TFM proposals 2023-24

Cosmology, Relativity, Fields and Particles

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1. Director: **Igor Bandos** (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 on.

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2. Director: **Jose J. Blanco-Pillado** (josejuan.blanco@ehu.eus)

Title: **Classical and Quantum decay of excited solitons**

Solitons are long lived configurations that appear in many non-linear field theories in many branches of physics; from String Theory to Condensed Matter. Many of these solutions also admit localized excitations that may decay by classical or quantum processes. In this work we will study some of these models with the aim of understanding these processes and numerically compute their decay lifetime. In this work, we will make extensive use of lattice field theory simulations so some experience with C++ would be required.

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3. Director: **Mariam Bouhmadi-López** (mariam.bouhmadi@ehu.eus)

Title: **The current inflationary era**

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.

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4. Directors: **David Brizuela** (david.brizuela@ehu.eus), **Leonardo Chataignier**

Title: **Semiclassical analysis of the canonical quantization of gravity and physical implications**

Extracting physical effects from any theory of quantum gravity is very challenging. In this master thesis the student will consider a canonical quantization of general relativity, which leadsto the Wheeler-DeWitt (WDW) equation. However, the interpretation of this formalism is problematic, in particular because time is not intrinsically defined and observables are not known. Therefore, certain semiclassical techniques will be applied to study the dynamics of the WDW equation. The focus will be in conceptual problems (like studying the relation between the gauge-fixing and the Page-Wootters approach to define the emergence of time; or using the Hamilton-Jacobi approach to find quantum observables in cosmology). Although an application to study quantum-gravity corrections to the Hawking radiation might also be considered.

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5. Director: **Ivan Esteban** (ivan.esteban@ehu.eus)

Title: **Neutrinos as microscopes**

The structure of nucleons cannot be calculated from first principles, yet it is key to perform many high-energy physics studies and shed light on how confinement arises from quantum chromodynamics. At the same time, 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. In this Master Thesis, both topics would be combined. The student would carry out original research on how neutrino experiments can probe nucleon structure. There are two main directions that could be followed: 1) Neutrinos from the LHC, related to the recent first detection of neutrinos from high-energy collisions. 2) Neutrinos from DUNE, related to the proposed multi-purpose experiment DUNE. Depending on the interests of the student, the work could be more analytic, numeric, theory-oriented, or experiment-oriented.

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6. Director: **Iñaki Garay** (inaki.garay@ehu.eus)

One choice between the two projects listed below.

Title: **Loop quantum gravity: implementation of dynamics in simple models**

Loop quantum gravity (LQG) is a well established proposal for the quantization of spacetime. Among its main results we find the description of the microscopic origin of the black hole entropy and, within the cosmological version of the theory (known as loop quantum cosmology), the avoidance of the initial singularity. Nevertheless, the implementation of the dynamics and the semiclassical limit are still open problems of the theory. In this project, we will explore the mathematical structure of LQG in order to explore these issues. More concretely, we will make use of the so-called spinorial formalism for LQG in order to propose dynamics for carefully constructed simple models with physical interpretation.

Title: **The handedness of entangled universes in quantum cosmology** [co-director: **Salvador Robles Pérez** (sarobles@math.uc3m.es)]

It has been recently proposed that the universes may most naturally be created in entangled universe-antiuniverse pairs. In this project we will study the correlation between the configuration of the spatial geometry in such a pair for non-isotropic spacetimes, in order to explore the observable consequences of this entanglement in the polarization of the primordial gravitational waves and in the parity or handedness of the particles created during the first moments after inflation.

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7. Director: **Miguel García Echevarría** (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 obviously crucial to perform any kind of phenomenological study at high-energy hadron colliders, like the LHC, and at the same time it is of great interest as a way to indirectly shed light on QCD confinement. The focus of the 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 international colleagues is expected.

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8. Director: **Ruth Lazkoz** (ruth.lazkoz@ehu.eus)

Title: **Forecasting cosmic chronometers datasets with machine learning**

The analysis of (independent) cosmological probes is at the heart of (computational) precision cosmology. This route is vital to keep their systematics under control, clarify the reasons for the current tensions between different measurements of cosmological parameters and, ultimately, improve the accuracy of these measurements. In general, those are highly non-linear and remarkably complex data analysis procedures which state-of-the-art computing resources allow to execute with unprecedented success. In other words, modern cosmology will certainly benefit from non-linear curve fitting, clustering and machine learning techniques to depict the evolution of the universe. This project will walk the pedagogical road from two dimensional curve fitting to multidimensional clustering and machine learning with neural networks or support vector machines for the analysis of

current cosmic chronometer data and eventual forecasts for future spectroscopic surveys (Euclid, Roman). Along the way the learning process will touch topics such as mathematical optimization or evolutionary algorithms. Cosmic chronometers are our observations of choice because of their growing relevance due to their ability to offer cosmological model-independent reconstructions of the Hubble parameter Universe based on minimal assumptions.The project will rely heavily on the commercial computing platform Mathematica and the Computational Intelligence Packages (CIP), a high-level open-source function library developed with Mathematica's programming language on top of Mathematica's algorithms.

