

# TFM proposals 2024-25

## Quantum matter, simulations, and technologies

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1. Director: **Maria N Gastiasoro** ([maria.ngastiasoro@dipc.org](mailto:maria.ngastiasoro@dipc.org))

Title: **Unconventional Superconductivity in Transition Metal Dichalcogenides**

Quantum materials with flat electronic bands are ideal playgrounds for the exploration of novel many-body phenomena driven by electronic interactions. Recent experiments on Ta-based heterostructures indicate the presence of an electronic flat band, charge density waves states and unconventional superconductivity. During this project we will develop a minimal theoretical model, study the superconducting channels allowed by symmetry in the system, and explore their response to applied magnetic fields. A combination of analytical methods and simple numerical routines will be implemented to characterize and predict the superconducting properties of the model. There will be a strong collaboration with experimental groups working on Ta-based heterostructures.

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2. Director: **Daniel Hernangómez-Pérez** ([d.hernangomez@nanogune.eu](mailto:d.hernangomez@nanogune.eu))

*One choice between the two projects listed below.*

Title: **Nonlinear photocurrents in magnetic 2D van der Waals systems for next-gen quantum technologies**

The charge and spin response of matter under light illumination holds great promise for next-generation energy-efficient optoelectronic and optospintronic devices, as well as for quantum technological applications like quantum and neuromorphic computation. In the absence of bulk inversion symmetry, a DC current can be generated via second-order nonlinear response through the bulk photovoltaic effect. A similar effect exists for spin currents, where time-reversal symmetry must be broken to generate pure nonlinear spin currents without associated charge flow.

The objective of this project is to investigate charge and spin photovoltaic effects in atomically-thin 2D van der Waals magnetic heterostructures, which exhibit a wide range of fascinating phenomena, including in-plane ferromagnetism and layered antiferromagnetism (both in-plane and out-of-plane) that can be manipulated by external fields. We will adopt a dual approach, combining ab initio calculations based on density functional theory with Wannier and model-based analytical methods.

Title: **Emergent many-body magneto-optics of van der Waals heterostructures for quantum technologies**

Excitons, bound quasiparticles resulting from the electrostatic interaction between electrons and holes in materials, play a vital role in the optical properties of two-dimensional van der Waals materials, particularly transition-metal dichalcogenides

(TMDCs). In this context, excitons dominate the optical spectrum, with the associated excited-state phenomenology influencing a broad array of applications, from photovoltaics to quantum applications. For this, understanding the behavior of excitons under applied external magnetic fields becomes crucial. This behavior can be quantified by the *excitonic g-factor*, which is involved in the exciton dynamics and for which the incorporation of the nuances in the exciton wavefunction has recently been found to be a crucial element. The objective of this project is to analyze by computational means the magnetic behavior of excitons in van der Waals heterostructures employing *first principles* and *state-of-the-art* numerical calculations (density functional theory, GW-Bethe-Salpeter equation). This project requires a combination of numerical skills (Python, basic Fortran) and analytical work. The project will be carried out at CIC NanoGUNE in San Sebastián, with the possibility of partially remote work.

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3. Director: **Aitor Bergara** ([a.bergara@ehu.es](mailto:a.bergara@ehu.es)), **Mikel Sanz** ([mikel.sanz@ehu.es](mailto:mikel.sanz@ehu.es))

**Title: Exploring Quantum Algorithms for Predicting Pathogenicity of KCNQ2 Gene Variants**

This project will explore quantum machine learning methods for predicting the pathogenicity of genetic mutations in the KCNQ2 gene, which is associated with conditions such as benign familial neonatal epilepsy and epileptic encephalopathy. Conventional machine learning has shown promise in pathogenicity prediction but remains limited in clinical reliability. Quantum computing, particularly in the Noisy Intermediate-Scale Quantum (NISQ) era, offers potential advantages in terms of accuracy and efficiency for small, noisy datasets. The project will evaluate various quantum algorithms to assess their effectiveness on clinical data of this kind. The aim will be to identify conditions under which quantum methods outperform classical models in these settings.

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4. Director: **Jon Lafuente Bartolomé** ([jon.lafuente@ehu.es](mailto:jon.lafuente@ehu.es)), **María Blanco Rey** ([maria.blanco@ehu.es](mailto:maria.blanco@ehu.es))

**Title: Spin relaxation in quantum materials for spintronics**

The active control of the spin degrees of freedom in solid-state systems is the ultimate goal of spintronics. A fundamental quantity in the design of efficient spintronic devices is the spin relaxation lifetime. This parameter is a descriptor for the spin precession (Dyakonov-Perel mechanism) and spin flip (Elliot-Yafet) dynamics of electrons. The aim of this project is to develop computational tools to model these spin-relaxation mechanisms from first principles. The calculations will be based on Density Functional Theory combined with more advanced many-body methods to account for the scattering of electrons by impurities and phonons. Given that the spin-relaxation events are a consequence of the relativistic spin-orbit interaction, topological and two-dimensional materials arise naturally as promising subjects of study.

The first proposed task is to calculate the so-called Elliot-Yafet parameter  $b^2$ , which is an intrinsic property of a given material that depends on its electronic structure and will condition the spin lifetime. A proper treatment of the spinorial wavefunctions in the Wannier formalism will allow us to determine the leading contributions and the degree of anisotropy of  $b^2$ . In a second stage of the project, the effects of phonons and impurities in the spin-relaxation processes will be explicitly considered, which will allow for a quantitative comparison between our theoretical results and available experiments. In a final stage, the developed computational tools will be used to propose new materials for potential applications in spintronics.

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5. Director: **Asier Eiguren** ([asier.eiguren@ehu.eus](mailto:asier.eiguren@ehu.eus)), **María Blanco Rey** ([maria.blanco@ehu.eus](mailto:maria.blanco@ehu.eus))

**Title: Advanced Electronic Structure Modeling Using Plane Wave and Localized Basis Sets**

The aim of this project is to develop a systematic approach for improving the basis sets of the SIESTA electronic structure code. The accuracy of plane wave codes is controlled by a single parameter, the cutoff energy, whose associated de Broglie wavelength determines the smallest detail that can be resolved in the charge density and wave functions. While atomic orbitals offer a relatively small and efficient basis set, they lack the straightforward tunability provided by the cutoff energy parameter in plane wave methods. Consequently, improving the basis set for atomic orbitals requires specialized expertise. We have some preliminary experience in this direction using orthogonal polynomials. However, the objective of this project is to refine, perfect, and develop a research-level software tool that can be integrated into the official versions of the SIESTA code. This tool will provide a systematic method for enhancing the accuracy and efficiency of localized basis sets in SIESTA, making advanced electronic structure calculations more accessible and robust. In the next step, the objective is to gain hands-on experience with the SIESTA code and calculate vacancy impurities in a real material comprising several hundred atoms. We will test the efficiency of the newly developed basis set and gain expertise in the real-space representation of wave functions and charge densities, including considerations in the relativistic limit.

