent electron systems.
Monte Carlo method stochastic series expansion, exact diagonalization, and the determinant method.

Teaching Methods and Learning Activities

Theoretical classes with the exposition of contents. Practical lessons with the computational implementation of the proposed problems.

Description of assessment

Class participation	10%
Written project	70%
project presentation	20%

During the semester, 3 written works will be done to be delivered. Of these works,

- Two will be shorter and will have the form of a guided project and will be evaluated with 20% each.

- The third will take the form of a project and must be presented in the form of a written work (30%) with oral exam (20%).

The activity in the practical classes will be evaluated by 10%.

Observations

The Jury of the unit is
João Viana Lopes
Vítor Pereira
Augusto Rodrigues

Quantum matterials

Code: FIS4043

Teaching components (total hours in semester)

T	TP	PL	Total Contact hours	ECTS	Total Hours
--	42	--	42	6	162

Lecturers

Vitor Manuel Pereira (vmpereir@fc.up.pt)

Goals

To develop skills for understanding the features and models of the electrical, optical, magnetic, and transport properties of quantum materials, with emphasis on two-dimensional materials and quantum condensed materials (condensates and superconductors).

To empower students for independent and critical assessment of the current literature, and to provide tools for subsequent research and/or technological development activities in the physics and applications of quantum materials.

Learning Outcomes and Skills

- Upon completion of this course unit, students will:
- Be acquainted with key physical properties, phenomena and representative materials that underpin the current and envisaged implementation of quantum technologies.
- Have a good perspective of the unique features of 2D materials and of many-body condensed states, with an eye on the opportunities they provide for exploring novel and intrinsically quantum-mechanical phenomena.
- Understand fundamental models and concepts of the theoretical description of these materials, and acquire skills to independently apply or extend such models.
- Understand the relations between the physics that underlines the properties of a material and the technologies and devices it enables.
- Have know-how and skills to engage effectively and in depth with the current research literature on these materials, the underlying phenomena, and their applications.

Subject Matter

1. *Two-dimensional materials* — Representative systems and their key feaures (structure, production, mechanical, electronic, transport and optical properties. Electronic structure based on tight-binding and effective low-energy models. Electronic structure of monolayers, bilayers and multilayers; twisted 2D crystals. Confined electrons: nanoribbons, quantum dots and other artificial microstructures. Crystalline lattice: phonons, elasticity, pseudomagnetic fields. Device applications.
2. *Quantum magnetism* — Exchange interactions and the origin of magnetism. Spontaneous symmetry breaking, ferro- and anti-ferromagnetism. Magnetic ground states and excitations. Novel magnetic states in 2D materials.

3. *Condensed materials I: Bose-Einstein condensates* — Broken gauge symmetry. Order parameter and superfluity. Fundamental properties. Condensate motion and phase of the order parameter. Vorticity quantization.
4. *Condensed materials II: superconductor*s — Broken gauge symmetry of charged particles and the Higgs-Anderson mechanism. Ginzburg-Landau theory. Meissner effect. Superconductors of type I and type II. Cooper instability and BCS theory. Ground state and excitations. Josephson's effect, SQUIDS and their applications. Superconductor devices. Particulars and unsolved questions of superconductivity in 2D; current forefront experiments using 2D materials.

Main Bibliography

1. Steven M. Girvin; Modern condensed matter physics. ISBN: 978-1-107-13739-4
2. Mikhail I. Katsnelson; The physics of graphene. ISBN: 978-1-108-61756-7 e-book
3. Phaedon Avouris; 2D materials. ISBN: 978-1-316-68161-9 e-book
4. Stephen Blundell; Magnetism in condensed matter. ISBN: 0-19-850591-4
5. James F. Annett; Superconductivity, superfluids, and condensates. ISBN: 0-19-850756-9
6. J. M. B. Lopes dos Santos; Lecture Notes, Unpublished

Complementary Bibliography

1. Neil W. Ashcroft; Solid state physics. ISBN: 0-03-083993-9 US College Edition
2. Gerald D. Mahan; Condensed matter in a nutshell. ISBN: 978-0-691-14016-2
3. P. W. Anderson; Concepts in solids. ISBN: 0-8053-0229-8
4. Alexandre M. Zagoskin; Quantum engineering. ISBN: 978-0-511-84415-7 e-book
5. Various authors; Research and review articles and other readings to be distributed during the course.