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9. Director: **Joanes Lizarraga** (joanes.lizarraga@ehu.eus)

Title: **The effect of the inflationary potential in the strong backreaction regime of axion inflation**

Axion inflation is one the most promising inflationary candidates rooted in particle physics. In this model a pseudo-scalar inflaton in coupled derivatively to gauge fields through an axion coupling. The gauge fields are always excited to high occupation states, both during inflation and during post-inflationary preheating. Due to the large excitation of the gauge fields the system becomes non-linear and enters into the strong backreaction regime. In this project, we will extend the study presented in our recent work [Figueroa, J. Lizarraga, Urio & Urrestilla, arXiv:2303.17436], where we studied the strong backreaction regime using lattice numerical techniques, i.e., including all degrees of freedom of the model. The main objective is to study the effect of including different proposals for the scalar potential beyond the most simple quadratic form. In order to do so, we will reproduce the strong backreaction regime, via lattice simulations, for different physically motivated inflationary potentials.

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10. Directors: **Asier Lopez-Eiguren** (asier.lopez@ehu.eus), **Jon Urrestilla** (jon.urrestilla@ehu.eus)

Title: **Primordial black hole formation from domain wall collapse**

The formation of primordial black holes is still an open question in cosmology, as well as the origin and nature of dark matter. Currently, the most viable dark matter candidate is the QCD axion, a particle that naturally appears form the mechanism proposed to solve the strong CP problem. In the axion production process domain walls play an important role. In this work, we will analyze the possibility of primordial black hole creation from collapsing axionic domain walls using advanced field theoretical simulations.

11. Director: **Gunar Schnell** (gunar.schnell@ehu.eus)

One choice between the two projects listed below.

Title: **The strange shape of protons**

Is the proton really round, or actually deformed, depending perhaps on the direction of its spin? And does it look different depending on which of its constituents we are looking at? One way to find out is to look at a specific parton distribution function: the Sivers function. The novel Sivers effect, characterized by the preference in the transverse momentum direction of quarks in a transversely polarized hadron, has become one of the major topics in hadron physics. Although predicted in the early days of Quantum Chromodynamics to be highly suppressed, various experimental results have since then managed to defy this expectation. The Sivers parton distribution can be accessed among others through the distribution of unpolarized final-state hadrons produced in deep-inelastic scattering of high-energy leptons by transversely polarized nucleons, which has been the most utilized way so far to study the Sivers effect. The dominance of the contributions from up and down quarks to this process makes it difficult, though, to probe anything but those quark flavors without currently overwhelming uncertainties. However, due to the apparently opposite signs of up- and down-quark Sivers distributions as well as the high sensitivity to strange quarks, a different process—-namely hyperon polarization—-might shed light on the difficult-to-measure strange-quark Sivers effect. In this work, the quark-parton model formalism for polarized hyperon production in deep-inelastic scattering will be reviewed and current parametrizations for parton distribution and fragmentation functions be used to make predictions for measurements at various facilities in order to estimate the feasibility of such measurements at existing and future experiments, and thus the possibility of accessing the shape of the strange-quark momentum distribution in transversely polarized protons.

Title: **Impact of HERMES data on proton PDFs**

Data from the world-only electron-proton collider HERA were included extensively in fits of the parton distribution functions (PDFs) of the proton, e.g., in the widely used HERAPDF sets. PDFs are indispensable parametrisation of the proton structure, needed for instance in the search for signatures of New Physics in the remnants of highly energetic proton-proton collisions at the Large Hadron Collider at CERN. The HERMES experiment at HERA focused mainly on the spin- dependent structure of the proton but also produced ample of data on unpolarised scattering from protons and deuterons. However, up to now these data sets have not been included in any of the HERAPDF fits. In this project, the commonly used xFitter framework will be employed to extract a new set of proton PDFs, one that includes for the first time also HERMES data.

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12. Director: **Iagoba Apellaniz** (jagoba.apellaniz@ehu.eus)

Title: **Quantum technology with Dicke states**

In quantum Information science, entanglement between two parties can pave the road for different quantum technology applications such as quantum teleportation, quantum communication and quantum error-correction. Dicke states are multipartite symmetric quantum states with a large entanglement. It is possible to create Dicke states experimentally with thousands of cold atoms. When such an ensemble is split into two spatially separated parties, a high level of bipartite entanglement can be detected. In this project we will study the quantum properties of states similar to the Dicke states. It is well known that Dicke states overcome the classically achievable precision in quantum metrology. We will also study the metrological gain of this family of states for different estimation tasks, compared to classical methods.

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13. Director: **Emilio Artacho** (e.artacho@nanogune.eu)

One choice between the two projects listed below.