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6. Director: **Lianao Wu** ([lianaowu@gmail.com](mailto:lianaowu@gmail.com))  
*One choice between the two projects listed below.*

**Title: Trotterization to simulate adiabatic evolution and adiabatic quantum computation**

In 2002, we proposed to use Trotterization to simulate adiabatic evolution of a time-dependent driving Hamiltonian to simulate BCS model. The experimental test of this BCS simulation was done at Massachusetts Institution of Technology. Now the idea have become a new type of quantum computation, the Trotterized (or digitized) adiabatic quantum computation. Along this line, we recently propose a static version

of this technique to perform the optical simulation of the adiabatic evolution of an arbitrarily given Hamiltonian. The dynamical process of the adiabatic evolution is mapped to a static linear optical array which is robust to the errors caused by dynamical fluctuations. We plan to propose experimentally implement the static adiabatic evolution of different dynamical processes in physical setups like photonic chips.

**Title: Developing and implementing Self-protected quantum algorithms and quantum simulations in the presence of noises**

Only a limited number of quantum algorithms are known to provide a speed-up over classical algorithms. Nevertheless, both these established quantum algorithms and any emerging ones play a pivotal role in driving the advancement of quantum computers. However, to enable execution of quantum algorithms, it is crucial to eliminate decoherence and noise for instance via dynamic decoupling and quantum error correction protocols. As potential alternatives we once introduced self-protected quantum algorithms many years ago. While these quantum algorithms are important in their own right, remarkably these quantum algorithms are innate immune to a large class of errors. Quantum algorithms of this kind can be used in the Noisy Intermediate- Scale Quantum regime. Lately, a class of self-protected quantum simulations in the presence of weak classical noises are noticed, and the equivalence between weak classical noise and noiseless quantum simulations can be demonstrated mathematically. This equivalence implies that a self-protected quantum simulation does not require any extra overhead in its experimental implementation. Since it has long suffered from great difficulties in, for example, experimentally implementations of qubit-encoding and stabilizers, a universal fault-tolerant quantum computer using quantum error correction are not likely to be available very soon. The idea of self-protected quantum algorithms against errors seems to be a bright alternative. The student will work on the implementation of one of our proposed algorithms on the 5 (or more) - qubit IBM platform(s).

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7. Director: **Íñigo L. Egusquiza** ([inigo.egusquiza@ehu.eus](mailto:inigo.egusquiza@ehu.eus))

**Title: The Schmid-Bulgadaev phase transition: a circuit phenomenological perspective**

In the 1980s, Schmid and Bulgadaev investigated the problem of a quantum particle moving in a periodic potential and coupled to a dissipative environment, and reached the conclusion that there are two distinct phases, one diffusive and one presenting localization, depending on the coupling strength. Almost as a footnote, Schmid proposed an experimental realization, in the form of a resistively shunted Josephson junction (RSCJ) in the limit of absolute zero. There is a lively, even heated scientific discussion on the existence or not of this quantum phase transition in that type of device, with contrary claims based on experiments. The impact or otherwise of compactness of a flux variable has also been very much debated. Using formalism recently developed, in this Master's thesis these topics will be summarized and revised.

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8. Director: **Xi Chen** ([xi.chen@csic.es](mailto:xi.chen@csic.es))

Title: **Suppressing Crosstalk in Quantum Dots via Shortcuts to Adiabaticity.**

This project aims to suppress crosstalk errors in quantum dot systems by employing shortcuts to adiabaticity, specifically inverse engineering techniques. Crosstalk, which arises from unintended interactions between qubits during gate operations, poses a significant challenge to scaling quantum processors. By designing precise, time-dependent control fields, we can guide qubit evolution along desired paths more efficiently than traditional adiabatic methods. The objectives are to develop inverse engineering protocols that shape magnetic fields for manipulating single and coupled spins, tailor control fields to suppress crosstalk during single- and two-qubit gate operations, ensure protocols are robust against parameter uncertainties, particularly in gyromagnetic factors, and validate these protocols experimentally by implementing and testing them in silicon-based quantum dots to demonstrate their effectiveness.

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9. Director: **Julen Ibañez- Azpiroz** ([julen.ibanez@ehu.eus](mailto:julen.ibanez@ehu.eus))

*One choice between the two projects listed below.*

Title: **Berry phases and nonlinear optical properties of materials**

In condensed matter physics, the optical response of a crystal is intimately connected to intrinsic topological properties such as Berry phases and more complex geometric quantities. For instance, the phenomenon known as optical activity describes how the polarization of light rotates as it traverses the material by acquiring a geometric phase. In this project we propose a combined theoretical and computational analysis in this area. As a first step, the student will work on the theoretical treatment of the response function associated to nonlinear optical properties. This will be done by employing localized Wannier functions as the basis set, a central tool that is heavily used in our group. Subsequently, the student will perform a first-principles study in concrete materials such as Weyl semimetals to predict and understand its optical properties. The project involves theoretical work using quantum theory of solids, combined with numerical calculations. Some experience in Fortran and/or Python programming languages would be required.

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10. Director: **Evgeny Sherman** ([evgeny.sherman@ehu.eus](mailto:evgeny.sherman@ehu.eus))

Title: **Quantum magnetism on nanoscale**

Quantum properties of matter, such as magnetism, strongly depend on the spatial scale of the systems of interest. A very interesting example is provided by nanoparticles, where magnetic properties critically vary as functions of size and shape.

The goal of this project is to understand the interplay between magnetism and nanoscale effects in novel materials such as topological insulators and in hybrid structures made of topological insulators and magnetic nanoparticles. In addition, we are going to study the effect of external electric fields on the nanoscale magnetism.

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11. Director: **Sebastian Bergeret** ([fs.bergeret@csic.es](mailto:fs.bergeret@csic.es))

Title: **Interplay between novel magnetic states and superconductivity**

The goal of this project is to theoretically investigate the interplay between magnetism and superconductivity in novel materials, such as altermagnets and p-wave magnets proximitized by conventional superconductors. Our approach involves designing devices to study their transport properties and predict new effects and functionalities. The analysis will employ both analytical and numerical methods, using recent quantum transport equations developed by our group. Collaboration with both local and international experimental teams is expected.

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12. Directors: **Aran Garcia-Lekue** ([wmbgalea@ehu.eus](mailto:wmbgalea@ehu.eus)), **Daniel Sánchez-Portal** ([daniel.sanchez@ehu.eus](mailto:daniel.sanchez@ehu.eus))

Title: **Quantum confinement effects in twisted nanoporous graphene**

Quantum confinement effects in nanostructured graphene are responsible for a wide range of physical phenomena, such as the emergence of topological states and magnetism, both of fundamental and practical relevance in nanoelectronics or quantum spintronics. Nanoporous graphene (NPG), a 2D array of covalently bonded graphene nanoribbons, is a particularly interesting platform due to its strong in-plane electronic anisotropy. In order to fully exploit its potential, NPG should ideally be on a substrate which preserves or enhances its unique anisotropic behavior. In this project, we will consider bilayers composed of NPG on graphene at different relative twist angles. Using state-of-the-art computational tools, besides the control of the twist angle, we will explore additional strategies to tune its electronic properties, such as strain or chemical doping. Our results are expected to be key for the design of future experiments.