Teaching Methods and Learning Activities

The contact hours blend lecturing, discussion of previously assigned readings and work with practical examples.

Key words

Quantum materials; 2D materials; quantum magnetism; many-body condensates; superconductivity; quantum technologies; quantum condensed matter theory; electronic, magnetic and structural properties of materials.

Description of assessment

The assessment comprises the submission of homework assignments (30%) and a final exam (70%). Each assignment will be announced in due time and may take different forms, such as: solve a problem, expand a calculation or provide further details on a selected topic, critically review a published research paper.

Observations

Unit evaluation panel: Vitor M. Pereira, Eduardo V. Castro, J. Agostinho Moreira.

Computational Complexity

Code: CC4011

Teaching components (total hours in semester)

T	TP	PL	Total Contact hours	ECTS	Total Hours
	42		42	6	162

Lecturers

Rogério Ventura Lages dos Santos Reis (rvreis@fc.up.pt)

Goals

We will study some techniques that prove or suggest that there are no known eficient method to solve some important problems in computer science. We will study several complexity classes and their relationship, namely: P, NP, co-NP, PH, RP, BPP, IP.

Learning Outcomes and Skills

Upon successful completion of this course, students will be able to:

a) Distinguish between complexity classes.

b) Classify decision problems into appropriate complexity classes, including P, NP, PSPACE and complexity classes based on randomised machine models and use this information effectively.

Subject Matter

1) Motivation and background

2) Complexity classes P and NP

3) Polynomial time hierarchy

4) Class PSPACE and Alternation

4) Non-uniform Models. Boolean Circuits, machines with advice. Class P/poly

5) Randomized complexity classes: RP, BPP and ZPP

6) Interactive protocols, classes IP, AM e MA

Main Bibliography

- Sanjeev Arora and Boaz Barak; Complexity Theory: A Modern Approach
- Oded Goldreich; Computational Complexity: A Conceptual Perspective, Cambridge University Press, 2008. ISBN: 978-0-521-88473-0

Complementary Bibliography

- Michael Garey and David Johnson; Computers and intractability: A guide to NP-Completeness, W. H. Freeman, 1979. ISBN: 0716710455

- C. Papadimitriou; Computational complexity, Addison Wesley Longman, 1994. ISBN: 0201530821
- D.Z. Du and K.I. Ko; Theory of Computational Complexity, John Wiley and Sons, 2000. ISBN: 978-0-471-34506-0

Teaching Methods and Learning Activities

Lectures with practical assignments.
Distributed grading.

Key words

Theoretical Computer Science, Computational Complexity,

Description of assessment

Distributed evaluation with final exam.

Eligibility for exams:

Two tests where the student needs to achieve a mark of 1/3 (in each), and an average of 1/2.

Calculation formula of final grade

The final classification will be the average of the classifications obtained in the tests.

Special assessment (TE, DA, ...)

Final exam

Classification improvement

Final exam

Sensing and Signal Analysis

Code:

Teaching components (total hours in semester)

T	TP	PL	Total Contact hours	ECTS	Total Hours
-	42	-	42	6	162

Lecturers

Nuno Azevedo Silva
José Luís Campos de Oliveira Santos

Goals

To give the students an insight to optical sensing, mainly interferometric based, supported by classical, semi-classical and quantum principles, addressing in each of the cases the relevant noise sources and signal analysis techniques.

Learning Outcomes and Skills

- The students will be able to understand the basic principles beyond interferometric sensing, including the effect of the source coherence in the sensing device performance
- They are expected to understand the homodyne, and heterodyne, techniques for signal recovery.
- The students should understand the evolution in optical sensing from the classical to the semi-classic paradigm and then to the one supported by the quantum system phenomenology.

Subject Matter

- *Classical Optical Interferometers for Measurement/Sensing.*

  Interferometric configurations (bulk and in fiber optics). Optical sources, beam splitters and polarization control elements. Photodetectors for multiple and single photon detection. Intrinsic and environmental induced noise sources in an interferometer. Signal-to-noise ratio and measurement merit factor in an interferometer. Homodyne and heterodyne techniques for phase recovery in optical interferometers and characterization of their performance.