Title: **Substrate and environment effects on protected spin states in graphene nanostructures**

Certain graphene nanostructures are known to display non-zero spin states associated to various positions at edges and/or corners [Friedrich *et al.*, Phys. Rev. Lett. 125, 146801 (2020); Pavliček *et al.*, Nat. Nanotechnol. 12, 308 (2017)] that are quite robust due to their topological origin and related protection [Rizzo *et al.*, Nature 560, 204 (2018); Lieb, Phys. Rev. Lett. 62, 1201 (1989)]. Robust spin states in novel, controlled systems are appealing for possible future developments in quantum sensing and other quantum technologies. Significant progress has been made in the generation and understanding of a variety of novel systems, for which theory and computational simulation have pre/postdicted such states. However, such systems are systematically measured on substrates, and the theory and simulations have been performed for nanostructures in isolation. In particular, the experimental group at Nanogune has been recently measuring on finite graphene nanostructures using scanning tunnelling spectroscopy. Although experimental results are still not definitive, it seems there are significant effects due to the substrate. Graphene on gold is known to represent a weakly coupled system, graphene retaining most of its magical properties. In recent cases of interest the gold substrate seems to be dictating on what is measured more than expected. The aim of this project is to extend previous calculations for isolated nanostructures to theoretical descriptions including the substrate. Theoretical modelling of open quantum systems described by a Hubbard model of correlated electrons coupled to a fermionic bath will be the base of the study, trying to address the particular spin states with those key theoretical ingredients, so as to better understand both the experimental results and their applicability for quantum technologies. Calculations performed within a density-functional-theory scheme might complement the study by offering estimates of the key parameters in the model.

Title: **The non-equilibrium Jarzynski equality and pure quantum dissipation in a fermionic bath**

An apparently simple but very powerful equation for non-equilibrium processes was proposed by C. Jarzynski in Phys. Rev. Lett. 1997, which relates the statistical average of the exponential of work performed in a process away from equilibrium with the exponential of the free-energy difference between initial and final states. In addition to its being quite surprising to find such a result so recently, it is counter-intuitive since we expect dissipation always to increase the work needed to drive the process. First proposed for weak-coupling classical systems, its applicability was later extended to strong coupling and quantum systems [Campisi *et al.*, Phys. Rev. Lett. 2009]. The idea of this project is exploring the implications of such equality to quantum dissipation, in particular to the case of a nucleus moving within a bath of fermions (electrons in a metal). There is significant knowledge accumulated on the problem from different perspectives, including scattering theory and explicit computational simulations of the quantum stopping processes, in addition to energy loss measurements, but which all relate to the average force (and average work). The project is of a highly exploratory character, for candidates ready to be creative and adapt the research direction according to ideas and findings, and to connect them to quantum dissipation in other contexts.

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14. Director: **Yue Ban** (yue.ban@tecnalia.com)

Title: **Quantum simulation on non-hermitian dynamics in topological SSH chains via quantum computers**

Already showing the advantage of simulating the dynamics in different materials, quantum simulation provides a valuable perspective to study the behaviors of complex physical systems [Daley *et al.*, Nature 607, 667 (2022)]. Among various quantum computing platforms, topological quantum systems have gained substantial attention due to their inherent robustness arising from topological protection mechanism [Field and Simula, Quantum Sci. Technol. 3 045004 (2018)]. The Su-Schrieffer-Heeger (SSH) model is a tight-binding model for the simplest 1D lattice and has catalyzed the exploration of topological properties across diverse quantum registers. Originally proposed for polyacetylene, it has been demonstrated experimentally by cold atoms in optical superlattices and by chlorine atoms on copper surface and many other quantum systems. We have presented a hybrid analog-digital protocol to transfer the robust edge state non- adiabatically in an SSH chain. Such an analog-digital transfer protocol, extending the methodology for quantum control, gives rise to robust edge state transfer via finding the optimized counter-diabatic drivings in variational quantum circuits. The optimized counter-diabatic drivings can be implemented across various quantum registers, such as superconducting quantum circuits, cold atoms confined in optical lattices, electrons trapped in quantum dot arrays, etc. Motivated by the above results and the promising hybrid analog-digital methodology, we further propose the analog and digital simulation on non-adiabatic transfer in a non-Hermitian SSH (nH-SSH) chain with the consideration of the environmental noise. We will simulate non-Hermitian dynamics with the application of counter-diabatic driving derived from by adiabatic gauge potentials utilizing nested commutators (NC) during the transfer process. Stability with the effects of disorder will be studied from the spectra by adding Rice-Mele model contribution. Quantum circuits will be designed to implement non-unitary operations of the transfer process in a more accurate way with shorter lengths, although the current NISQ device naturally hosts the unitary quantum gates. We will also simulate

the non-Hermitian skin effect (nHSE) for the nH-SSH model [Lin *et al.*, arXiv: 2302.03057 (2023)] and investigate other non-Hermitian topological phenomena. on a noisy real quantum processor. We will check all the above results in a noisy IBM quantum processor.

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15. Director: **Dario Bercioux** (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 investigate the spectral properties of non-Hermitian Hamiltonian systems [Bergholtz, Budich & Kunst, Rev. Mod. Phys. 93, 01500 (2021); Bender & Boettcher, Phys. Rev. Lett. 70, 947 (1998); Martinez Strasser *et al.*, arXiv:2307.08754]. Specifically, we will focus on the dice lattice, a bipartite two- dimensional lattice system characterized by three sites in the unit cell [Bercioux *et al.*, Phys. Rev. A, 80, 063603 (2009)], resulting in a flat band at zero energy. One of the goals of the master project is to introduce a non-Hermitian dimerization of the hopping parameter of the system and characterize the properties of the systems similarly to higher-order topological insulators [Herrera *et al.*, Physi. Revi. B 105, 085411 (2022)]. In the specific, we will investigate the accumulation of eigenvectors of the system of the boundary of a finite-size piece of dice lattice. The project will involve both analytical and numerical calculations.

