Master's Thesis Topics for the academic year 2024-2025

Efficient Simulation of Large Quantum Circuits via Circuit Cutting and Clustering

Based on recent advances such as CutQC and cluster-based simulation, investigate scalable methods for simulating quantum circuits that exceed the hardware limits of quantum devices. Thesis will focus on partitioning quantum circuits into smaller subcircuits executable on limited-qubit hardware, with classical postprocessing to reconstruct global outcomes. Key mathematical tools include graph theory and mixed-integer programming (for optimal circuit partitioning), tensor networks (to represent and simulate quantum operations), linear algebra and operator theory (to handle matrix decompositions and gate simulation). Applications will include VQE and/or Hamiltonian simulation, with the goal of developing practical hybrid quantum-classical workflows.

Master thesis examination committee.
Ioannis Karafyllidis (Supervisor)
Georgios Sirakoulis
Kyriakos Zoiros

Quantum algorithm for ligand-protein docking based on the pharmacophore model.

Pharmacophore modelling is a computational technique used in drug discovery to identify and represent the key chemical features of a molecule that are essential for its biological activity. These features, such as hydrogen bond acceptors or donors, hydrophobic areas, and aromatic rings, are represented in a 3D spatial arrangement. Ligands will be represented by their pharmacophore model and a quantum algorithm will be developed to search and find possible docking sites of the ligands in proteins. Proteins will be modelled using the protein lattice model.

Master thesis examination committee.
Ioannis Karafyllidis (Supervisor)
Christos Schinas
Georgios Sirakoulis

Expainable Quantum Machine Learning (XQML)

This thesis investigates the explainability of quantum machine learning models by developing interpretation techniques for various quantum algorithms. The aim is to analyse the internal behaviour of purely quantum models, using approaches such as entanglement analysis, gradient-based sensitivity, and circuit structure inspection. The project will leverage frameworks like Qiskit and PennyLane and evaluate performance and interpretability on benchmark datasets via quantum simulators.

Master thesis examination committee.
Ioannis Karafyllidis (Supervisor)
Georgios Sirakoulis
Kyriakos Zoiros

Quantum Markov models for choice modelling and decision making.

Classical Markov models introduce a dynamic dimension to choice modelling by capturing the sequential nature of decision-making. Quantum Markov Models (QMMs) incorporate contextuality, superposition of preferences, interference effects, and order-dependent outcomes, features inadequately modelled by classical models. QMMs use superposition, entanglement, and interference in choice and decision processes. A quantum algorithm for QMMs will be developed and applied in both choice modelling and decision making.

<u>Master thesis examination committee.</u>

Ioannis Karafyllidis (Supervisor)
Christos Schinas
Kyriakos Zoiros

Quantum hidden Markov models.

Classical Hidden Markov Models (HMMs) consist of a set of hidden states that follow a Markov process, with observable outputs probabilistically dependent on these states. In choice modelling, HMMs can uncover unobserved heterogeneity in preferences. Quantum Hidden Markov Models (QHMMs) are effective in modelling complex decision-making processes, capturing the intricacies of human cognition that classical models often overlook. By incorporating quantum processes, QHMMs provide a deeper understanding of choice behaviour, particularly in contexts characterized by uncertainty and contextual influences, where states are hidden and all information stems from the results.

<u>Master thesis examination committee.</u>

Ioannis Karafyllidis (Supervisor)
Ioannis Boutalis
Kyriakos Zoiros

Quantum walks on decision trees.

A decision tree is a flowchart-like structure used for decision making, visualizing possible outcomes, costs, and consequences of different choices. It's a hierarchical model that breaks down complex decisions into a series of simpler decisions and their potential results, often used in machine learning and data analysis. A quantum walk algorithm will be developed to simulate the decision process on trees in which multiple paths in the tree will be examined in superposition.

<u>Master thesis examination committee.</u>

Ioannis Karafyllidis (Supervisor)
Georgios Sirakoulis
Georgios Dimitrakopoulos

Parrondo quantum games.