  Semi-Classical Optical Interferometers for Measurement/Sensing

  Squeezed light and the Heisenberg phase resolution limit in an optical interferometer. Generation of squeezed light from light in a coherent state using optical non-linear interactions (optical parametric amplification and frequency doubling). The case study of the LIGO interferometric observatory.

  Optical Interferometers for Quantum Measurement/Sensing.

Interferometers with entangled photons. The entangled N00N quantum state in a Mach-Zehnder interferometer. The signal-to-noise ratio in these interferometers. Super sensitivity and super resolution. Optical sources for emission of entangled photons and optical detectors with the ability to distinguish photon numbers at the level of single photons. The environment problem. Evolution of the signal processing techniques mastered in classical optical interferometry to address the phase recovery in quantum interferometers. Quantum sensor and the sensing protocol. Figures of merit in quantum sensing. Quantum metrology and its future impact in the International System of Units.

Main Bibliography

- Guenther, Robert D.; "*Modern Optics*". ISBN: 0-471-51288-5

Complementary Bibliography

- Born, Max; "*Principles of Optics*". ISBN: 0-08-018018-3
- Reitze, David; Saulson, Peter; Grote, Hartmut (Editors), "*Advanced Interferometric Gravitational-wave Detectors: Essentials of Gravitational Wave Detectors*". ISBN: 978-9813146075
- Hans-A. Bachor, Timothy C. Ralph; "*A Guide to Experiments in Quantum Optics*". ISBN: 978-3-527-41193-1

Teaching Methods and Learning Activities

- Classes for presenting and discussing theoretical topics, with relevant examples, and for problem solving.
- Some visits to laboratories to see some relevant experiments ongoing on the research labs.

Key words

[Sensing, Optical Sensing, Interferometric Optical Sensing, Classical, Semi-classical and Quantum Optical Sensing, Noise Sources, Signal Processing Techniques, Sensing Systems]

Description of assessment

Assessment by final exam. Optional written report can be considered for 30% of the grade.

Observations

[...]

Topics in Theoretical Physics

Teaching components (total hours in semester)

T	TP	PL	Total Contact hours	ECTS	Total Hours
-	42	-	42	6	162

Lecturers

Eduardo Vieira Castro (evcastro@fc.up.pt)
João Viana Lopes (jlopes@fc.up.pt)

Goals

To provide students with the basic tools to describe condensed matter systems and phenomena using Quantum Field Theory.

Learning Outcomes and Skills

- Being able to understand how the physics of many-body condensed matter systems can be described using Quantum Field Theory methods.
- Knowing how to apply perturbation theory to many-body condensed matter systems starting with a Quantum Field Theory description.
- Understanding symmetry broken phases of condensed matter many-body systems using the language of Quantum Field Theory

Subject Matter

- *Second quantization and coherent states.*
- *Functional path-integral*
- *Perturbation theory*
- *Order parameters and broken symmetry*

Main Bibliography

- Condensed Matter Field Theory, A. Altland and B. Simon, Cambridge University Press.

Complementary Bibliography

- Quantum Many-Particle Systems, J. W. Negele and H. Orland.
- Introduction to Many-Body Physics, P. Coleman, Cambridge University Press.

Teaching Methods and Learning Activities

- Classes for presenting and discussing theoretical topics, with relevant examples, and for problem solving.

Key words

[Quantum Field Theory, Many-Body, Condensed Matter, Path-Integral, Perturbation-Theory, Order-Parameter, Broken-Symmetry]

Description of assessment

Assessment by final exam.

Observations

[...]

Examples of Internship Projects

1. Experimental Optical analogues for the simulation two-dimensional quantum fluids

Providing Institution

INESCTEC

Place of work

Center of Applied Photonics, Department of Physics and Astronomy, Faculty of Sciences, UPorto

Supervisor(s)

Nuno Azevedo and Tiago D. Ferreira

Start date and duration

March 2024; 14 weeks

Goals

We will break the Internship and the study of Quantum Fluids of Light (QFLs) into two operational blocks:

1. Theoretical model: Understand the basic concepts behind the light fluid analogy focusing on the paraxial geometry configuration. Derive the Nonlinear Schrödinger equation (NLSE) and understand the connection to nonlinear optics and quantum fluids, discussing its limitations. Basic review of the state-of-the-art of QFLs in nonlinear optical materials.