Title: **Volkov-Pantrakov states in topological cold atoms systems**

In this project, we will study the emergence of Volkov-Pankratov states in cold atom systems. Volkov-Pankratov states are boundary modes observed in topological systems when the parameter driving the topological phase does not change abruptly but smoothly [Volkov & Pankratov, JETP Lett. 42, 178 (1985); van den Berg, Calvo, Bercioux, Phys. Rev. Research 2, 013171 (2020); van den Berg *et al.*, Phys. Rev. Research 2, 023373 (2020)]. We will consider a topological cold atoms system as proposed in [Goldman *et al.*, Phys. Rev. Lett. 105, 255302 (2010); Goldman, Urban, & Bercioux, Phys. Rev. A 83, 063601 (2011)], and we will consider different shapes for the confining trap that could lead to the appearance of Volkov-Pankratov states [Buchhold, Cocks, & Hofstetter, Phys. Rev. A 85, 063614 (2012)]. The project will involve both analytical and numerical calculations.

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16. Director: **Aitor Bergara** (a.bergara@ehu.eus)

Title: **Alchemical Transformations for Calculating Free Energy Changes**

It is increasingly common to use techniques based on molecular dynamics in the design of small organic peptides or molecules that can be used as drugs. Through these techniques, the properties of a molecule can be optimized by making chemical substitutions and selecting the replacement that minimizes the free energy of the system. Among the techniques used for evaluating this free energy, alchemical transformations are the most common. In these transformations, the chemical nature of the atoms in an initial molecule is changed to the atoms of another molecule, and the change in the resulting free energy is calculated. Due to their precision and efficiency, these techniques are widely used in the biotechnology industry today.

17. Director: **F. Sebastián Bergeret** (fs.bergeret@csic.es)

One choice between the two projects listed below.

Title: **Diode effect in superconducting systems**

There is currently significant interest in studying non-reciprocal transport properties in superconducting systems. The primary motivation is the creation of superconducting diodes that could be integrated into low dissipation circuits. The diode effect is associated with the breaking of two symmetries: time-reversal and inversion, and has therefore been observed in a wide variety of systems. In this project, the student will theoretically explore the diode effect in hybrid structures composed of superconducting elements and materials with strong spin coupling. The student will gain expertise in quantum kinetic equations, which enable the study of transport in real structures, accounting for disorder and out-of-equilibrium situations. It is worth noting that a significant portion of the project calculations will be done analytically, with numerical calculations used only for the study of intermediate cases. The Project will be carried out in the Mesoscopic Physics Group at the Material Physics Center in San Sebastian, with the possibility of partially remote work. Close collaboration with international experimental groups, with whom we actively collaborate, is anticipated.

Title: **General theory of Spin Hall Magnetoresistance**

Through the spin Hall effect, charge currents can be converted into spin currents. This effect can be observed in conductors with strong spin-orbit coupling. In particular, measurements of the so-called SMR (Spin Hall Magnetoresistance) are actively used to quantify this conversion and determine the fundamental parameters in transport. In this project, we will generalize the theory of SMR for hybrid systems, including terms allowed by the symmetry of the system. specifically, we will solve the kinetic transport equations for various geometries and combinations of materials using analytical methods and express measurable observables, such as conductance, in terms of the microscopic parameters of the theory. The Project will be carried out in the Mesoscopic Physics Group at the Material Physics Center in San Sebastian, with the possibility of partially remote work. Once the results are obtained, experiments will be proposed and discussed with local experimental groups at the Centro de Física de Materiales (Dr. Celia Rogero) and Nanogune (Dr. Felix Casanova), with whom we have a close collaboration.

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18. Director: **Jorge Casanova** (jorge.casanova@ehu.eus)

Title: **Quantum sensing at the nanoscale enhanced by entanglement**

Entanglement is a fundamental resource for quantum information processing, whilst it could also provide a systematic route to detect structural parameters of complex systems with unprecedented resolution. Among them we have, e.g., ensembles of unstable nuclei that could transmute to other nuclear isotopes (thus, effectively changing their magnetic moment), biomolecules involved in relevant metabolic routes, or highly protonated samples appearing in solid-state systems and cells. Current approaches to explore these scenarios use single quantum sensors, as well as ensembles where each sensor is considered as an independent quantum register. In this Master thesis we will design appropriate radiation patterns involving laser and radio-frequencies leading to entangled sensors arrays. Then we will study the properties of these arrays for the efficient detection of parameters in

physically relevant scenarios where the presence of entanglement could lead to quantum advantage. This is an interdisciplinary theoretical project that requires knowledge in quantum mechanics, as well as an open attitude of the candidate to investigate and incorporate different programming paradigms (such as machine learning of Bayesian inference) to the burgeoning field of quantum information processing.

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19. Director: **Xi Chen** (xi.chen@ehu.eus)

Title: **Error analysis of digitized counter-diabatic quantum optimization algorithms**

Shortcuts to adiabaticity are well-known methods for controlling the quantum dynamics beyond the adiabatic criteria, where counter-diabatic (CD) driving provides a promising means to speed up quantum many-body systems. In recent years, we have shown the applicability of CD driving to enhance the digitized adiabatic quantum computing paradigm in terms of fidelity and total simulation time. In this program, we begin with the state evolution of an Ising spin chain using the digitized CD driving derived from the variational approach. Later, we apply this technique in the preparation of Bell and Greenberger-Horne-Zeilinger states with high fidelity using a very shallow quantum circuit, demonstrating the acceleration of adiabatic quantum computing in noisy intermediate-scale quantum devices. Finally, we focus on the error analysis, including Trotter errors and adiabatic error, to understand the outperformance of digitized CD quantum optimization algorithms with different use cases.