Parrondo's paradox, a paradox in game theory, describes how a combination of losing strategies can be combined to form a winning strategy. The classical Parrondo game will be quantized, and a quantum algorithm that implements the Parrondo game will be developed.

<u>Master thesis examination committee.</u>

Ioannis Karafyllidis (Supervisor)
Georgios Sirakoulis
Ioannis Boutalis

Quantum algorithm for reference-guided DNA sequence alignment.

Reference-guided DNA sequencing and alignment is a very important process in computational molecular biology. The amount of DNA data grows very fast, and many new genomes are waiting to be sequenced while millions of private genomes need to be resequenced, necessitating a major leap in computing power. A quantum algorithm for reference-guided DNA sequence alignment will be developed. Grover's quantum algorithm will be used as the basic tool for searching the alignment positions of the DNA fragments to the reference DNA in superposition.

<u>Master thesis examination committee.</u>

Ioannis Karafyllidis (Supervisor)
Georgios Sirakoulis
Christos Schinas

Strategies for efficient initialization of quantum dot spin states under Voigt geometry

Spin states of electrons and holes in semiconductor quantum dots play a central role in the development of next-generation quantum information technologies, with applications ranging from quantum communication to quantum computing. A key challenge in this field is the precise and reliable control of these spin states, which can be achieved through tailored electromagnetic pulses. One particularly important and actively researched platform involves the manipulation of quantum dot spin states in the Voigt geometry, where the magnetic field is applied perpendicular to the growth direction of the quantum dot.

A fundamental and technologically relevant problem in this context is the initialization of the electron spin state: how to prepare a well-defined spin state starting from the natural thermal state, which is typically an equal incoherent mixture. Efficient initialization is a critical first step for any quantum information processing protocol.

In this master thesis project, the student will explore and compare two quantum control techniques for the initialization of electron spin states: optical pumping and adiabatic preparation. The project will involve numerically simulating the quantum dynamics under both schemes and systematically analyzing their initialization fidelity as a function of key system parameters. The results will provide insight into the advantages, limitations, and potential applications of these methods in realistic quantum dot platforms, contributing to the broader effort to realize reliable quantum technologies.

<u>Master thesis examination committee</u>

Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Geometric approaches to optimal control in basic quantum systems

This master's thesis explores theoretical methods for the optimal control of qubit and qutrit systems, using tools from differential geometry and variational optimization. The central idea is to view quantum evolution as a trajectory on a curved geometric space, where the most efficient control strategy corresponds to following a geodesic path between the initial and target quantum states. By assigning suitable cost functions—such as the energy or time required for a given evolution—the project aims to derive control protocols that minimize resources while maintaining high-fidelity quantum state transformations.

The work may focus on either or both of the following main directions: (1) the design of energy-efficient control schemes, including shortcut-to-adiabaticity methods, where the cost is evaluated via norms of the control Hamiltonian, and (2) time-optimal quantum control, where the evolution is completed in the shortest possible duration under given constraints. Both analytical methods (in systems with symmetry) and numerical optimization techniques will be employed to study a variety of representative scenarios in closed and weakly open quantum systems. The results are expected to contribute to a deeper understanding of resource-efficient quantum dynamics in low-dimensional Hilbert spaces.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Optimization of nonadiabatic holonomic quantum gates for robust quantum computation

This master's thesis focuses on the design and optimization of nonadiabatic holonomic quantum gates, a promising class of geometric gates for realizing robust and fault-tolerant quantum computation. Holonomic gates are based on non-Abelian geometric phases, making them inherently resilient to certain control errors and fluctuations. However, in realistic experimental setups, imperfections in pulse shaping and external noise still degrade gate performance. To address this, the project investigates how optimization techniques (analytical and numerical) can be applied to design high-fidelity holonomic gate sequences under nonadiabatic evolution.