2. Development of an experimental case study, either:

    a. Exploring quantum turbulence with QFLs – possible experimental verification of [R1];

    b. Observation of the Bogoliubov dispersion relation and drag force suppression – possible experimental verification of [R2];

Learning Outcomes and Skills

Quantum simulation is one of the pillars of quantum technologies and concerns the controllable emulation of quantum systems. In this project the students will be introduced to the field of optical quantum fluid analogues, exploring how one can use nonlinear optics to emulate quantum-like phenomena and thus create a quantum simulator. The students will also have contact with experimental setups and methodologies, learning concepts of advanced optical system design and wavefront shaping, and observing nonlinear optics phenomenology with photorefractive crystals.

Project description

The project and research internship aim to introduce the student to the fundamental concepts of Quantum Fluids of Light (QFLs) in an integrated but increasingly autonomous research

environment. The training covers mathematical foundations, numerical and computational tools, and hands-on experimental research.

Main Bibliography

[R1] Silva, Nuno Azevedo, Tiago D. Ferreira, and Ariel Guerreiro. "Exploring quantum-like turbulence with a two-component paraxial fluid of light." Results in Optics 2 (2021): 100025.

[R2] Ferreira, Tiago D., Nuno A. Silva, and A. Guerreiro. "Superfluidity of light in nematic liquid crystals." Physical Review A 98.2 (2018): 023825.

[R3] Carusotto, Iacopo. "Superfluid light in bulk nonlinear media." Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 470.2169 (2014): 20140320.

Complementary Bibliography

[R4] Fontaine, Quentin, et al. "Interferences between Bogoliubov excitations in superfluids of light." Physical Review Research 2.4 (2020): 043297.

[R5] Michel, Claire, et al. "Superfluid motion and drag-force cancellation in a fluid of light." Nature communications 9.1 (2018): 1-6.

2. Tuning properties of novel quantum 2D materials

Providing Institution
IFIMUP

Place of work
Department of Physics and Astronomy, Faculty of Sciences of the University of Porto

Supervisor(s)
Catarina Dias and João Ventura (cdias@fc.up.pt and joventur@fc.up.pt).

Start date and duration
March 14 weeks

Summary

2D materials (such as graphene, molybdenum disulfide or the novel MXene family) have attracted great attention due to their unique electronic and optical properties [1-3]. Furthermore, enhanced quantum confinement and edge effects can be obtained by further reducing their dimension to zero. Quantum dots (QDs) derived from 2D materials have been successfully synthesized with high stability and new optical properties for a large range of applications. In particular, hybrid QD-polymer composites offer the feasibility of fabricating memristors for data storage or neuromorphic computing. This approach, based on solution-processed methods, provides unique advantages such as low cost and large scale integration. The use of low-dimensional nanomaterials has provided astonishing first results by conferring neuromorphic devices high scalability, higher switching control, more spatial and temporal reproducibility, and much lower power consumption and fabrication cost. However, there still exists a lack of fundamental understanding on the physical mechanism, including the consideration of quantum effects. There is thus an urgent need to explore and understand novel QD-based devices and structures. The aim of this project is then to fabricate and study thin films with quantum dots (QDs) of MXenes, a novel family of 2D materials. Our approach of using composite stacks, combining organic polymers (such as PMMA, PVA or PVP) with 2D materials brings unique advantages such as low cost, simplicity and large- scale fabrication potential. The work will be carried out at IFIMUP (www.ifimup.up.pt), together with a team specialized in microfabrication and characterization of low dimensional materials. Besides the two supervisors, the group currently has a Postdoc, a research fellow, two PhD (funded by FCT and Quantum Portugal Initiative) and a MSc student. Existing collaborators include INL (International Iberian Nanotechnology Laboratory), INESC-MN (*Instituto de Engenharia de Sistemas e Computadores – Microsistemas e Nanotecnologias*) and i3S (*Instituto de Investigação e Inovação em Saúde da Universidade do Porto*).