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20. Director: **José A. Fernández** (josea.fernandez@ehu.eus)

Title: **Structural determination of molecular aggregates using mass-resolved laser spectroscopy and DFT methods**

Intermolecular interactions are weak forces of pure quantum nature. Despite their small module, they are of paramount importance for life on Earth, due to their influence in the environment. In addition, life makes extensive use of such forces. They are used to control fundamental processes such as docking of a ligand into a protein, or molecular recognition. Thus, having a deep knowledge of such forces is required to understand such processes, and therefore, there is a strong demand for high-quality experimental data from systems attached by intermolecular forces. In the “Grupo de Espectroscopía”, we form molecular aggregates using supersonic expansions, which cool the molecules to a few Kelvin, preparing them to be probed by means of a combination of UV and IR lasers. Using several mass-resolved spectroscopic techniques, important structural information is extracted from the aggregates, which is afterwards interpreted on the light of quantum-mechanical calculations.

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

Title: **Towards carbon-based quantum nanocircuitry**

Controlling electron propagation at the nanoscale is essential for future nanoelectronics, quantum computing, or sensing applications. To accomplish this, the design of atomically precise platforms with low-loss propagation channels is essential. In particular, carbon-based nanoarchitectures have emerged as promising candidates due to the recently demonstrated possibility of phase-coherent electron transport along 1D graphene nanoribbons integrated into a 2D platform. In this theory project, quantum electronic transport calculations will be performed in order to address different strategies aimed at manipulating and guiding electron propagation in 1D or 2D graphenic platforms. To this end, density functional theory (DFT) or tight-binding approximation in combination with non-equilibrium Green's function (NEGF) method will be employed. As a way of example, the effect of including heteroatoms in the nanoribbons or building lateral as well as vertical heterostructures might be investigated. The addition of dopants and/or functional groups that might add additional functionalities like magnetic moments, spin-selective transport or optical switching might be also considered. Our results would be very useful towards developing carbon-based nanocircuits and could guide future experiments in this direction.

22. Director: **Maia G. Vergniory** (maiagvergniory@dipc.org)

Title: **Band structure renormalization induced by correlations in the topological superconductor FeTe0.55Se0.45**

Topological superconductors are a class of materials that exhibit a unique combination of superconducting and topological properties. In these materials, superconductivity coexists with nontrivial topological electronic band structures. This distinctive feature gives rise to novel and fascinating physical phenomena, such as Majorana fermions and topological edge states, which have potential applications in quantum computing and other advanced technologies. In particular FeTe0.55Se0.45 (FTS) holds a distinctive position in contemporary condensed matter physics, where it intersects the realms of electron correlation, topological properties, and unconventional superconductivity. The bulk electronic structure of FTS is anticipated to possess topological non- triviality owing to the band inversion between the dxz and pz bands along the Γ-Z axis. In order to study the effect of correlations, an analytical tight-binding model was develop in this group [Li *et al.*, arXiv:2307.03861v2] and a renormalization scheme was proposed based on experimental data. In this project we propose to explore further this model by adding correlation via a Hubbard U and study its topology.

Title: **Phonon instabilities and charge-density waves in layered transition metal dichalcogenides** [co-director: **Ion Errea** (ion.errea@ehu.eus)]

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 [Schröter *et al.*, nat. Phys. 15, 759 (2019); Science 369, 179 (2020); Flicker *et al.*, Phys. Rev. B 98, 155145 (2018)]. 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-TaS2 or 1T-TiS2. Recently it has been proved that 1T-TaS2 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 [Bianco *et al.*, Nano Lett. 19, 3098 (2019); Errea, Calandra & Mauri, Phys. Rev. B 89, 064302 (2014); Bianco *et al.*, Phys. Rev. B 97, 214101 (2018)].

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23. Director: **Tasio Gonzalez-Raya** (tgonzalez@bcamath.org)

Title: **Coupled Hodgkin Huxley Quantum neurons**

The increasing interest in artificial intelligence, together with developments in quantum technologies have given rise to the interdisciplinary area of quantum machine learning. An interesting approach to combining both areas would be to replicate the behavior of brain neurons using an electric circuit, which can be done through the Hodgkin-Huxley model, and to study the quantum effects arising if the circuit was implemented on a quantum platform. In this thesis, we will study how two Hodgkin-Huxley quantum neurons can be connected, and specifically the dynamics and quantum effects arising in such a system. This study could be completed by looking at the possible applications in hardware-based quantum machine learning.