The goal is to construct gate protocols that satisfy the cyclic and parallel transport conditions required for holonomy, while minimizing sensitivity to experimental imperfections and decoherence. Theoretical models will be developed for basic quantum systems and the performance of the optimized gates will be benchmarked through simulation of fidelity and robustness under various control and system parameters. This work aims to advance the practical feasibility of geometric quantum computation by offering a flexible and efficient approach to implementing high-quality holonomic gates in diverse quantum platforms.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Control of quantum dynamics in semiconductor quantum dots under acoustic phonon-induced decoherence

Semiconductor quantum dots (QDs) are promising systems for quantum information processing, but controlling their quantum dynamics is challenging due to environmental noise and complex interactions. Several studies have shown that exciton-phonon coupling, related to acoustic phonons, significantly reduces control efficiency, leading to reduced fidelity and increased decoherence. In this thesis, we investigate the effects of exciton-phonon coupling on the control of quantum dynamics in QDs using quantum control techniques giving emphasis to the problem of efficient exciton generation. The student will employ a theoretical framework to simulate the quantum dynamics of a QD system and study with numerical, and potentially approximate analytical, calculations the impact of exciton-phonon coupling on control efficiency in the QD. The results will contribute to the development of robust and scalable quantum information processing technologies with QDs.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Controlled entanglement dynamics of excitons in colloidal quantum dots
Colloidal quantum dots (CQDs) are a promising platform for quantum information processing due to their ability to generate and manipulate entangled excitons. This thesis aims to investigate the controlled entanglement dynamics of excitons in CQDs using optical control techniques. The student will employ a theoretical framework to simulate the dynamics of the excitons in CQDs and study the potential to control the entanglement dynamics using specific laser pulses. Specific CQDs will be studied where their characteristics have been obtained from ab initio electronic structure calculations. This thesis contributes to the understanding of the controlled entanglement dynamics of excitons in CQDs and provides insights into the development of novel control strategies for quantum information processing. The results have potential applications in quantum computing, quantum communication, and quantum metrology.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Machine learning methods for efficient quantum state transfer in spin chains
Quantum state transfer (QST) is a crucial process in quantum information processing, where a quantum state is transmitted from one end of a quantum system to the other. Spin chains are a popular platform for QST due to their scalability and potential for high fidelity. However, the dynamics of spin chains are complex and often require careful optimization to achieve efficient QST. This thesis proposes a novel approach to optimize QST in spin chains using machine learning (ML) methods.
The proposed approach uses a deep reinforcement learning algorithm to learn the optimal control sequence for QST in a spin chain. The algorithm is trained using a simulated environment, where the RL agent interacts with the spin chain and receives rewards based on the fidelity of the transferred state. The goal is to maximize the fidelity of the transferred state while minimizing the control time.
The proposed approach has several potential benefits, including improved fidelity, reduced control time, and scalability to larger spin chains. The thesis aims to investigate the feasibility of this approach and demonstrate its effectiveness in optimizing QST in spin chains. The results will contribute to the development of efficient and scalable quantum information processing technologies.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Solving inverse quantum control problems using Physics-Informed Neural Networks
This master’s thesis focuses on applying Physics-Informed Neural Networks (PINNs) to solve inverse quantum control problems in a low-dimensional quantum system, such as a qubit. The goal is to develop and train neural network models that incorporate the underlying physics, specifically, the time-dependent Schrödinger equation or Lindblad master equation, as constraints during learning. This approach enables the neural network to infer the optimal control fields that drive a quantum system from a known initial state to a desired target state, even in the presence of decoherence or other open-system effects.
The project will begin with the simulation of the forward problem, where the system's evolution is predicted given a fixed Hamiltonian. It will then progress to solving the inverse problem, where the control fields are reconstructed from the desired system dynamics. The use of PINNs offers a flexible and data-efficient framework for tackling these problems, especially in situations where traditional numerical methods become costly or unstable. The work combines techniques from quantum