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13. Directors: **Daniel Sánchez Portal** ([daniel.sanchez@ehu.eus](mailto:daniel.sanchez@ehu.eus)) , **María Camarasa Gómez** ([maria.camarasa@ehu.eus](mailto:maria.camarasa@ehu.eus))

Title: **Searching for excitonic properties in two-dimensional materials from ab initio**

Excitons are quasiparticles composed of an electron and the hole that occur when a semiconductor is excited with light. They have been recently attracted a great amount of attention as essential components for quantum technologies, such as quantum

sensors and energy storage devices. These particles are especially important in low dimensions, since they can completely dominate the optical spectrum. However, its prediction and characterization remain a challenge within the current numerical methods at the atomistic level due to the large computational cost. Density functional theory has been proven to be an excellent alternative to capture excitonic effects when hybrid functionals are employed. In this project, we aim at implementing one of these hybrid functionals in ab initio codes, such as Siesta, to capture the electronic structure and excitonic effects in van der Waals 2D materials, thus greatly reducing the typical computational cost. We will as well employ alternative computational techniques based on many-body perturbation theory methods to benchmark our results. Some experience with ab initio codes, programming and Python scripting is desirable. As the field evolves quickly, several directions of the project will be discussed to fit the interest of the candidate.

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14. Director: **Dario Bercioux** ([dario.bercioux@dipc.org](mailto:dario.bercioux@dipc.org))

*One choice between the two projects listed below.*

**Title: Skin effect in two-dimensional non-Hermitian lattice system with a flat band**

This project will explore the intriguing spectral properties of non-Hermitian Hamiltonian systems, with a focus on the dice and the Lieb lattices— bipartite, two-dimensional lattices characterized by three sites per unit cell, resulting in a distinctive flat band at zero energy. By introducing non-Hermitian dimerization of the hopping parameters, we aim to uncover novel properties in this system, drawing parallels to higher-order topological insulators. A vital aspect of this project is to investigate the non-Hermitian skin effect, where eigenvectors accumulate at the boundaries of a finite-sized dice lattice. Understanding this phenomenon could provide valuable insights into the behavior of non-Hermitian topological matter and its unique boundary states. The research will involve analytical approaches and numerical simulations, allowing students to learn advanced quantum theory and computational methods.

This project presents an exciting opportunity for students passionate about non-Hermitian physics, topological systems, and lattice models. The work contributes to the growing field of non-Hermitian quantum mechanics and provides a platform for discovering novel physical phenomena in topological lattice systems.

**Title: Exploring Volkov-Pankratov States in Topological Cold Atom Systems**

This thesis will investigate the emergence of Volkov-Pankratov states, a fascinating type of boundary mode, in topological cold atom systems confined within optical lattices. Unlike typical topological edge states, Volkov-Pankratov states arise when the parameter driving the topological phase transition varies smoothly rather than abruptly. These exotic states represent a rich and less- explored aspect of topological quantum matter, offering new insights into the behavior of quantum systems with non-trivial topological properties. Leveraging recent theoretical models, we will explore how different trap geometries for confining cold atom systems can induce the appearance

of these states. This work will combine analytical and numerical techniques, comprehensively exploring the interplay between topological phases and confinement conditions. Students will be able to work on cutting-edge research at the interface of condensed matter and cold atom physics, gaining hands-on experience in advanced computational simulations and mathematical modeling. This project contributes to a more profound understanding of topological quantum matter and opens pathways for future experimental realizations in quantum simulators. It is ideal for students passionate about quantum mechanics, cold atom systems, and topological phenomena.

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15. Director: **Unai Aseguiolaza Aguirreche** ([uaseguiolaza@mondragon.edu](mailto:uaseguiolaza@mondragon.edu))

**Title: Quantum Kernel Design and Optimization for Machine Learning**

In the last years the combination of deep neural networks and big data has created many success cases in the field of machine learning. However, there exist other algorithms to perform machine learning. Among others, there are kernel methods. A subclass of these methods is the Quantum Embedding Kernel (QEK) method. In this method a quantum parametric circuit is used to maximize the separation between learning data in the Hilbert's space. It has been argued that this method can be more efficient than analogous classical methods when the separation of the learning points is complex. The objective of this project is to study the accuracy of different parametric circuits with different architectures and levels of entanglement in a classification machine learning problem.

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16. Director: **Alexey Nikitin** ([alexey@dipc.org](mailto:alexey@dipc.org))

**Title: 2D Nanophotonics**

This project focuses on exploring the fundamental and applied physics of light propagation in novel two-dimensional (2D) materials, such as graphene. These materials possess the unique ability to "trap" light and confine it to extremely small volumes, resulting in extraordinary optical phenomena. For instance, confined light in 2D materials can exhibit unconventional properties like negative refraction and superfocusing. Due to these unusual behaviors, 2D materials have significant potential for a range of advanced optoelectronic applications, including (bio)sensors, hyperlenses, photodetectors, and even future quantum computers. Our approach combines theoretical research with cutting-edge experimental validation, conducted in state-of-the-art laboratories. The findings of this project will contribute to the development of nanoscale devices where light can be manipulated similarly to electrical currents in semiconductor processors.

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17. Director: **Ane Blazquez** ([ablazquez@ikerlan.es](mailto:ablazquez@ikerlan.es))

One choice between the two projects listed below.

Title: **Optimization of Logistics Using Quantum Annealing.**

This project aims to optimize logistical problems, specifically the assignment of parts to pallets and their distribution to work orders, using Quantum Annealing (QA). Through this quantum technique, the goal is to solve complex problems with multiple operational constraints (e.g., pallet capacity, costs) more efficiently than traditional methods. The approach includes formulating the problem into a QUBO model and solving it using quantum hardware.

Title: **Shadow models for Quantum Machine Learning**

Co-director: **Paul San Sebastian** ([psansebastian@ikerlan.es](mailto:psansebastian@ikerlan.es))

Quantum Computing has shown an incredible potential to solve certain problems more efficiently than classical computers. However, the quantum advantage is yet to prove in the context of Quantum Machine Learning (QML). The most studied type of algorithms in QML are called Variational Quantum Circuits (VQC), which consist of parameterized quantum circuits whose parameters are optimized classically. Flipped circuits, a special type of VQC, allow us to create Shadow Models, which are classical approximations of the quantum models. Therefore, once trained a flipped circuit for a given learning task, shadow models should allow us to make the inference without the need of a quantum computer. The objective of this project is to gain a deep understanding of this type of models and to make theoretical and experimental comparisons with other type of models.