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24. Director: **Julen Ibañez-Azpiroz** (julen.ibanez@ehu.eus)

Title: **Optical activity of materials: theory and calculations**

In condensed matter physics, the optical activity of a material describes how the polarization of light rotates as it traverses the medium. The quantum-mechanical description of this phenomenon is given in terms of response functions that are calculated using perturbation theory. In this project we propose a combined theoretical and computational analysis in this area. As a first step, the student will work on the numerical implementation of the response function associated to optical activity. This will be done by employing localized Wannier functions as the basis set, a central tool that is heavily used in our group. Secondly, once the expression is successfully implemented, it will be used to study and understand the properties of optical activity in chosen materials of particular interest. 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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25. Directors: **Jon Lafuente Bartolomé** (jon.lafuente@ehu.eus), **María Blanco Rey** (maria.blanco@ehu.eus)

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 (SOI), 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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26. Director: **Aritz Leonardo** (aritz.leonardo@ehu.eus)

Title: **Prediction of Free Energy Changes through Artificial Neural Networks**

While traditional methods to calculate free energy changes of molecules have their utility, they often come with a significant computational cost, which can limit their practicality. A recent alternative that has gained traction is the use of artificial neural networks. Instead of relying on physically-based principles, artificial neural networks harness the power of modern databases. These neural networks, once trained on available data, are capable of efficiently predicting the values of the free energy changes we are interested in, offering a compelling trade-off with significantly reduced computational overhead. This shift toward artificial neural networks represents a paradigm shift in how we approach the prediction of free energy changes. Rather than relying solely on traditional simulations that demand extensive computational resources, neural networks leverage vast datasets to extrapolate insights into energetic phenomena. Once trained, these models become invaluable tools for rapidly and accurately estimating free energy changes, saving both time and computational resources. In this way, artificial neural networks have opened up new avenues for researchers and scientists to explore complex energy landscapes, making the prediction of free energy changes a more accessible and efficient endeavor in modern computational chemistry and biophysics.

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27. Director: **Hegoi Manzano** (hegoi.manzano@ehu.eus)

Title: **Training of DFT accurate Machine Learning potentials**

Quantum methods, and particularly Density Functional Theory (DFT), are a valuable tool in materials science. They are robust and accurate, yet their computational cost limits their application to <1000 atoms and make them prohibitive for molecular dynamics simulations. The raise of Machine Learning (ML) methods give us a chance to bypass that limitation. It is possible to train a neural network with sufficient data to reproduce accurately DFT energies and forces in atomic systems at a much lower computational cost. In this master

project the student will build a DFT database for calcium carbonates and train a neural network using the GPU-based aenet-pytorch code.

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28. Director: **Ana Martin Fernandez** (ana.martinf@ehu.eus)

Title: **Exploring Quantum Sensing at the Nanoscale: NV Centers in Diamond for Characterizing Organic Samples**

A nitrogen-vacancy (NV) center is an electronic spin that can be manipulated and read out with high precision, making them excellent detectors for various physical quantities, such as magnetic fields and temperature, at the nanoscale. A diamond crystal can contain a large number of NV centers distributed throughout its lattice structure. It is possible to place a sample of interest on or near the surface of the diamond crystal, close to the ensemble of NV centers. The sample could be a molecule, a nanoscale object, or even another quantum system. The NV centers in the diamond can be used to interact with and sense the properties of the sample. In this thesis, we will explore the use of NV-ensembles located just a few nanometers from an organic sample on a diamond's surface, to study and characterize it. The student will learn the characteristics of the nanoscale regime and study different techniques to address the challenges posed by this environment.

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29. Director: **Ana Isabel Martinez** (AIMartinez@ikerlan.es)

One choice between the two projects listed below.

Title: **Solving the TSPTW Problem Using Quantum Annealing**

The TSPTW problem (Traveling Salesman Problem with Time Windows) involves determining the optimal route for visiting a specific number of locations or nodes while minimizing the total distance traveled. This must be done under the constraint that each node has a deadline for visitation. It is an adaptation of the classic combinatorial optimization problem known as the Traveling Salesman Problem (TSP), with variations like TSPTW aimed at making it more realistic by adding practical constraints that often occur in real-world scenarios. The resolution of the TSP and its variants has numerous applications in various industrial and commercial fields, including logistics, land and naval freight transport, planning, printing, lithography, microchip manufacturing, and more. Improving the accuracy or reducing the time required to determine the optimal route can lead to energy savings, reduced greenhouse gas emissions, significant cost savings, and enhanced resilience in global freight transportation systems against bottlenecks. This is of extreme importance both in the current international context and in addressing humanity's major challenges, such as climate change. Mathematically, TSPTW is an NP-hard problem that becomes intractable to solve exactly when the number of nodes is large due to the factorial growth in the number of possible combinations with the number of nodes. Therefore, its resolution requires the use of heuristic algorithms that provide approximate solutions, especially for a large number of nodes, demanding substantial computational capacity and yielding suboptimal results. One of the most common and promising short-to-medium-term applications of quantum computing (QC) and Quantum Machine Learning (QML) is the resolution of combinatorial optimization problems. In fact, significant progress, both theoretically and practically, has already been made in addressing TSP and TSPTW using various QC/QML techniques, with promising outcomes. At Ikerlan, we aim to explore

the state-of-the-art in exact TSPTW resolution by employing QC and QML techniques and methodologies that could be applicable to this problem. The significance of TSPTW and the feasibility of its resolution in the short-to-medium term make it attractive in offering practical solutions to our customers' real-world problems.