Main objectives:

(i) Fabrication of thin films based on 2D materials composites (synthesis and spin-coating);

(ii) Characterization of the structural, morphological and chemical properties of the fabricated materials (XRD, SEM, AFM, PPMS);

(iii) Analysis of the electrical transport (vertical and parallel configurations) and light interaction. Due to the novelty of the proposed topic, one publication is expected. Afterward, the candidate is welcomed to pursue a PhD under funding opportunities such as national (FCT, Quantum Portugal Initiative) and international calls (Marie Skłodowska-Curie Actions).

Bibliography

[1] Sariga et al. Adv. Mater. Inter. 10, 514 (2023), 10.1002/admi.202202139.
[2] Einafshar et al. Top. Curr. Chem. 381, 5 (2023), 10.1007/s41061-023-00439-4. [3] Hazan et al. Adv. Mater. 35, 11 (2023), 10.1002/adma.202210216.

[...]

3. *Manipulating phonons at the nanoscale level*

Providing Institution

IFIMUP

Place of work

Department of Physics and Astronomy, Faculty of Sciences of the University of Porto

Supervisor(s)

Rui Vilarinho Silva, Estelina Lora and J. Agostinho Moreira (rvsilva@fc.up.pt,

estelina.silva@fc.up.pt, jamoreir@fc.up.pt)

Start date and duration

March, 14 weeks

Summary

Phonons are quantum states of crystal lattice vibrations that behave like propagating waves. They can reflect and transmit at the interfaces between two different materials with different elastic properties, and they can also be scattered at domain walls in ordered phases in ferroelectrics and (anti)ferromagnetics. As phonons transport thermal energy, these mechanisms can be used to confine and control heat transport at the nanoscale [1].

The objective of this project is the simulation and realization of interference experiments with phonons and to control the energy propagation by phonon interference and different phonon transport regimes in artificial heterostructures. We aim at exploring phonon interference and transport in planar superlattices with atomically terminated interfaces. We propose to use planar heterostructures made with n unit cell thick of $SrTiO_3$ (n = 3, 6 and 9) and m unit cell thick $RFeO_3$, R a trivalent rare-earth cation (m = 5 and 10), as the platform for investigating and designing the phonon interference effects, taking advantage of the atomic connectivity between the building blocks of the crystal structures of the chosen compounds. Moreover, the room-temperature soft mode and ferroelectric like polarization in $SrTiO_3$ ultrathin films [2] are potential tools to control thermoconductivity, because they are expected to affect the 'space' of the acoustic phonons. Phonon interference will be probed by means of inelastic light scattering, THz-pump-probe experiments and thermal transport experiments.

The complexity and diversity of the envisioned experiments, which are key for the success of the proposed research project, requires computational simulations to guide experiments and interpret results. From the computational perspective, it is therefore proposed to perform *ab initio* calculations by employing Density Functional Theory to compute the structural and electronic properties of the systems of interest. Moreover, for a structural phase to be synthetically accessible one should

also probe the dynamical stability of the system, which requires the study of the phonon frequencies. If imaginary frequencies emerge (usually represented by negative modes in the phonon dispersion curves), this would indicate that the system is at a potential-energy maximum (transient state), undergoing a phase transition and thus cannot be kinetically stable at the given temperature and/or pressure conditions. Respective information will also provide insights into the phonon dispersion, more specifically to the optical phonon modes and if these increase the available phase space of the phonon-phonon scattering of the heat-carrying acoustic phonons. If so, such an effect will cause low values for the lattice thermal conductivity (due to the interplay between the phonon-phonon Umklapp scattering rates and the soft phonon frequencies), and thus interest also lies in performing calculations based on the third-order phonon interactions.

The proposing team has the scientific competences and tools to perform this project, and resources in relevant HPC facilities are available to pursue the proposed computational tasks [3-5]. This proposal benefits of the financial support of a running project PTDC/FIS/03564/2022, and running collaborations with expert groups on nanofabrication and characterization.