dynamics and control, numerical simulation, and machine learning, and is well-suited for students interested in a combination of quantum control, artificial intelligence, and computational techniques.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Efficient quantum control of three-level quantum systems via Physics-Informed Neural Networks
Three-level quantum systems play a central role in the development of quantum technologies, serving as essential building blocks in quantum computing, quantum communication, and quantum sensing. Their rich structure enables the realization of fundamental protocols such as quantum state transfer, quantum gates beyond two-level systems, and advanced schemes for quantum memory and entanglement generation. Achieving accurate and efficient control of these systems, particularly under realistic environmental conditions, remains a critical challenge.
In this master thesis, we investigate the use of Physics-Informed Neural Networks (PINNs) as a modern computational framework for quantum control of three-level quantum systems. PINNs offer a data-efficient and flexible method for solving the governing differential equations of quantum dynamics while incorporating physical constraints directly into the training process. We apply this approach to state-to-state transfer problems in both closed and open three-level systems, focusing on achieving high-fidelity control protocols with minimal energy consumption and short operation times. Moreover, we demonstrate the adaptability of PINNs in handling variations in system parameters and initial conditions, highlighting their potential advantages over traditional optimization-based control techniques.

Fast and efficient creation of quantum gates with machine learning methods
This master's thesis proposes a novel approach to the control of a qubit using machine learning (ML) techniques, with the goal of fast creation of single and/or two-qubit gates with very high efficiency by using different ML methods. In this project, the student will develop a machine learning framework that learns to optimize the control pulses for single qubit and two-qubit quantum gate operations, such as the controlled NOT and the controlled-phase, like the controlled Z, gates, by interacting with two qubits in a specific quantum platform, and receiving feedback on its performance. The ML agent will apply pulsed excitation to the qubit and measure its response, using the reward function to maximize the fidelity of the quantum gate operation. The expected outcomes of this project are optimized control pulses for high-fidelity quantum gate operations, improved scalability, and increased flexibility. Different ML methods will be applied. This research will contribute to the development of more efficient and scalable methods for creating quantum gates, essential for large-scale quantum computing and quantum information processing.

<u>Master thesis examination committee</u>
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Exploring single-photon generation in an asymmetric quantum dot molecule
The generation of single photons is of major importance in several quantum technology applications. On demand single photon generation from semiconductor quantum dots has been shown with high efficiency in several cases and different quantum dot structures. This diploma thesis explores single photon generation in an asymmetric quantum dot molecule consisting of two quantum dots coupled by tunneling. The band structures of the quantum dots are different, while the rate at which the

tunneling effects take place is determined by the value of the applied voltage. The two-time intensity correlation function of the emitted photons, focusing on the bunching–antibunching transition of the photons in resonance fluorescence, is studied. The behavior of the two-time intensity correlation function is analyzed for different parameters of the tunneling coefficient and the detunings of the system.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Quantum sensors and transistors based on the optical properties of a monolayer MoS_2 nanoresonator

This thesis proposes a theoretical and computational study of the optical properties of a monolayer MoS_2 nanoresonator. This system is promising for quantum technologies, particularly in quantum sensing and nanoscale quantum transistors, due to its tunable optical properties. The project focuses on deriving and analyzing relevant expressions for the linear and higher-order nonlinear optical susceptibilities of the system. The linear susceptibility is expected to show a single resonance whose position depends on the exciton energy and the exciton–phonon coupling. The higher-order susceptibility spectra typically feature resonances which are narrower or broader resonances than the linear spectra, influenced by the exciton–phonon interaction. Using MoS_2 instead of graphene with a quantum defect, which is also studied for such applications, allows for enhanced exciton–photon coupling due to its direct bandgap and stronger light–matter interaction. The project will involve analytical modeling, numerical simulations, and investigation of the system's potential for quantum sensors and nanoscale quantum transistors.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Quantum sensing based on the nonlinear optical response of a semiconductor quantum dot–DNA nanohybrid: A comparison of cross-Kerr and self-Kerr nonlinearities