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18. Director: **Enrique Rico** ([enrique.rico@ehu.eus](mailto:enrique.rico@ehu.eus))

One choice between the two projects listed below.

Title: **An Atomic Quantum Simulator of Quantum-Glue** [co-director: Daniel Barredo (U. Oviedo)]

The student will exploit a method in which a quantum Rydberg simulator can serve as a rich playground for exploring quantum lattice gauge theories. Subsequently, they will be able to simulate string physics "on a chip," using the Rydberg simulator as a platform for studying the propagation of open-loop and closed-loop quantum excitations. This task will prepare them for the engineering of Rydberg quantum platforms where deterministic quantum effects can be experimentally investigated. To achieve this goal, the following two tasks will be undertaken: 1) The student will focus on exploring frustrated quantum systems. Numerical and perturbative methods will be employed to characterize these frustrated systems. 2) The student will explore potential implementations of these models in a Rydberg quantum simulator and develop simple realizations in finite size lattices, taking into account the relevant experimental parameters. They will assess the robustness of the observables in the face of experimental imperfections.

Title: **GPUs implementation of tensor network states** [co-directors: Elias F. Combarro Alvarez, Jose Ranilla Pastor (U. Oviedo)]

Tensor network methods are a computational framework for approximating ground states and low-lying excited states of strongly correlated quantum systems. Their accuracy is controlled by the so-called bond dimension, with higher values yielding higher accuracy. While offering a computationally efficient route to treating strongly correlated quantum systems, the effort often scales as a high power of the bond dimension, which can severely limit the applicability of these methods in practice. On the other hand, the past decade has seen tremendous progress in the development and commoditization of hardware accelerators, for example, graphical processing units (GPUs), custom-built processors used to train and run large-scale machine-learning tasks, for example, AlphaGo. In this work, the student will investigate how GPUs can be leveraged to scale tensor network algorithms to unprecedented bond dimensions, speed, and accuracy. To this extent, the student will approach the following three tasks: Study the capabilities and limitations of existing computational libraries for tensor networks, to select the optimal platforms and frameworks for our simulations. Develop GPU-accelerated algorithms with tensor networks for specific problems in quantum many-body simulations, such as magnetic systems. Benchmark the implemented algorithms on different instances of the target problems and on different hardware platforms.

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19. Director: **Jens Siewert** ([jens.siewert@ehu.eus](mailto:jens.siewert@ehu.eus))

Title: **Absolutely maximally entangled states for four parties**

One of the characteristics of quantum mechanics is that correlations between several parties of a composite system cannot be arbitrarily distributed. This fact is central for any (quantum) many-body physics and is expressed in the so-called quantum marginal problem (QMP). Nonetheless it is not well understood even for few-party finite dimensional quantum systems. Absolutely maximally entangled states  $AME(N,d)$  have a simple definition for  $N$  parties with  $d$  dimensions each and represent one of the simplest instances for the action of the QMP: It is not known in general whether or not, for a given pair  $(N,d)$ , an AME state exists. Recently, the famous case of the existence of  $AME(4,6)$  was solved and answered in the positive (the quantum solution to Euler's famous 36 officers problem). This TFM project aims at constructing certain AME states based on general principles, starting from  $N=4$  where we are sure that such solutions do exist at least for any odd local dimension. If successful, the project bears the potential for many new constructive solutions. The project is highly ambitious and requires strong skills in linear algebra as well as in analytical and numerical calculations.

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20. Director: **Luis Hueso** ([l.hueso@nanogune.eu](mailto:l.hueso@nanogune.eu))

Title: **Exploring devices with van der Waals Heterostructures**

Conventional monolithic materials have dominated electronic and optical devices for decades, mostly thanks to our ever-increasing ability to control the properties of bulk materials. However, as we approach the range of the single nanometre scale in our fabrication capabilities, it is necessary for the industry to be able to create, control and profit from novel materials and architectures. In this context, the rich library of 2D layered materials presents multiple opportunities to design novel spintronics and valleytronics devices.

Making use of the possibility to create 2D artificial van der Waals heterostructures, in this project we will overcome single materials by focusing on the interface as an active playground. For instance, we will perform interface engineering by combining different magnetic and non-magnetic 2D layers in an unprecedented fashion, exploring new magnetic ground states which are not accessible neither in single materials nor in conventional multilayers. We will also explore spin and valley physics in van der Waals heterostructures by combining 2D layered materials with complementary properties.

In this project, the Master student will be responsible for the design and preparation of structures by exfoliation and stamping of 2D materials in controlled atmosphere and device fabrication by standard electron-beam lithography. (S)he will be also involved in the magneto-transport measurements (high magnetic fields and low temperatures), data analysis, and drafting of results. We offer an international and competitive environment, state-of-the-art equipment (including a class 100 cleanroom for nanofabrication capabilities), and the possibility of performing research at the highest level.

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21. Director: **Fèlix Casanova** ([f.casanova@nanogune.eu](mailto:f.casanova@nanogune.eu))

Title: **Exploiting the spin-orbit coupling in spintronic nanodevices**

Spin orbitronics is an expanding field in Condensed Matter Physics that aims to utilize different phenomena in magnetism and spintronics caused by the spin-orbit coupling. One of the most studied phenomena is the interconversion between spin currents and charge currents in novel materials and interfaces, which has a strong potential to be harnessed for energy-efficient logic and memory tasks for processing of information. In this project, we aim to explore the spin Hall effect in heavy metals, the Edelstein effect at Rashba interfaces or the spin-momentum locking at topological insulators to help implementing the recent proposal by Intel of a magneto-electric spin-orbit logic.

In this project, the Master student will be responsible for the design and the fabrication of nanodevices (thin film deposition, electron beam lithography, etching). The student will be also involved in the magneto-transport measurements (high magnetic fields and low temperatures), data analysis, and drafting of results.

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22. Director: **Beatriz Martín-García** ([b.martingarcia@nanogune.eu](mailto:b.martingarcia@nanogune.eu))

Title: **Raman spectroscopy in 2D materials**

The significant growth, development, and evolution of technologies such as optoelectronics and spintronics have been always accompanied by the access to materials with targeted and extraordinary properties. Among these materials, 2D materials such as graphene, transition metal chalcogenides, metal phosphorus trichalcogenides or hybrid organic-inorganic metal-halide perovskites have attracted the attention due to their extraordinary electronic, optic, and magnetic properties and the possibility of control them by fine tuning the composition, crystal structure and dimensionality. In this project, we will focus on micro-Raman spectroscopy as a non-destructive and powerful tool for gaining insight into phase transitions, crystal structure or molecules arrangement and how they change with the composition, structure, and dimensionality of the 2D materials. For this purpose, we will use single crystals and flakes of 2D materials as material platform.