This project will strengthen the understanding of the physics of phonons. Furthermore, since phonons are responsible of heat transport, this project will also have an impact on thermal management applications at the nanoscale. So, it is expected that further studies can be developed in a PhD program.

Bibliography

[1] APL Mater. 9, 070701 (2021).
[2] Sci Rep 7, 2160 (2017).
[3] Physical Review B 94, 214103 (2016).
[4] Physical Review B 99, 064109 (2019).
[5] Phys Rev B 104, 024103 (2021).

4. Interaction-free quantum imaging and computation

Providing Institution

INL - International Iberian Nanotechnology Laboratory

Place of work

INL - International Iberian Nanotechnology Laboratory

Supervisor(s)

Ernesto Galvão (ernesto.galvao@inl.int)

Start date and duration

To be defined (flexible) from 3 months up to 12 months

Goals

The goal is to study protocols for interaction-free imaging and computation, with the possibility of proposing new photonic interferometric schemes for these protocols. Starting with the original proposal by Elitzur-Vaidman [Elit93], which uses a two-mode Mach-Zehnder interferometer for probabilistic identification of an absorbing object with no photon absorption. Then we will look at generalizations that have been proposed, with the goal of establishing communication without exchange of particles [Sali13], computation [Mitc01, Sali21], imaging [Lem14, Yan23]. The basic idea is to review these proposals, understand the underlying assumptions, and gauge the possibility of implementing them in the lab, or using cloud-based photonic chips made available by company Quandela [Quan23].

Learning Outcomes and Skills

The student will learn the quantum description of multimode interferometers, how to calculate the probabilities of different outcomes, and how to use them for interaction-free imaging. They will review protocols using nested interferometers for counterfactual communication [Sali13], quantum computation [Mitc01, Sali21], and imaging [Lem14, Yan23]. A helpful online virtual lab can be used for small demonstrations of some of the simplest interferometers [flyt23]. The student will be confronted by the different possible interpretations for these protocols, and we will try to analyse to what extent the counterfactual claims are justified. An optional task involves learning how to program cloud-based photonic quantum computers made available by the French company Quandela, for possible implementations of simple versions of some of these protocols.

Project description

We will start by reviewing the basics of the Mach-Zehnder interferometer, and how it can be used to implement the interaction-free imaging experiment proposed by Elitzur and Vaidman. Then we will review how nested interferometers allow for improved performance at the imaging task, and look at generalizations, for example imaging of semi-transparent objects.
We will analyse the related counterfactual communication protocols, and look also at different versions of counterfactual computation protocols, and their possible implementations in currently available photonic devices.

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5. Excitonic instability and exciton condensation in 2D materials with nontrivial electronic topology

Providing Institution

Centro de Física das Universidades do Minho e do Porto

Place of work

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Supervisor(s)

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Start date and duration

To be defined (flexible)

Background and Goals

Two-dimensional Van der Waals materials (2DM) are privileged platforms to engineer quantum electronic behaviour on many fronts [1]. Research in 2D materials (2DM) is among the most competitive and promising directions in quantum condensed matter physics, comprising an ever-growing portfolio of atomically thin materials with a remarkable scope of properties of interest to applications, as well as a fruitful playground to discover and validate new phenomena and fundamental physics [2,3].

In particular, being easily integrated into gated planar devices and amenable to on-demand doping over large density ranges by field-effect, 2DM are a privileged platform to assess and manipulate electronic interactions; for this, in recent years they have materialized the idea of tunable correlated states in quantum materials. In addition to the reduced screening in 2D, which natively enhances interaction effects, we find several classes of 2DM with nontrivial electronic topology. This combination of tunability, enhanced interactions, and nontrivial topology, drives a strong theoretical and experimental interest in studying the interplay between different (often competing) correlated electronic states, such as magnetism, superconductivity, charge-density wave states, and other may-body condensed states. [3]

The focus of this thesis proposal will be to theoretically study how the excitonic instability (which drives an electron-hole electronic system into a macroscopic condensed state of excitons: a Bose-Einstein condensate of excitons), and the resulting condensed state are affected when the underlying electronic bands carry nontrivial topology. A model of a 2D quantum spin hall (QSH) insulator will be explored to assess the interplay between the nontrivial topology, the stability of the excitonic state, and the stability (or feasibility) of the QSH state itself.

