TFM proposals 2022-23

Cosmology, Relativity, Fields and Particles

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.

Director: **Jose J. Blanco-Pillado** (joseblancopillado@gmail.com)

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.

Director: **Mariam Bouhmadi-López** (mariam.bouhmadi@gmail.com)

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.

Director: **David Brizuela** (david.brizuela@ehu.eus)

one choice between these two projects:

Title: **Quantum-gravity effects for the inflationary universe**

In this proposal we would analyze certain aspects of the quantization of both matter and geometric degrees of freedom in the primordial universe. In particular, in the context of a semiclassical approximation to the geometrodynamical (Wheeler-DeWitt) quantization the possibility of constructing a well-defined Hilbert space by using the PT invariance of the Hamiltonian would be considered. On the other hand, backreaction effects on a polymeric (loop) quantization would be analyzed.

Title: **Canonical derivation of the Hawking radiation**

Most of the works that derive the Hawking radiation for a collapsing body are formulated in a Lagrangian framework. Nonetheless, recently a number of approaches have been put forward in order to provide a Hamiltonian formulation of this effect. In this master project one would first perform a literature review of such proposals and then consider the computation of quantum-gravity corrections to the Hawking radiation via a semiclassical method based on the moment decomposition of the wave function.

Director: **Miguel García Echevarría** (miguel.garciae@ehu.eus)

One choice between the two projects listed below.

Quarks and gluons are the fundamental constituents of nucleons. But how are they distributed in space? How much and in which way do they contribute to the spin of the nucleon? How does their dynamics generate other nucleon properties and affect high-energy processes? Nucleon inner structure is parametrized in terms of different 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 Physics 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 confinement in QCD.

Title: **Quarkonia production as a tool to probe TMDs**

We will focus on quarkonia production as a tool to access TMDs, which give the 3D structure of the nucleon. We will use the machinery of effective field theories to analyze some quarkonium-production process which can be relevant at the LHC or future experiments like the electron-ion collider (EIC) and fixed-target experiments, and give predictions which can be tested with experimental data.

Title: **GTMDs in Ultra-Peripheral Collisions at the LHC**

Ultra-Peripheral Collisions (UPCs) at the LHC are recently gaining more and more attention as a tool to probe nucleon structure. Within this project we will analyze the potential of UPCs in proton-ion collisions at the LHC to access GTMDs, which give the 5D structure of the nucleon.

Directors: **Ruth Lazkoz** (ruth.lazkoz@ehu.es), **Jon Urrestilla** (jon.urrestilla@ehu.es)

Title: F**orecasting 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.

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

Title: **Characterisation of Gravitational Wave backgrounds generated at preheating**

Gravitational wave backgrounds of stochastic nature are expected to have been formed at many phenomena of the early universe, which include inflation and/or (p)reheating at the end of it. In fact, the measurement and characterisation of such backgrounds is one of the major goals of future GW observatories. This research proposal aims to explore the properties of the formation and evolution of GWs produced at some standard preheating scenarios. We will try to improve the standard approach to GW phenomenology to characterise such backgrounds through different components and also to investigate possible backreaction effects onto the background dynamics. In order to accomplish this, we will employ lattice simulations of the underlying field theories, where full dynamics, including non-linear effects, can be accurately described.

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

one choice between these two projects:

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 (QCD) 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: **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.

Directors: **Matthias Burkardt** (Burkardt@comcast.net)

one choice between these two projects:

Title: **Model dependence of the QCD evolution description in the analysis of Sivers asymmetries**

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 non-perturbative Quantum Chromodynamics (QCD). One of its striking signatures is its cause of transverse single spin asymmetry in semi-inclusive deep-inelastic scattering, i.e., hadron produced in coincidence with the scattered lepton in highly energetic lepton-nucleon scattering. Since such experiments are typically performed at different energy scales, a comprehensive analysis requires including QCD evolution effects using known equations. However, these evolution equations require off-diagonal quark-gluon correlation functions that cannot be directly measured and are thus modelled. We plan to compare different models to elucidate the dependence of employing different models in such an analysis.