The Master student will be responsible for the design and preparation of the 2D materials by exfoliation and stamping on substrates. The student will be also involved in the Raman spectroscopy measurements (including low temperature or polarization tests), data analysis, and drafting of results.

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23. Director: **Ion Errea** ([ion.errea@ehu.eus](mailto:ion.errea@ehu.eus))

*One choice between the two projects listed below.*

Co-director: **Đorđe Dangić** ([dorde.dangic@ehu.eus](mailto:dorde.dangic@ehu.eus))

Title: **Novel methods to calculate the thermal expansion of magnetic materials from first principles**

Thermal expansion is a fundamental property of materials, highly relevant for technological applications. As is commonly known, most materials expand when heated. However, there exists a notable group of materials that behave counterintuitively—they shrink as temperature increases. This phenomenon, known as negative thermal expansion (NTE), is often observed in functional materials such as ferroelectrics and ferromagnetics, most commonly in the vicinity of the phase transitions.

This project aims to unravel the physical origins of negative thermal expansion in ferromagnetic materials. We will employ first-principles methods coupled with the quasiharmonic theory of phonons to uncover the microscopic mechanisms behind this intriguing phenomenon. The student will gain experience with state-of-the-art techniques for modeling material properties and will be introduced to the fundamentals of condensed matter theory. The expected outcomes include a method for calculating the thermal expansion coefficient in magnetic materials, with the potential for publication of results in a prestigious international physics journal.

Title: **Superconductivity in hydrogen based compounds**

Co-director: **Yuewen Fang** ([fyuewen@gmail.com](mailto:fyuewen@gmail.com))

In the past decade, the progress achieved in both experiment and theory has led compressed hydrides to set numerous records in pushing the critical temperature,  $T_c$ , of superconductivity to approach and even exceed room temperature. These hydrides feature multihydrogen atoms and have to be synthesized at extreme high pressures above 100 GPa. Not only do these multi-hydrogen superconducting hydrides show poor ductility [6], but also the diamond anvils used for hydride synthesis frequently fracture during depressurization due to hydrogen embrittlement.

On the other hand, elemental superconductors and metallic alloy superconductors generally demonstrate excellent ductility and excellent mechanical properties due to the unique metal bonds [8, 9], despite that their critical temperatures generally below 25 K are much less than that of highly compressed superconducting hydrides.

Very recently, several metal-bonded hydrides with few hydrogens have been theoretically reported to show high  $T_c$  at ambient pressures, e.g.  $Al_4H$ ,  $Pb_4H$ , and  $MgHCu_3$ . In particular, the predicted  $T_c$  of perovskite-structured is as high as 54 K at ambient pressures, and the metallic bond between Al and H is suggested to enhance the structural stability and ductility. In addition, we note that some few-hydrogen hydrides have been synthesized in earlier experiment at ambient pressures (e.g.  $AlHTi_3$  and  $TiHPd_3$ ) although the study on their superconductivity is still absent. These earlier and recent discoveries imply that the few-hydrogen metal-bonded superconducting hydrides would be a great platform to investigate the promising materials that can combine the excellent ductility and the high- $T_c$  superconductivity at ambient pressures.

In this project, combining the stochastic self-consistent harmonic approximation (SSCHA) method with ab initio calculations, we aim to study the ionic quantum and anharmonic effect on the superconductivity in the recently reported few-hydrogen metal-bonded superconducting hydrides at ambient conditions, e.g.  $Al_4H$ . Furthermore, we will perform high-throughput screening by using the template methods and crystal structure prediction methods to predict novel few-hydrogen hydrides that could demonstrate comparable  $T_c$  as  $AlH_4$ . Particular interest will be casted onto the perovskite structured  $X_4H$  and  $XHY_3$  hydrides, where the mechanism of driving large electron-phonon coupling constant will be addressed as a comparison with the widely studied multihydrogen hydrides, and the potential maximal  $T_c$  in such few-hydrogen hydrides will be discussed theoretically.

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24. Director: **Ivo Souza** ([ivo.souza@ikerbasque.org](mailto:ivo.souza@ikerbasque.org))

Title: **Wave propagation in magnetic crystals**

Magnetic crystals display a range of optical effects depending on the type of magnetic order: ferromagnetism, antiferromagnetism, or the newly-discovered altermagnetism. This project consists of a critical survey of the phenomenology of wave propagation in

magnetic crystals with zero net magnetization. The standard approach is based on the multipole theory of electromagnetism, which however becomes problematic for bulk crystals: the delocalized charge distribution precludes a multipole expansion. After reviewing the multipole theory of wave propagation (Ch. 5 of the book "Multipole Theory in Electromagnetism" by Raab and De Lange), a bulk formulation based on the wavevector-dependent optical conductivity will be pursued, combined with a symmetry analysis to identify magnetic point groups hosting various effects. The project, in combination with a recently-developed microscopic theory, paves the way to ab initio calculations of optical effects in antiferromagnets and altermagnets.

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25. Director: **Emilio Artacho** ([e.artacho@nanogune.eu](mailto:e.artacho@nanogune.eu))

*One choice between the two projects listed below.*

**Title: Quantum computing for first-principles calculations of correlated electrons**

The solution of quantum many-particle systems is one of the most natural problems to be addressed with quantum computing, since the exponential growth of the system's Hilbert space with the size of the system is matched by the exponential growth of the space associated with growing numbers of entangled qubits. In a collaboration between the Theory group at Nanogune and IBM Quantum at Zurich we are working on the connection of a large-scale first-principles method for addressing weakly correlated systems from first principles on conventional supercomputers (SIESTA) with a program running on quantum computers (IBM's QISKIT) that can address the (nearly) exact solution of the correlated system given by an active space embedded into a larger, less correlated one. For a first proof of concept, the variational quantum eigensolver method will be used on IBM's quantum computers to obtain correlated solutions for the complete active space spanned by the relevant orbitals of a few atoms (e.g. a transition-metal ion substitution) in a material that can be otherwise sensibly treated using density-functional theory, which is a widely used mean-field-like method for first-principles calculations. Other quantum solvers will be explored henceforth, for a more powerful use of the numbers of qubits available in IBM's quantum computers. The student will engage in the development, testing, and first applications of the software, using supercomputers linked to IBM's quantum computers.