This project is directly motivated by recent experimental results suggesting that the QSH state in WTe_2 (the first experimentally established QSH insulator) might be stabilized by an underlying excitonic instability [4-6]. The mechanisms of this interplay and the possibility of stabilizing more robust combined correlated/topological states at higher temperatures is under active scrutiny by the community. The work on this project will build on previous work by the supervisor on excitonic instabilities, excitonic condensation and their interplay with superconductivity, as well as topological states in 2DM [4,7,8].

Tackling this project will require that the student has an interest and an adequate background in quantum condensed matter theory, namely: dexterity with second quantization, setting-up and handling simple tight-binding models of electrons in crystals, preliminary experience with self-consistent mean-field calculations applied to many-body problems (e.g. BCS superconductivity, Bose-Einstein condensation).

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6. *Ab-initio* modeling of carbon-based minerals

Providing Institution

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Start date and duration

To be defined (flexible)

INTRODUCTION

Research in Materials Science has many implications in Physics, Chemistry, Geology/Geophysics, and Astromineralogy, where many minerals (sulfides, pyroxenes, carbonaceous compounds) can be applied to several fields, such as photonic crystal fibers, waveguides for applications in all-optical switches and optical logic elements, IR transmitting materials, photovoltaics and, more recently for catalytic applications, with particular interest for the modern chemical and pharmaceutical industries. Additionally, there is substantial interest among the mineral physics, geophysics and astrophysics communities to study phase-transitions of compounds that are constituents of the mantle of the Earth, i.e. ABO_3 compounds, like $MgSiO_3$ or even exotic carbonaceous systems which compose meteorite dusts. Therefore, studying the high-pressure behavior of minerals is important to understand the possible structural transitions of many materials at extreme conditions in the Earth mantle, planetary interiors and other cosmic environments where specific conditions are met.

Carbon microcrystals with unique structural peculiarities have been prowling in the dust, and these are left behind by meteors when entering the atmosphere of the Earth. High temperature and high pressure cause tiny particles to break away from the main body, forming a cloud of meteorite dust. Usually, this fine dust simply dissipates into the atmosphere or is mixed with terrestrial soil, making it impossible to recover and analyze such crystalline structures. Examples of dust constitutes, such as those originated from the Chelyabinsk meteor (2013), which blew apart high in the atmosphere, fortunately where possible to recover and study due to the low temperatures that occurred in Chelyabinsk at the time of the event. While analyzing the well-preserved grains through different experimental techniques, it was possible to observe that the crystals were in fact formed by layers of graphite surrounding a central carbon nanocluster. Further studies were engaged in order to try and understand the formation of respective structure. Therefore, by carrying out a series of computational simulations it was found that the crystals consisted of either a cage-like ball of 60 carbon atoms called buckminsterfullerene or a molecule called polyhexacyclooctadecane. While conclusions were drawn to the fact that the formation of these crystals were a result of the conditions of high temperature and pressure (with impact in the atmosphere of the Earth), the precise mechanisms that resulted in their formation still remain a mystery [1].

The project therefore will be based on quantum chemical modeling studies on novel carbon-based materials (i.e. 2D carbon allotropes). These theoretical computational frameworks are a powerful and accurate tool for investigating detailed relevant properties of a wide range of minerals (electronic, optical, elastic, thermodynamics). Such a project may provide a new platform for an accurate and detailed understanding of minerals under different conditions to those which are well known at room conditions – the unique structures found in the meteorite or cosmic dust that have not been observed before demonstrate the unlimited potential of nature to synthesize new materials.

It is foreseen, continuation of the dissertation work based on the present proposal, with the possibility of pursuing a PhD program. For such, financial support from the Portuguese Foundation for Science and Technology will be applied for to support the stipendship during the four years of the PhD and respective tuition fees.