This master's thesis presents a theoretical investigation of the nonlinear optical response of a semiconductor quantum dot (SQD)–DNA nanohybrid, with the aim of exploring its application as a quantum sensor. The study focuses on the system's bistable behavior and its sensitivity to physical parameters such as DNA length and concentration, which modulate the coupling strength between the SQD and the DNA molecule. A central objective of the thesis is to compare the sensing performance of the system under cross-Kerr and self-Kerr nonlinearities. We analyze how each nonlinearity affects the system's optical response and determine their respective capabilities for enhancing sensitivity and control in biosensing contexts. Special attention is given to the form and features of the nonlinear susceptibility spectra associated with each nonlinearity, including the position, width, and amplitude of key resonances. The findings are expected to contribute to the design of biologically integrated, label-free optical quantum sensors with tunable nonlinear properties for advanced molecular diagnostics.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Quantum correlations in qubits near graphene nanodisks
This thesis will investigate the quantum correlations that arise between qubits near graphene nanodisks. Graphene has unique electronic properties that make it an attractive material for quantum information processing. The interaction between quantum emitters and graphene nanodisks can lead to interesting quantum phenomena, such as strong coupling at the single photon level, quantum interference in spontaneous emission, and strong coupling between the emitters. These effects can be explored for a large degree of quantum correlations, like entanglement and quantum discord. The project will use theoretical models and numerical simulations to study the quantum correlations between qubits when placed in close proximity to graphene nanodisks. Various parameters, such as the distance between the qubits and the nanodisks, the size of the nanodisks, and the strength of the interactions, will be varied to understand their effects on the quantum correlations. Understanding these correlations is crucial for the development of quantum technologies, such as quantum computing and quantum communication. The results of this study will provide insights into the potential applications of graphene in quantum information processing and pave the way for further research in this field.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Quantum simulation of dynamics of open quantum systems
Accurate simulation of the time evolution of a quantum system in the presence of an environment is crucial for making reliable predictions in various scientific and technological fields. While a closed quantum system can typically be described by unitary time evolution, simulating open quantum system dynamics presents a challenge due to the non-Hermitian nature that results in nonunitary evolution. Recent advances have been made in this area, paving the way for further exploration. This Master thesis project will involve a thorough review of relevant literature on methods for simulating the dynamics of open quantum systems. The student will select one of these methods, thoroughly explain its steps, and apply it to simulate the dynamics of a basic quantum system. A comparison of the results obtained will be made with existing literature. Furthermore, the methodology may be extended to explore the dynamics of a new problem not yet studied in the literature.
Proficiency in quantum mechanics, quantum computing, and open quantum systems is essential for this project. The student will also need to be skilled in programming languages commonly used for quantum computing simulations, such as Python or Qiskit and should also be competent in analytical calculations. Conducting a comprehensive literature review, implementing the chosen simulation method, and analyzing the results will be part of the student's responsibilities. Access to a quantum computer or quantum simulator will be required for running simulations.
Overall, this Master thesis project offers an opportunity to develop valuable knowledge and skills in quantum computing and open quantum systems, contributing to advancements in quantum simulation research.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Modeling non-Markovian dynamics in controlled open quantum systems with tensor networks

Accurately numerically simulating the dynamics of quantum systems interacting with their environments is essential for the advancement of quantum technologies. While the behavior of open quantum systems under weak environmental influence is relatively well understood, modeling their dynamics beyond this regime, where memory effects and strong coupling emerge, remains a significant challenge. Most existing methods rely on specific approximations about the nature of the system-environment interaction, often limiting their generality.
This thesis adopts a different approach, utilizing a recently developed, general, and efficient numerical technique for computing observables of open quantum systems. The method is based on reformulating the exact equations of motion of the open quantum system as a tensor network. This formulation enables decomposition into matrix product forms, which can be efficiently compressed and manipulated, allowing for accurate simulation of complex environments with reduced computational cost.
The objectives of this work include gaining a thorough understanding of the method, reviewing the relevant theoretical background and literature, implementing the necessary computational tools, and applying the technique to an original problem in quantum control of open quantum systems beyond the Markovian limit. Special emphasis is placed on exploring non-Markovian effects within controlled quantum dynamics in complex environments.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Ioannis Thanopulos
Dionisis Stefanatos

Controlling unconventional photon blockade using numerical optimization and machine learning methods
Photon blockade is a quantum phenomenon in which the emission of additional photons is inhibited by the presence of a previously emitted photon. This effect has been experimentally demonstrated in a variety of systems, including superconducting circuits, optical fibers, and atomic ensembles. More recently, attention has turned to unconventional photon blockade, where photon suppression arises not from strong nonlinearity, but from quantum interference between distinct excitation pathways.
The objective of this thesis is to enhance the performance of unconventional photon blockade within a specific quantum structure by applying advanced quantum control techniques. These techniques leverage numerical optimization strategies, including genetic algorithms and machine learning approaches. The outcomes of this research are expected to contribute to the efficient design of single-photon sources - an essential component in modern quantum communication technologies.