Title: **Quantum Sparse Representation: Development of a Hybrid Classical-Quantum Computer Vision Algorithm via Quantum Annealing**

Sparse Representation is an unsupervised classification technique in which we represent our data in a latent space using a feature map. This technique, which can be considered a type of autoencoding, differs from variational autoencoders in that it imposes sparsity on the representation, meaning that for each instance in the dataset, most of the feature values in the latent space are equal to zero. This has the advantage that the dimensionality of the latent space can be higher than that of the original space without the autoencoder tending to replicate the identity function. This technique has various applications, such as restoring old or damaged images, as it learns patterns present in imperfect data very well. In fact, several studies suggest that this technique is a model that adequately replicates the functioning of the part of the neocortex responsible for processing visual data in mammals (including humans). This technique serves as a gateway to spike neural networks, where a neural network is constructed using layers that constitute sparse representations. Finally, there are reasons to believe that this technique could prevent the occurrence of so-called adversarial examples, which are images that can cause any Computer Vision model to fail through modified images that appear identical to the original ones at first glance. The natural way to implement the sparse autoencoding algorithm is by using the L0 norm of feature values as a regularization term. Avoiding this using L1 or L2 norms worsens the results. However, calculating the L0 norm is classically intractable, which is why classical algorithms do not use L0 norms. Nevertheless, quantum annealing allows for the natural and straightforward generation of this representation, performing a calculation that is classically intractable but feasible today (with some degree of approximation). In essence, this opens the door to implementing a new technique that is not feasible for classical computers: the Quantum Sparse Representation technique, a hybrid Quantum Machine Learning technique that involves replacing the calculation of sparse representation in a Machine Learning model with a quantum annealer-based calculation. The task at hand involves implementing this algorithm and developing the Machine Learning model, including the classical component.

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30. Directors: **Sofía Martínez-Garaot** (sofia.martinez@ehu.eus), **Mikel Palmero** (mikel.palmero@ehu.eus)

One choice between the two projects listed below.

Title: **Quantum System Dynamics Control for Metrology**

We have developed a set of analytical and numerical tools known as Short- cuts to Adiabaticity (STA), which play a pivotal role in the art of controlling quantum systems. Notably, these methods can significantly contribute to the implementation of quantum technologies, such as quantum computers, by substantially enhancing fidelity levels currently constrained by state-of-the-art technology. Applications span a wide range, encompassing information transfer and processing through gate-based or analog paradigms, as well as interferometry and metrology. The flexibility of STA paths for the controlling parameters may be used to boost robustness against noise and perturbations

or to optimise relevant variables. For this master's thesis, we propose to make substantial contributions to the development of both fundamental and applied aspects of STA in the field of metrology, with the aim of enhancing precision measurements. Given that the implementation of shortcuts is still in a very initial phase within this field, our plan consists of a two-stage approach. In the initial phase, we will try implementing a specific shortcut to a known problem and study the improvement in efficiency. In the second stage (subject to available time), we will refine shortcut-based results to mitigate the effects of noise and perturbations.

Title: **Develop a Python module for numerical evolution of time-dependent Hamiltonians**

We propose developing a full set of functions useful for numerical simulation of time dependent Hamiltonians in python, writing documentation for it, testing and optimising the code in real problems, and finally gathering it in a python library format. The student will be able to base this work in a number of MATLAB codes that have been previously tested and applied for research applications. The library will span from writing supporting functions (e.g. different ways of defining the grid), to writing different time evolution solvers for different situations (1D and 2D Schrödinger, Gross Pitaevskii, etc.). Once the minimum basic library is built tests will be run to compare performance vs the original code. Depending on the available time, more complex functionalities can be developed for this library (e.g. parallelisation of some of the functions, include more options to the functions, etc.). This project is a good opportunity not only to get in touch with useful code for quantum dynamics, but also to develop coding skills, and develop a full working library in a professional manner.

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31. Director: **Michele Modugno** (michele.modugno@ehu.eus)

Title: **Ultracold atomic gases: a toolbox for quantum physics**

Ultracold quantum gases represent one of the most fascinating research areas in modern physics. They are employed in many laboratories worldwide to investigate fundamental problems at the frontiers of different fields, including superfluidity, nonlinear and disordered systems, solid-state physics, to mention a few. Quantum gases stand out as versatile platforms for quantum simulations, making this research field exceptionally rich and stimulating. The student will work on a project aimed at investigating the physics and phenomenology of these quantum systems. Possible projects include: 1) Modulation instability of a Bose-Einstein condensate (BEC) with attractive interactions; 2) Kelvin-Helmoltz instability of an array of quantum vortices in a single-component 2D superfluid, in both planar and annular geometries. Both projects will involve the use of analytical and numerical methods. Students will gain proficiency in mastering the Gross-Pitaevskii equation and computing the excitation spectrum of a BEC using the Bogoliubov theory. Other project possibilities are also open for discussion.