THEORETICAL STUDY

Density Functional Theory (DFT) is a computational *quantum mechanical* modelling *method* widely applied to study the ground-state electronic properties of many-body systems (molecules, nanosystems, periodic crystalline systems). Within this methodology, the electron orbitals are obtained as solutions of a set of single-particle Schrödinger-like equations, referred to as the Kohn-Sham equations[2-5], in which potential terms depend solely on the electron density, n(**r**), instead of a many-body function of *3N* electronic degrees of freedom. One of the terms of the Kohn-Sham potential takes the form of a functional derivative over the density and is called the exchange-correlation (xc) functional. This term cannot be described exactly and thus is constructed by employing approximations, with many different forms and developed for a wide variety of physical systems and applications. The simplest approximation to the xc potential is the Local-Density Approximation (LDA), for which the potential depends solely on the value of the density at point **r**. The generalized-gradient approximation (GGA) is a simple extension of the LDA, and can be seen as an improvement in accuracy, since it attempts to incorporate the effects of inhomogeneities by including the gradient of the electron density (making it a semi-local method). New approaches to xc functionals have been implemented over the years to try and correct for several properties which cannot be accurately described by the (semi-)local functionals (i.e. underestimation of the band-gaps; incorrect description of long-range correlation in particular van-der-Waals interactions; strongly localized *d*- and *f*- states are incorrectly described as being delocalised states). The different fucntionals have been grouped into different rungs in a sequence of chemical accuracy, known as the Jacob's ladder of density functional approximations[6]. As the ladder is ascended, the functionals incorporate higher levels of theory with increasingly complex parameters.

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7. Exploring novel electronic devices based on topological insulators grown by molecular beam epitaxy

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INL – International Iberian Nanotechnology Laboratory

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Start date and duration

To be defined (flexible)

Summary

Topological insulators are a new class of quantum materials that offer unique physical properties and the potential to revolutionize future electronics and information technology, from more energy-efficient spintronics to robust quantum computing. Topological insulators are insulating in the bulk but possess topologically protected conducting states at the surface. These topological surface states exhibit spin-momentum locking and could allow for dissipationless transport.

At INL we can grow topological insulators, such as Bi_2Se_3, by molecular beam epitaxy with excellent crystalline quality. By using the state-of-the-art cleanroom facilities available at INL, we can fabricate functional micro- and nanodevices based on these topological insulators.

At INL the MSc student will participate in the growth of the topological insulators and in the fabrication and characterization of the devices, from structural characterization of the materials to electrical transport measurements of the devices. This will be accompanied by a theoretical understanding of the physics behind topological insulators and the functionality that can be obtained from these materials through literature review. From this, novel electronic device concepts based on the functionality of the topological insulators will be discussed and explored.

After finishing the MSc thesis, there could be possibilities to continue in the group and pursue a PhD by applying to the yearly Portuguese national call for PhD scholarships funded by the Portuguese national agency Fundação para a Ciência e a Tecnologia (FCT - https://www.fct.pt/en/).

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8. Decreasing the sign problem with the sampling of sets

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Start date and duration

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Summary

Strongly correlated electronic systems remain an enormous numerical and analytical challenge. The Monte Carlo method is one of the most powerful methods to tackle problems with strong interactions and correlations [5,6]. Usually, this technique is applied to a classical problem. To apply it to a quantum problem with interactions (Quantum Monte Carlo- QMC), the problem has to be mapped into a classical problem, and the partition function is converted into a sum over classical configurations. This sum could be sampled with polynomial time using the importance sampling approach. The sign problem appears because the quantum to classical transformation induces negative signs in some sum terms. This negative sign invalidates the direct association of each parcel with a weight and imposes the modification to the absolute value. This problem can be rewritten as the average sign that could make the measurements impossible due to the relative error (huge variance and very small mean) [3]. During last years many attempts were done to ease this problem [1,2,4].
We intend to use the fermionic Hubbard model in a one-dimensional and two-dimensional square lattice as a laboratory to study the QMC properties. The student will write his code of the determinant Monte Carlo and characterize the sampling of the sign problem and its dependence on the temperature and chemical potential.
To improve the quality of the sampling, we will approach this problem. By introducing a deterministic map between classical configurations, the sampling between configurations is changed to a sampling between sets. This approach could decrease the sign problem and open the door to a new perspective of the Quantum Monte Carlo.

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