**Title: Time-dependent many-body effective Hamiltonians for highly correlated systems**

Highly-correlated many-particle problems in condensed matter have been very successfully addressed within the paradigm of the Hubbard model and variants thereof, formulated using second quantisation, referring to a basis set with very few states per site (canonically just one). Very easily formulated, these models describe rich, complex physics, stemming from quite non-trivially entangled many-body states. Recent experimental advances with optical lattices have extended that physics to the realm of periodically-driven time-dependent systems, in what is being called Floquet

physics (the Floquet theorem is analogous to Bloch's theorem but referring to periodicity in time instead of space). Novel states of matter are being devised in this context. The same Hubbard-like models described above are being extended to the time-dependent domain, so far quite tentatively, with time-dependent (time-periodic) dependences of their parameters. Some of the new physics relate to time-periodic displacements of the confining potential wells defined by the lasers used to obtain optical lattices. In this project we want to obtain the transformation of those models needed to describe such time-dependent displacements. If the underlying basis moves with the confining wells, a gauge potential appears that can be understood in terms of the Hilbert space becoming a curved manifold in a differential geometry context. We will formulate an extension of the simplest Hubbard model for a periodically moving basis, and will explore its effects in a Hubbard dimer as simplest non-trivial system. The solutions will be compared with the presently used conventional model with time-dependent parameters. In addition to an initial study of the relevant literature, the work will be mostly analytic, with the help of numerical solution of the final equations, accessible to simple python coding in e.g. Jupyter notebooks.

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26. Directors: **Maia G. Vergniory** ([maiaqvergniory@dipc.org](mailto:maiaqvergniory@dipc.org)) and **Ion Errea** ([ion.errea@ehu.eus](mailto:ion.errea@ehu.eus))

**Title: Phonon instabilities and charge-density waves in layered transition metal dichalcogenides**

Chiral materials have attracted significant research interests as they exhibit intriguing physical properties, such as exotic topology, quantized optical response or large robust surface states. The chiral electronic structure can emerge alternatively in materials with achiral crystal structure. Due to the limited material choice, such emergent chiral electronic structure and its unique physical properties has not been investigated. This is the case of the layered transition metal dichalcogenide such as 1T-TaS<sub>2</sub> or 1T-TiS<sub>2</sub>. Recently it has been proved that 1T-TaS<sub>2</sub> transit to an incommensurate charge-density wave at 550K. During this project we plan to study phonon instabilities and the contribution of anharmonic effects to calculate at which temperature the phonon frequencies of the high-temperature high-symmetry phase collapse and determine whether a CDW can occur.

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27. Director: **Koushik Paul** ([koushikpal09@gmail.com](mailto:koushikpal09@gmail.com))

**Title: Resolving ground states through controlled inverse quantum annealing**

Solving ground state problems for many body systems is of prime interest due to its diverse applicability in solving optimization problems. This project aims to explore the potential of quantum control techniques in inverse quantum annealing (IQA) for resolving ground states in complex optimization problems. Unlike traditional quantum annealing, which begins with a quantum superposition of all possible states and a known initial Hamiltonian, IQA works by refining solutions through quantum evolution

with carefully controlled parameters. The research will focus on the tunability these parameters, such as annealing schedules and transverse fields to enhance the discovery of optimal solutions, particularly in challenging energy landscapes. Simulations will be developed to benchmark the performance of IQA against classical optimization techniques and conventional quantum annealing, with a focus on solving NP-hard problems and applications in machine learning and quantum chemistry.

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28. Director: **M. Fernando Gonzalez Zalba** ([f.gonzalez@nanogune.eu](mailto:f.gonzalez@nanogune.eu))

Title: **Silicon-based quantum computing: Electrical specifications of the control and readout electronics.**

Solid-state quantum processors rely on classical electronic controllers to manipulate and read out the quantum state of the qubits. As the performance of the quantum processor improves, non-idealities in the classical controller and receiver can become the performance bottleneck for the whole quantum computer. In this Master's project you will work to determine the electrical specification of the classical control layer of a quantum processing unit based on silicon spin qubit technology. More particularly, you will (i) learn the basics of silicon-based quantum computing with spins, (ii) you will learn how spin qubits are controlled and readout, (iii) you will understand the how classical electronics interacts with quantum systems, (iv) you will determine the electronics specifications needed to achieve an overall quantum processor performance which will enable better selecting and designing the classical control layer. At the end of this master's project, you will be ready to design the classical control layer of a silicon-based quantum computer and be prepared to perform experiments with silicon quantum computing devices.

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29. Title: **Processing NV's sensor signal with artificial intelligence**

Director: **Jorge Casanova** ([jorge.casanova@ehu.eus](mailto:jorge.casanova@ehu.eus))

Quantum sensors exploits quantum properties of matter to measure and/or detect, with high precision and sensibility, different physical magnitudes. This capacity to disclose changes in the environment implies that collects information from all the sources the ones under study as well as others present around. This, together with the quantum randomness, means that the experimental recorded signals direct analysis can sometimes be difficult.

Among the different types of available quantum sensors, those based on nitrogen-vacancy (NV) centers offer the possibility to work at room temperature. This makes suitable for its use in a wide range of applications from chemical analysis to magnetic field measurements.

In this master thesis we will work on the application of artificial intelligence tools to NVs quantum sensors' signal processing. It will require previous knowledge in quantum



mechanics, quantum sensors (specially in NVs' based ones) and artificial intelligence (signal processing, machine learning and deep learning).

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30. Director: **Aitor Moreno** ([ai.moreno@ibermatica.com](mailto:ai.moreno@ibermatica.com))

*One choice between the two projects listed below.*

**Title: Quantum Digital Twin. Simulator of physical systems using quantum computing**

A digital twin is a virtual model of a machine or process that functions as an exact copy of a real system or a physical model. Digital model makes it possible to compare continuously and in real time the differences in behavior between the machine, material, or drugs interactions with a theoretically ideal process. Digital twins make it possible to simulate, study and understand how complex real systems would behave, for example, in the generation of new materials or new drugs, modeling the molecular interaction of their components. The objective of this work is to build a system about internal differential equations with a quantum system, described by Partial Derivative Equations (PDE) or Ordinary Derivative Equations (ODE) in an industrial simulation environment. The massive under activation of multiple "ODEs", the high dimensionality of the system and the design and/or location of distributed systems are currently the major limitations in the calculation of classic automation and control simulations. With this work we intend to develop an algorithmic approach based on quantum simulation models, taking advantage of the linear algebra over real quantum processors. Quantum techniques make it possible to emulate particle reactions in a "more natural" way: how molecules associate and dissociate, how materials behave at high temperatures, how it is possible to generate new materials through the analysis of particle interactions in physics of high energy, thermodynamics, materials science, or biological processes. In short, addressing simulation challenges that are intractable with classical computing means.

**Title: Quantum Natural Language Processing and Quantum Language Generation Project.**

NLP is an area of study with elements from linguistics, computer science and artificial intelligence that focuses on the interaction between computers and human language. Loosely speaking the goal in NLP is to make computers capable of understanding text and spoken language in much the same way that humans do. NLP has countless use cases such as machine translation, text summarization, chatbot creation, and spam detection. Recent interest in the creation of quantum algorithms for NLP has given birth to a new field of research, which is now known as quantum natural language processing (QNLP). Much of what we'll cover is related to Natural Language Generation (NLG), which is a topic at the intersection of procedural generation and Natural Language Processing (NLP). Generative AI and quantum computing can offer great features from both worlds that can help accelerate research work and the related quantum supremacy in developing a practical quantum computer. Few of the advantages are:

- 1) GPT can help improve design of better quantum architectures, especially for the co-design of various interdisciplinary optimizations

- 2) Improve the training and generation speed of large data assets for fine tuning LLMs, and other data-warehouse, big data batch operations
- 3) Leverage the inherent quantum security features
- 4) Autonomous self-directed agents can help improve the speed of job completions with a minimal human prompt input.
- 5) Assist researchers in visualizing the areas that might not be easy to illustrate.