32. Director: **Aitor Moreno** (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.

33. Director: **Koushik Paul** (koushikpal09@gmail.com)

Title: **Variational Quantum Algorithms with Photonic Quantum Computing**

In recent years, photonic quantum computing has generated attention for its potential as an alternative computational paradigms for quantum computing through the manipulation of quantum states encoded in photons. This project will investigate the application of photonic quantum computing to develop and optimize variational quantum algorithms (VQAs) using Quantum Machine Learning and/or conventional optimization. The scope will involve implementing photonic quantum computing by designing tailored VQAs, comparing their performance with classical approaches, and offering insights into practical applications. Additionally, the project will explore the integration of shortcuts to adiabaticity (STA) techniques within VQAs to enhance algorithmic efficiency and speed up quantum computations. The expected outcomes will include valuable contributions for understanding the potential of photonic quantum computing and STA in the noisy intermediate scale quantum computing era.

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34. Director: **Jose M. Pitarke** (jm.pitarke@nanogune.eu)

One choice between the two projects listed below.

Title: **Silicon-based quantum computing: Quantum state readout**

Electron spin qubits in silicon quantum dots are consolidating their position as a leading candidate to build scalable high-fidelity quantum computing processors, a machine that could solve many of today's computational challenges such as for example the simulation of new materials and medicines. Several recent demonstrations have shown single- and two-qubit gate fidelities exceeding the requirements for fault tolerant thresholds in the same device. Combined with the dense scaling potential, advanced manufacturing, and prospects for integration with cryogenic classical electronics, these results present a promising future for spin-based qubits in silicon. Silicon spin qubit are typically readout by ultrasensitive charge sensors such as the single-electron transistor (SET) and the single-electron box (SEB). More particularly, the SEB has attracted recent interest due to its small footprint that enables the realisation of highly connected qubit architectures. In this master's project, you will design and simulate a new type of SEB based on multi-electron quantum dots. More particularly, you will (i) learn the basics of spin qubit readout via spin-to-charge conversion, (ii) you will learn the fundamentals of the SEB, (iii) you will reproduce the simulations of the standard SEBs and (iv) you will extend these results to a new type of SEB based on multi-electron quantum dots. At the end of this master's project, you will be ready to design optimized SEBs and be prepared to start experiments on spin qubit readout. [Relevant literature: arXiv:2202.10516]

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 experiment silicon quantum devices. [Relevant literature: arXiv:1803.06176v1]

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35. Director: **Ricard Ravell** (rravell@bcamath.org)

Title: **Memory effects and degeneracy of Liouvillians**

In Open Quantum systems the dynamics of the reduced state of interest evolves due to a Liouvillian superoperator. Properties of these superoperators have been extensively studied. For instance, there are works that investigate the relationship between the degeneracy of the eigenvalue 0 and the chaotic behaviour of the dynamics of the system. The aim of this project is to study the degeneracy of the spectrum of the Liouvillian and relate it to some measure of the memory effects of the evolution (its non-Markovianity.)

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36. Director: **Enrique Rico** (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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37. Director: **Mikel Sanz** (diracmatrix@gmail.com)

One choice between the two projects listed below.

Title: **Mathematical aspects of quantum computing and quantum algorithms**

Quantum computation employs quantum resources to speed up certain algorithms and tasks. This field has blossomed during the last years due to the advances in quantum platforms and algorithmics, but there are still multiple open problems which must be addressed. Some examples are the generation of efficient methods for data loading in quantum processors, the design of efficient classical-quantum interfaces, or a proof of speedup in variational quantum algorithms, just to mention a few. In this thesis, we will develop mathematical tools to address some of these questions, depending on the interest of the student.

Title: **Applications of the quantum model of light-matter interaction in anti-resonant optical fibers** [co-director: **David Novoa** (david.novoa@ehu.eus)]

Anti-resonant optical fibers are a recently developed quantum platform which provides a huge flexibility in the design and physical properties. In this Thesis, the student will study the quantum properties of this new technology from the fundamental model describing them. Afterwards, the student will employ this machinery to design applications in quantum technologies, particularly in quantum communication and sensing.

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38. Director: **Evgeny Sherman** (evgeny.sherman@ehu.eus)

Title: **Simulation and design of quantum materials**

Modern experimental techniques can produce on demand rich varieties of quantum materials by appropriate multiple gating of two-dimensional electron systems. The goal of this Master project is to provide a theoretical description of these experiments and to design gating patterns for producing materials with requested quantum properties.

39. Director: **Jens Siewert** (jens.siewert@ehu.eus)

One choice between the two projects listed below.

Title: **Bloch-ball type representation of two-party composite systems with different local dimensions**

The Bloch representation (that is, the mathematical description of quantum-mechanical density operators in terms of a matrix basis) is a powerful — yet far from fully developed — tool to solve quantum mechanics problems. Its language is deeply rooted in geometry and therefore its concepts are amenable to geometric intuition. Only recently, methods have been presented to adequately visualize higher-dimensional state spaces, such as the Bloch-sphere analog of a three-level system (qutrit) and that of bipartite systems, and there is much potential for further research. In particular, these investigations of bipartite systems are fundamental for our understanding of which quantum correlations are possible and which are not. The central theme of this master thesis project is to study two-party systems of different local dimension. While we know the complete solution for equal local dimensions, it is evident that the opposite case has rather different geometrical properties which require precise description. The results of the project will open the possibility to study multi-party systems which are of tremendous importance to extend this research to a variety of physics applications. The project is highly ambitious and demanding. Involving both analytical and numerical work it requires strong motivation and excellent technical skills, especially in linear algebra.

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 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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40. Director: **Lianao Wu** (lianaowu@gmail.com)

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).