Master thesis examination committee
Emmanuel Paspalakis (supervisor)
Dionisis Stefanatos
Ioannis Thanopulos

Time-optimal charging of a spin-pair quantum battery in the presence of field inhomogeneities.
This thesis investigates the time-optimal charging of a quantum battery composed of a coupled spin pair in the presence of field inhomogeneities. By leveraging the reduction of the spin-pair battery model to an effective two-level quantum system, we apply advanced methods from optimal control theory to achieve robust and efficient energy transfer. In particular, we exploit recent developments in the application of the Pontryagin Maximum Principle to two-level systems, which enable the derivation of control protocols that are both time-optimal and resilient against imperfections such as

field inhomogeneities. The primary objective is to identify control strategies that minimize the charging time while maintaining robustness, ensuring the battery reaches its maximal stored energy despite the presence of unavoidable experimental imperfections. This approach bridges concepts from quantum batteries and quantum control, providing insights into the practical realization of fast and reliable quantum energy storage devices.

<u>Master thesis examination committee</u>
Dionisis Stefanatos (supervisor)
Emmanuel Paspalakis
Ioannis Thanopulos

Rapid charging of a quantum battery composed of a pair of spins with Heisenberg coupling using optimal control
In the context of quantum thermodynamics, quantum batteries are a new concept aimed at storing and releasing energy efficiently. In this thesis, we focus on the development of an optimal control strategy for fast charging a quantum battery composed of a pair of spins with Heisenberg coupling. The Heisenberg coupling is a fundamental interaction commonly encountered between two spin-1/2 particles. In this project we will employ optimal control techniques to design and optimize the control fields that minimize the charging time of the aforementioned quantum system. The optimal control problem will be formulated as a maximization problem, where the objective function is the energy transfer from the external energy source to the quantum battery. The outcome of this thesis has potential applications in various fields, including quantum computing, quantum communication, and energy storage. The findings can also contribute to the development of new technologies that rely on efficient energy transfer and storage.

<u>Master thesis examination committee</u>
Dionisis Stefanatos (supervisor)
Emmanuel Paspalakis
Ioannis Thanopulos

Maximizing entanglement in a pair of spins with Ising coupling using optimal control
Entanglement is a fundamental concept in quantum mechanics, which is essential for various quantum information processing applications. In the context of spin systems, entanglement is a key resource for quantum computing, quantum sensing and quantum communication. One of the most popular spin systems is the Ising model, which consists of two spins interacting via an Ising coupling. In this project we aim to use optimal control for maximizing entanglement is such a pair of spins. Specifically, the goal is to find the optimal time-dependent magnetic fields which drive the system to the state with maximum concurrence and thus entanglement in the least possible time. The results of this research are expected to contribute to the development of more efficient quantum algorithms and protocols for modern quantum technology applications, like computing, sensing and communications.

<u>Master thesis examination committee</u>
Dionisis Stefanatos (supervisor)
Emmanuel Paspalakis
Ioannis Thanopulos

Improving unconventional photon blockade with optimal control
Photon blockade is a phenomenon in which the emission of photons from a quantum system is suppressed due to the presence of an already emitted photon. This phenomenon has been experimentally observed in various systems, including superconducting circuits, optical fibers, and

atomic systems. In recent years, unconventional photon blockade has been explored, where the suppression of photon emission is induced by exploiting the quantum interference between different transition pathways. The goal of this thesis is to improve unconventional photon blockade in a bosonic Josephson junction using optimal control methods for the design of the coupling between the two nonlinear bosonic modes. Specifically, we aim to find lower values of the second-order correlation function obtained at earlier times than with constant coupling, with larger one-photon populations and for longer time windows. The present research is expected to find application in the efficient design of single-photon sources, which are an essential element for modern quantum communications.