In this TFM we will work about Quantum NLP and Quantum Text Generative at an industrial context.

## Cosmology, Relativity, Fields and Particles

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31. Director: **Ivan Esteban** ([ivan.esteban@ehu.eus](mailto:ivan.esteban@ehu.eus))

Title: **Neutrinos as messengers in fundamental physics**

Neutrinos interact weakly, making them hard to detect. But, at the same time, their weak interactions make them clean messengers of extreme environments. Because of this, research on neutrino properties is a very active area in fundamental physics, linking to particle physics, astrophysics, and cosmology. Many neutrino experiments are currently being built and planned, with large amounts of high-quality data forecasted for the near future.

This Master Thesis will explore how neutrino experiments can be used as a window into fundamental physics. There are two possible directions: 1) Neutrinos and proton structure: we still do not understand how the constituent quarks arrange to form a proton. Since neutrino-quark interactions are spin- and flavor-dependent, probing a nucleus with neutrinos could provide unique insight. The student will determine the physics reach of upcoming neutrino detectors. 2) Neutrino signals from Dark Matter: understanding the nature of Dark Matter is among the most pressing problems in fundamental physics. The absence of signals so far might be due to Dark Matter preferentially interacting with neutrinos. The student will determine the signals that this would leave on neutrino detectors, with the chance of analyzing real data.

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32. Director: **Miguel García Echevarría** ([miguel.garciae@ehu.eus](mailto:miguel.garciae@ehu.eus))

Title: **QCD and Hadron Structure in High-Energy Colliders**

Quarks and gluons are the fundamental constituents of nucleons (protons and neutrons). However, even now - after 50 years of Quantum Chromodynamics (QCD) - many questions about them remain. How are they distributed? How do they form hadrons? How much and in which way do they contribute to one of the most basic properties of nature, the nucleon spin? Nucleon inner structure is parametrized in terms of several multi-dimensional functions, like parton distribution functions (PDFs), transverse-momentum-dependent functions (TMDs), generalized transverse-momentum-dependent functions (GTMDs), etc., which encode different correlations

between the momentum and spin of the considered quark/gluon and the parent nucleon. These functions are probed in high-energy processes, and tools like factorization, resummation and perturbative calculations, together with phenomenological data analyses, are needed to constrain them. However, for now we only have a reasonable understanding of these distributions in 1 dimension, i.e. PDFs, since the multi-scale processes needed to probe other multi-dimensional functions (like TMDs and GTMDs) are challenging both theoretically and experimentally. Understanding and constraining these functions is essential, on one hand because they are needed to perform any kind of phenomenological study at high-energy hadron colliders, like the LHC, and on the other because they are of great interest as a way to indirectly shed light on QCD confinement. The focus of the master project will be adapted depending on the interest and skills of the student, being possible to tackle theoretical aspects, phenomenological analyses, computing, quantum simulations, etc. Collaboration with university as well as international colleagues is expected.

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33. Directors: **David Brizuela** ([david.brizuela@ehu.eus](mailto:david.brizuela@ehu.eus)), **Leonardo Chataignier**

Title: **Quantization of cosmological and black-hole models**

A number of topics in the context of the quantization of cosmological and black-hole models are proposed, which will be pursued depending on the specific interests of the student. i/ Rigorously analyze the definition of path integrals in quantum cosmology (minisuperspace gauge systems): check the gauge invariance of the path-integral measure and connect it to the canonical approach. ii/ Carry out the Feynman quantization procedure based on the on-shell action for minisuperspace cosmological models: this is a method that is equivalent to path integrals, but it directly yields the Schrödinger equation with a fixed factor ordering based on nothing more than the classical action. iii/ Carry out a reduced phase-space quantization of black-hole toy models: this entails the calculation of classical gauge orbits and quantization of functions on these orbits. iv/ Study the postquantum theory of classical gravity, which consistently couples gravity, as a stochastic classical field, to quantum fields, and analyze its physical implications.

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34. Directors: **David Brizuela** ([david.brizuela@ehu.eus](mailto:david.brizuela@ehu.eus)), **Marc Schneider**

Title: **Violation of Lorentz symmetry in black-hole spacetimes and universal horizons**

In general relativity, black-hole horizons serve as a causal boundary for light, that is, light can enter but never escape. This property is related to the finite value of the speed of light, which is intimately connected to Lorentz symmetry. Since in quantum gravity Lorentz symmetry is not necessarily present, one may ask what happens to a black hole if higher propagation speeds are allowed. In particular, Einstein-aether gravity studies general relativity coupled to a timelike vector field, the aether, that represents a preferred clock. In this context, Lorentz symmetry becomes an emergent low-energy

phenomenon, which may be absent at high-energy scales. This permits, in principle, infinite speed signals that put the notion of the black-hole horizon at stake. However, for vacuum static black holes, it has been shown that the interplay between geometry and aether forms a new sort of universal horizon inside the usual Schwarzschild horizon, which even captures infinite-speed signals. The goal of this master-thesis project will be to extend such analysis to charged black holes.

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35. Director: **Mariam Bouhmadi-López** ([mariam.bouhmadi@gmail.com](mailto:mariam.bouhmadi@gmail.com))

*One choice between the two projects listed below.*

Title: **Quantum cosmology and classical singularities resolution.**

The quantum fate of classical singularities can be addressed in the setup of quantum cosmology: the application of quantum theory to the universe as a whole. This framework has proven that many cosmological singularities (and also gravitational singularities) like the big bang, can be avoided as a result of quantum effects emerging as the universe approaches the classical singularity. In this work, we will further analyse the quantum behaviour of some classical singularities beyond the big bang that can be described classically in the framework of general relativity as well as in some extended theories of gravity. For that purpose, we shall focus on the quantum cosmology scheme given by the Wheeler-DeWitt equation and its possible extensions within a quantum geometrodynamics approach. More information about our research can be found by checking our list of publications at inspirehep.

Title: **The current speed up of the Universe**

The observations of distant SNIa, CMB and the Baryon acoustic oscillations indicate that the expansion of the Universe is presently accelerating. This fact implies that the Hubble rate has grown faster than previously foreseen and, therefore, the universe has recently come into an epoch of accelerated expansion, which is incompatible with a universe described by general relativity and filled exclusively with matter (dark and baryonic). The origin behind this acceleration is still a mystery up to date and it is one of the biggest problems open nowadays in theoretical physics. The goal of this Master thesis project is to contribute actively in understanding this mysterious acceleration. Please notice that some of these models will not only include a classical analysis but also a quantum study. More information about our research can be found by checking our list of publications at inspirehep.