Title: **Model dependence of extractions of the proton's generalized parton distributions**

Generalized parton distributions (GPDs) have a very physical interpretation in terms of impact-parameter dependent parton distributions in the nucleon. What makes them appealing, among others, is the fact that they have been related to orbital angular momentum of quarks and gluons inside the proton and thus to one of the missing pieces in the description of the proton spin. However, GPDs cannot be measured directly and can only be determined indirectly from the Compton cross section. We plan to study whether or not the latter can be done model-independently if known QCD evolution equations are included in the data analysis.

Quantum matter, simulations, and technologies

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

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 carbon triangulenes using scanning tunneling spectroscopy. Although experimental results are still not definitive, it seems as if there would be significant effects due to the gold substrate. Graphene on gold is known to represent a weakly coupled system, graphene retaining most of its magical properties, albeit with small shifts of the Fermi level away from the Dirac-cone tip, which can be controlled by gating. In the case of the spin states in triangulene so far 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 5-triangulene to computational simulations including the gold substrate. The calculations will be performed within a density-functional-theory scheme, which is known to give realistic descriptions of weakly correlated condensed matter. They will be complemented by qualitative theoretical modeling trying to address the particular spin states with key theoretical ingredients, so as to better understand both the experimental and computational results.

Director: **Dario Bercioux** (dario.bercioux@dipc.org)

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

In this project, we will study the emergence of Volkov-Pankratov states in cold atoms 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 et al., Phys. Rev. Research **2**, 013171 (2020); 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); 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 et al., Phys. Rev. A **85**, 063614 (2012).]. The project will involve both analytical and numerical calculations.

Directors: **Aitor Bergara** (a.bergara@ehu.eus), **Aritz Leonardo** (aritz.leonardo@ehu.eus)

Title: **Simulating cotranslational protein folding in the ribosome**

A human cell contains over 100.000 types of unique proteins, and the information contained in its sequence of amino acids is sufficient for it to adopt its folded structure. Protein synthesis occurs on ribosomes, where the nascent chain is progressively synthesized and passes through a tunnel inside the ribosome. When the chain is formed, folding occurs and the final structure is adopted. For years this official paradigm established that the ribosomal tunnel was a passive conduct; however, today we know that protein folding begins in the ribosome tunnel itself. What happens during this transit is enigmatic since all the experimental evidence is indirect, and poses a major theoretical-experimental challenge. It implies the experimental capacity to observe the process of creation and folding of the peptide in real time and to be able to create quantitative models through molecular dynamics in sufficiently wide time intervals. This MASTER project deals with the theoretical-computational part of an ambitious collaboration with the University of Marseille, that has the challenge of taking real-time images of the process described above, using High Speed Atomic Force Microscopy. This project aims to clarify, through theoretical simulations accompanied by HS-AFM images, the crucial role played by cotranslational folding in the formation of neuronal potassium channels.

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

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

Entanglement is a fundamental resource for quantum information processing, whilst it could also provide a route to access parameters of complex systems with unprecedent 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 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 programing paradigms (such as machine learning of Bayesian inference) to the burgeoning field of quantum information processing.

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

Title: **Shortcut Towards Optimal Quantum Algorithms**

Shortcuts to adiabaticity (STA) are well-known methods for controlling the quantum dynamics beyond the adiabatic criteria, where counter-diabatic driving provides a promising means to speed up quantum many-body systems, with the applications in digitized adiabatic quantum computing. In this project, we will explore the application of shortcuts to adiabaticity in quantum adiabatic computing, quantum annealing and quantum variational algorithms. We will first focus on two quantum variational algorithms, including QAOA and VQE, assisted by counter-diabaticity, which will be used to construct non-trivial ground states for various models, including integrable and non-integrable quantum spin systems. Later, approximate counter-diabatic potentials satisfying locality constraints will be optimized by machine learning (ML) algorithms. This approach, combined with RL-based QAOA will show parameter schedules clustering around optimal or quasi-optimal smooth trajectories. Here STA and ML approaches will be jointly pursued to seek the appropriate evolution trajectories rapidly, by avoiding small energy gap and/or suppressing the energy excitation. Finally, applications to theoretical chemistry, pattern recognition, logistic networks and other optimization problems, such as battery optimization for electric cars where the input data is provided from industry, are foreseen, implemented in NISQ quantum processors with shallower circuit depth, towards quantum advantage.