Master thesis examination committee
Dionisis Stefanatos (supervisor)
Emmanuel Paspalakis
Ioannis Thanopulos

Polychromatic adiabatic passage scheme for quantum information encoding
Polychromatic adiabatic passage schemes combine the high-selectivity between different target states achieved by coherent control methods with the effectively complete transfer of population under few-level adiabatic passage schemes. Such quantum control schemes have been in the center of the research on quantum control since its inception due to their evident potential for manipulating quantum systems and developing quantum technological applications. In this diploma thesis, the use of polychromatic adiabatic passage schemes for quantum encoding and decoding purposes is investigated on non-degenerate quantum systems. The dynamics of such processes are studied in the relevant quantum state subspace of dark states. The necessary parameters of the encoding laser fields required for achieving a target quantum information state by given a known initial state are determined. Also, the inverse process of developing a decoder for a given quantum information state is addressed.

Master thesis examination committee
Ioannis Thanopulos (supervisor)
Emmanuel Paspalakis
Dionisios Stefanatos

Controlling the quantum-light group velocity by cavity induced transparency: single-photon emission and interference effects
The propagation of a quantized probe field in a dense medium composed of three-level Λ-type quantum systems under conditions of electromagnetically induced transparency conditions is a topic which has attracted the interest of recent research activity due to its fundamental scientific importance as well as numerous potential applications in nanophotonics and quantum technologies. In this diploma thesis, the group velocity of a probe pulse propagating under such conditions in a cavity is investigated in the weak and strong light-matter coupling regime. The possibility of photon-number selectivity on the group delay and the creation of single-photons on demand is studied. Also, the possibility of interference effects between different photon components in the probe pulse is addressed.

Master thesis examination committee
Ioannis Thanopulos (supervisor)
Emmanuel Paspalakis
Dionisis Stefanatos

Degree of non-Markovianity and quantum speed limit under strong coupling at the nanoscale

The proposed master thesis project aims to study the degree of non-Markovianity and the quantum speed limit in the spontaneous emission evolution of a quantum emitter coupled to a specific photonic nanostructure. The study will investigate how various vacuum decay rates and distances affect these key quantum properties in the system. The research will employ well-established measures of non-Markovianity to quantify the extent to which memory effects are present in the evolution of the quantum emitter. Additionally, the possibility for substantial dynamical quantum speedup will be analyzed, considering how the coupling to the photonic nanostructure can influence the emission dynamics of the quantum emitter. By exploring these aspects, the project aims to deepen our understanding of the quantum behavior of coupled systems and contribute to the development of quantum technologies. The study will utilize theoretical tools and computational simulations to investigate the dynamics of the system under different conditions, with the ultimate goal of shedding light on the interplay between non-Markovianity and quantum speed limits in the context of spontaneous emission processes, which is crucial for various application in quantum technologies.

<u>Master thesis examination committee</u>
Ioannis Thanopulos (supervisor)
Emmanuel Paspalakis
Dionisis Stefanatos

Cluster Distribution Study for Applications in Quantum Cryptography Protocols

In the context of the diploma thesis, the production and distribution of quantum entangled photons will be studied theoretically and experimentally. The principle of operation of the source of production of entanglement, the methodology for validating the violation of Bell inequality through non-classical correlations, and its limitations of loss in real provisions. A production source will be used for the experimental validation tests of photon-associated polarization coding for photons in the telecommunications C-band, analysis of device polarization with variable angles of polarization axes. In addition, the effect of fiber optical/wireless channels on the distribution of entanglement will also be investigated. In the final stage of the work, the results for applications in next-generation entanglement-based quantum cryptography protocols (ENT-based QKD) will be demonstrated. The thesis will be deployed at the PCRL – NTUA in collaboration with Dr John Giannoulis.