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36. Directors: **Matthew Elley** ([matthew.elley@ehu.eus](mailto:matthew.elley@ehu.eus)) and **Jose J. Blanco-Pillado** ([josejuan.blanco@ehu.eus](mailto:josejuan.blanco@ehu.eus))

Title: **Primordial Black holes from the Nucleating Domain walls**

Spherical domain walls can be formed via quantum mechanical processes in the Early Universe. If these bubbles are created with perfect spherical symmetry, their subsequent evolution would lead to gravitational collapse and the formation of black

holes. However, quantum mechanical fluctuations inherent in their formation introduce a calculable spectrum of deviations from perfect sphericity. This study aims to investigate, through numerical simulations, the fraction of these initial configurations that result in black hole formation. By estimating the percentage of bubbles that collapse into black holes, we can place constraints on early universe models involving domain walls. This project offers an opportunity to gain deeper understanding of these phenomena through computational methods in numerical General Relativity, so we welcome students with an interest in engaging with complex numerical simulations and coding but also have a strong interest in the analytical aspects of General Relativity and Quantum Mechanics that underpin these simulations.

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37. Director: **Alberto Garcia Martin-Caro** ([agmcaro@gmail.com](mailto:agmcaro@gmail.com))

Title: **Quantum interaction of solitons and radiation**

Topological solitons are semi-classical solutions that can appear in some interacting quantum field theories. Due to their non-perturbative nature, the computation of their static properties and dynamics in the full quantum theory using standard QFT tools is extremely difficult, and usually they are studied in the classical limit, in which it is well known that they can interact non-trivially with the perturbative radiation. Recently, a new formalism for computing some static properties of solitons in the full QFT has been developed and applied to solitons in 1+1 (kinks) and 2+1 dimensions (domain walls). In this project, the student will explore such formalism, with the final goal of describing a simple dynamical process involving the radiation emission of a perturbed domain wall at the quantum level.

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38. Director: **Igor Bandos** ([igor.bandos@ehu.eus](mailto:igor.bandos@ehu.eus))

Title: **Modern problems of String/M-theory**

The strategic goal of the research will be to gain new insights in the theory of fundamental interaction and in the structure of the Universe in the framework of String/M-theory. The characteristic predictions of this are supersymmetry, the symmetry between bosons and fermions, and extra spacetime dimensions. The project will deal with supergravity, a supersymmetric generalization of the Einstein General Relativity, which describes the low energy limit of String/M-theory, and with supersymmetric extended objects, supermembrane and higher p-branes in multidimensional spacetime, which appear as non-perturbative states in String/M-theory. As the field is progressing very rapidly and new interesting directions might appear, a more detailed specification of the research project will be defined later.

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39. Director: **Joanes Lizarraga** ([joanes.lizarraga@ehu.eus](mailto:joanes.lizarraga@ehu.eus))

Title: **Axion kinetic fragmentation in periodic potentials**

The axion, a light pseudo-scalar field, is one of the most promising dark matter candidates. Recently a new plausible mechanism for axion generation, called the kinetic misalignment mechanism has been proposed. The most important consequence of this new scenario is that the parameter space that current and future observatories could probe is considerably enhanced. The model considers an initial non-null velocity that makes the scalar field roll over a number of maxima in periodic potentials until confinement happens. During this rolling fragmentation of the homogeneous axion field could happen, where most of the energy of the homogeneous axion goes to fluctuations, i.e. inhomogeneities. These could backreact in the evolution altering the prediction provided by linear studies. In this work we consider a toy model for kinetic misalignment mechanism, where the most important features of fragmentation will be studied. This model could later be embedded in more realistic scenarios, where an actual prediction of axion dark matter abundance, hence the axion mass, could be provided.

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40. Director: **Gunar Schnell** ([gunar.schnell@ehu.es](mailto:gunar.schnell@ehu.es))

*One choice between the two projects listed below.*

Title: **Hadronization models for high-energy experiments**

Most high-energy physics experiments to date observe among others final-state hadrons in their detector, hadrons that stem from the elementary interactions of the various physics processes. However, our present-day tools of describing the formation of color-neutral hadrons from colored partons (quarks and gluons) within the quantum field theory of Quantum Chromodynamics are still rather limited and insufficient for first-principle calculations and the description of this color-confining process. A multitude of tools have been developed to lessen the dependence on such first-principle calculations, albeit all with their own short-comings. One of the more successful approaches presently available in high-energy physics is the application of Monte Carlo event generators, which employ perturbative methods where possible and parametrizations as well as modeling where perturbative methods cannot be used. One example is the widely used PYTHIA event generator, incorporating the JETSET hadronization model. It is used for a number of processes, from lepton-nucleon scattering, electron-positron annihilation, to hadron collision as, e.g., done at the Large Hadron Collider at CERN. Indeed, it is often the only way of evaluating the Standard Model background in searches for physics beyond the Standard Model. As such a reliable reproduction of the Standard Model physics is often pivotal. Still, it is only a model, continuously adjusted and tuned to existing data. In this work, comparisons of previous PYTHIA tunes with the latest reincarnation of PYTHIA as well as to real data will be performed, in particular for observables relevant to electron-positron annihilation with the goal of establishing a framework to coherently fit model parameters for a better reproduction of annihilation data for the recently started Belle II experiment, the luminosity frontier of particle physics.

## Title: **Spinning baryons from spinning neutrinos**

The spin of the proton,  $1/2 \hbar$ , is still a mystery when it comes to explaining its origin. How the proton's constituent, quarks and gluons conspire to produce  $1/2 \hbar$  has thus been subject of intense research for the past decades latest when it was found that the proton spin does not come from just the spin of its two up valence and one down valence quarks. As intriguing or even more is the question of how polarised baryons, e.g., protons, neutrons, lambda hyperons and so on, are produced from the hadronization of a single quark into the final baryon. Here, polarization refers to a preferred orientation of the particles spin. There is another family of particles that exhibit a preferred spin orientation: all neutrinos that we have detected are actually left-handed. This can be used to select a well-defined polarisation of quarks that then can hadronize into polarised baryons, making it almost an ideal tool to shed light on the above-mentioned mystery of polarization transfer to final-state baryons.

The "almost" here is the property of neutrinos to only interact weakly with matter. For that reason, large numbers of them are needed to extract precision information from a scattering experiment with neutrinos. Several experiments are being build or are proposed that are promising to provide sufficient events for that purpose. In this project, we will explore how well the frontier neutrino experiment DUNE (Fermilab), or the proposed Forward Physics Facility at the Large Hadron Collider (CERN), would perform in this respect, by calculating or modelling the production of lambda hyperons in deep-inelastic scattering of neutrinos.

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