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.

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

Title: **Addressing spin states in graphene nanostructures**

Spins are expected to become key elements in the second quantum revolution as qubit elements for quantum computations. For this purpose, optimal materials that combine properties such as spin localization and long-range spin-spin interactions are required. In particular, the recent discovery of stable spin-polarized states in graphene nanostructures make such nanomaterials promising candidates for their use as quantum platforms. In this project, density functional theory (DFT) and model calculations will be employed to unravel the basic mechanisms giving rise to spin polarized states in selected graphene nanostructures, with special focus on the evolution of the spin arrangement and spin-spin interactions from 1D chains to 2D networks. Our results would be very useful towards developing carbon-based 2D materials with optimal magnetic properties and could guide future experiments in this direction.

Director: **Ion Lizuain** (ion.lizuain@ehu.eus)

Title: **Control of quantum system dynamics for quantum technologies**

Quantum dynamics offers a vast potential of applications but they are hindered by decoherence. A general way to mitigate decoherence is to implement "Shortcuts to adiabaticity" (STA), a set of techniques developed by the group to speed up the processes without residual excitations. STA work by inverse engineering the time-dependent external controls. They have been applied to a broad range of systems such as qubits in different physical platforms (trapped ions, superconducting circuits, neutral atoms in optical lattices,...) for motional control or to implement interferometry, metrology or quantum information processing. STA extend as well beyond quantum mechanics, to make optical devices or mechanical systems more compact and robust. In this project we would address some application of STA in one of the many systems or operations in which they are useful. Examples for this project, in the context of quantum technologies, could be to design state transfer between two coupled oscillators or manipulations of ion chains.

Directors: **Ion Errea** (ion.errea@ehu.eus) and **Maia G. Vergniory** (maiagvergniory@dipc.org)

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

[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 dichalcogenides 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., Phys. Rev. B **97**, 214101 (2018); Nano Lett. 19, 3098 (2019) ; Errea et al., Phys. Rev. B **89**, 064302 (2014)].

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 of modern physics. They are being employed in many laboratories around the world for investigating fundamental problems from disparate areas (including e.g. solid state physics, superfluids, non-linear and disordered systems), representing one of the current platforms for quantum simulations. The student can choose a project in any of the above areas, to be carried out with analytical and numerical methods. Collaborations with international experimental groups are also possible.

Director: **Aitor Moreno** (ai.moreno@ibermatica.com)

one choice between these two projects:

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 Process Mining System applied to the optimization of planning in an industrial production**

The proposed work consists of a process optimization system, based on industrial data from a real plant, which adjusts its production priorities, operating restrictions and shifts, recommendations regarding maintenance, in order to find the best scenarios in terms of costs, minimization of incidents or improvement in production (optimization of the OEE, minimizing stops). These scenarios will be "suggested" based on technology based on quantum computing, where the execution is regulated by a flow of processes with certain restrictions (process mining). The classic methods of programming plant operations (MRP systems) are not very effective in real production plants since they presuppose unrealistic hypotheses that are hardly met in practice. Quantum algorithms constitute one of the most promising techniques as an alternative to classical techniques, due to their scalability and flexibility, avoiding local minima.

Director: **David Novoa** (david.novoa@ehu.eus)

Title: **Design and optimization of a quantum molecular modulator**

We are witnessing a second quantum revolution in which quantum mechanics is enabling new tools with applications in, for example, sophisticated quantum networks. In this endeavour, it is of utmost importance to develop technologies capable of addressing long-standing challenges in "real-life" quantum applications, whose solutions have for many years remained elusive. In photonics, this is the case, for example, of quantum frequency conversion of single photons and entangled photon pairs, where most current approaches are either inefficient, offer limited spectral shifts, and suffer from the addition of noise and decoherence. In this thesis we will design a novel type of quantum frequency convertor based on synchronous molecular motion in specialty optical fibers. We will analyze all the relevant parameters of the system to find an optimum design that could be implemented in real laboratory tests.

Director: **Eneko Osaba** (eneko.osaba@tecnalia.com)

Title: **Quantum Optimization Algorithms for real-world oriented Vehicle Routing Problems**

Quantum Computing is considered as the next frontier in computing, and it is attracting a lot of attention from the current scientific community. This kind of computation provides to researchers with a revolutionary paradigm for addressing complex optimization problems with a significant advantage. Anyway, although high expectations are pinned on this field, Quantum Computing is still in an incipient stage of development. Despite this, the application of quantum computing has already been explored in various fields such as industry, energy, economics, or logistics. It is precisely this last field, logistics, in which quantum computing has shown a great adaptability, having been applied to various optimization problems of different kinds (almost always from an exploratory perspective). This master's thesis will focus on this specific field. Delving into the specific issue of work, the efficient distribution of goods is a major challenge for the main agents in the sector. It is a problem with different facets, where customers can have their own restrictions, and where, in turn, other factors such as municipal restrictions, the type of vehicle used or typical density of traffic on the routes to follow can influence. Therefore, the main objective of this master's thesis will be to explore the application of quantum annealing based solvers to the Vehicle Routing Problem. Being more specific, it will deal with problems that take into account restrictions coming from the real world, such as flexible time-windows. Among the paradigms to be explored, priority will be given to the resolution method known as the Quantum Approximate Optimization Algorithm (QAOA), without ruling out the use of other approaches such as D-WAVE. The work will explore the resolution of i) small problems: directly solved by quantum processing units; ii) large problems: applying hybrid approaches and exploring the possibility of carrying out knowledge transfers in the resolution of different tasks (Transfer Optimization).

Directors: **Enrique Rico** (enrique.rico@ehu.eus)

one choice between these two projects:

Title: **Symmetry protected qubit in an open quantum system**

We will consider a particular limit of a very light particle on a circle, in the presence of half of the flux quantum. With this flux, the ground state of the system is doubly degenerate and the rest of the spectrum is separated by large energy gaps from the ground state. At low- temperatures, we can neglect contributions of all states except for the ground state. The ground state space coincides with the one for a spin-1/2. We will consider a superconducting circuit implementation, considering any source of noise, that must be described by an open quantum system. Problems to be addressed: (1) Discuss the symmetry and topological aspects of the problem and characterize the symmetry protected subspace that realizes a qubit. Check how is changing in the presence of noise. (2) Couple two protected qubit and study any interaction that respects the symmetries of the combined system. (3) Study the quantum computational power of the proposed qubit. (4) Analyze a particular implementation of a single and two protected qubits in terms of superconducting circuits. (5) Propose a minimal quantum circuit realization for a set of symmetry protected qubits in realistic scenario, i.e., described by an open quantum system.

Title: **Quantum simulation of particle physics**

We will consider the simplest gauge model, a Z(2) lattice gauge model, and we will study in detail how to implement in a quantum simulator any possible gauge invariant expectation value, including real-time dependent quantities which are essential to describe physical processes like scattering of particles. Problems to be addressed: (1) Study and get familiar with the physics of lattice gauge models in the case of a Z(2) gauge model. (2) Propose a physical realizable implementation of a quantum simulator with all the degrees of freedom and interaction terms of the gauge model. (3) Understand how to measure gauge invariant quantities that depend on real-time. (4) Analyze all the previous steps in the description of scattering of particles.

Directors: **Mikel Sanz** (diracmatrix@gmail.com)

one choice between these two projects:

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: **Secure microwave quantum communication with satellites**

Microwaves are present in almost every wireless communication process nowadays, from local area networks to mobile communications. The use of quantum degrees of freedom allows for provable secure communications, so understanding the limits of microwave quantum communications is crucial. In this thesis, we will study the limits due to decoherence and diffraction losses in the security and distance of microwave quantum communication in satellite-satellite and Earth-satellite communication. Additionally, depending on the interest of the student, we could also focus on the development of missing pieces for this protocol, such as the design of quantum collimators to focalize the signal or a receptor antenna.

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

one choice between these two projects:

Title: **Electron motion in solids with isotopic disorder**

Disorder is the key element that determines electron transport in solids. Usually disorder is produced by charged impurities or other lattice defects. However, another type of disorder is possible and is of real interest. Chemical elements have various isotopes, having different atomic masses with all other absolutely equivalent electronic properties. Isotopes are randomly distributed in crystals and, thus, produce a disorder in the mass distribution. At zero temperature this disorder can considerably influence conductivity of the system due to randomness in the zero-point quantum oscillations of the atoms. The proposed project will be focused on the studies of the effects of the isotopic disorder on the electron transport in solids.

Title: **Driven motion of solitons**

Solitons (self-localized objects) in nonlinear systems play an important role in modern physics, from optics to spin systems and cold atomic gases. Understanding of the motion of solitons is important in all these branches of quantum physics. As localized objects, solitons strongly interact with the impurities and other defects in their host systems. Therefore, motion of solitons can be initiated and controlled by the motion of these defects. In this project, we will study motion of solitons driven by controlled displacement of the defects the solitons are pinned to. Thus, we will understand their dynamics and also formulate new rules for design of properties of dynamical nonlinear quantum systems.

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

Title: **Maximally entangled mixed states**

Entanglement theory is one of most important branches of quantum information. Although it has been developed for more than two decades now, many of the supposedly simple questions remain unanswered. Part of the reason for this is that it is notoriously hard to quantify and even to detect entanglement in mixed quantum states. Consider the following problem for two-party quantum states: It is well known that entanglement does not increase under local unitary operations of the parties, whereas a global unitary operation including both parties is often capable of augmenting the amount of entanglement in the state. Then, which are the states whose entanglement cannot increase under any global unitary (for a given purity)? These states are called 'maximally entangled mixed states' (MEMS), and they are known only for the case of two qubits ($d=2$), but not for local dimensions $d>2$. In this TFM project we want to develop a more thorough understanding of the analytical solution for two qubits and try to transfer aspects of this insight to higher local dimensions, i.e., to devise ways for finding MEMS at least for $d=3$. This is a highly ambitious project that involves both analytical and numerical work, thereby providing valuable insight into the fundamental concepts of entanglement theory as well as hands-on experience for 'how things work in practice'.

Directors: **Ivo Souza** (ivonuno.saldanha@ehu.eus), **Stepan S. Tsirkin** (tsirkinss@gmail.com)

Title: **Natural optical activity of crystals from first principles**

As light propagates through a chiral medium its plane of polarization rotates, a phenomenon known as "optical rotation" or "natural optical activity". Due to the fundamental and practical importance of chirality in chemistry, the molecular theory of this phenomenon is well developed. Chiral crystals are being intensively studied nowadays, but the theory of optical activity in crystals is not nearly as well developed as for molecules. The goal of this project is to develop and implement ab initio methodologies for calculating the optical activity of crystals, using either finite-frequency perturbative approaches or real-time propagation schemes.

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

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 in our paper, Phys. Rev. Lett. **89**, 057905 (2002). The experimental test of this BCS simulation was done by Massachusetts Institution of Technology. Now the idea have become a new type of quantum computation, the Trotterized (or digitized) adiabatic quantum computation [Nature **534**, 222 (2016)]. Along this line, we recently propose a static version of this technique to perform the optical simulation of the adiabatic evolution if 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 mimic different physical systems with the static adiabatic evolution using the idea in Phys. Rev. Lett. **89**, 057905 (2002).