<u>Master thesis examination committee</u>
Panagiotis Dimitrakis (supervisor)
Georgios Syrakoulis
Ioannis Karafyllidis

Optical Fiber-based Power Network SCADA Quantum Communication

This subject addresses the status, future trends, and practical challenges of optical fibre-based Power Network SCADA quantum communication, enabling the leveraging of this technological platform's potential in real-world Power system SCADA communications that involve vast amounts of data generated in real-time, as well as managing, encoding, and applications such as quantum cryptography. Quantum key distribution (QKD) sharing is central to the quantum communication cybersecurity paradigm. While quantum computing through individual circuits entails a probabilistic outcome for every problem, managing real-world datasets is a significant challenge due to their intricacy. The traditional cybersecurity triad of confidentiality, integrity, and availability (CIA) is thus applicable in reverse sequence, i.e., (AIC), giving availability of electric power the utmost importance.

The diploma thesis aims to apply BB84, E91, B92, and SARG04 cryptographic protocols to large-scale Power system SCADA open-source multivariate datasets and compare the results thereon.

Master thesis examination committee.

Kyriakos Zoiros (Supervisor)
Ioannis Karafyllidis
Christos Schinas

Genetic Algorithms with Quantum Computing

Quantum algorithms that can be used in various aspects of genetic algorithms implementation will be selected and implemented. First, genetic algorithms and their variants will be reviewed from classical literature. Then those aspects of genetic algorithms that could benefit from implementing them with quantum computing will be selected. Moreover, the advantages in terms of computational complexity will be studied, and the effect that quantum computing will have on the correctness of the results in relation to classical algorithms will be presented.

Master thesis examination committee
Ioannis Boutalis (supervisor)
Georgios Syrakoulis
Ioannis Karafyllidis

Data Clustering with Quantum Computing

First, a literature review of classical clustering techniques will be conducted. Next, a review will be made of the above techniques that have been implemented with quantum computing. Selected algorithms will be implemented to show the results in relation to the benefit in computational cost and accuracy of the solutions

Master thesis examination committee
Ioannis Boutalis (supervisor)
Georgios Syrakoulis
Ioannis Karafyllidis

Quantum algorithms in Artificial Neural Networks

Quantum algorithms will be implemented and tested to run various aspects of ANN training and operation on a quantum computer. Classical ANN algorithms will be studied first, and a set of classical algorithms will be selected that could be quantized and benefited from quantum implementation. Aspects of computational complexity, accuracy and generalization performance will be investigated in order to derive useful conclusions on the appropriateness of the quantized versions of the algorithms.

Master thesis examination committee
Ioannis Boutalis (supervisor)
Georgios Syrakoulis
Ioannis Karafyllidis

Magnetic characterization of a polynuclear transition cluster.

Polynuclear transition metal clusters (PTMC) have been proposed as possible candidates for the realization of qubits. In the present master thesis, the student will apply experimental methods in order to characterize the magnetic properties of a PTMC, based on transition metal and lanthanide ions. The characterization involves application of variable temperature, variable magnetic field static and dynamic magnetic susceptibility measurements, variable temperature Mössbauer Spectroscopy and variable temperature Continuous wave Electron Paramagnetic Resonance EPR spectroscopy. These studies will provide information about the nature of the spin value of the ground state, the exchange coupling scheme between the ions, the contribution of non-isotropic exchange terms, the composition of the eigenstates, and the temperature dependence of the spin relaxation time.

Master thesis examination committee
Yiannis Sanakis (supervisor)
George Mitrikas
Michael Pissas

Photosystem II Inspired Spin-Based Quantum Computing Devices

Photosystem II (PSII) is a naturally occurring system that can be isolated from higher plants and catalyzes the photoinduced water oxidation. The PSII apparatus comprises paramagnetic species positioned in a well-organized topology dictated by the proteinic environment. The light induced electron transfer that occurs within PSII can be controlled and certain paramagnetic species can be trapped leading to pairs comprising these species. These magnetically exchanged pairs could constitute the prototype to realize a spin-based quantum computing device (SBQCD). In order to do this, it is necessary to characterize in fine detail the magnetic interactions within these pairs by applying continuous wave EPR at X (9.5 GHz) and Q (34 GHz) and pulsed EPR at X-band at liquid helium temperatures.

Master thesis examination committee
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Topological superconducting qubits

Recently, Microsoft has announced a controllable topological qubit chip, which is crucial in producing error-corrected quantum computers within a few years. The topological qubit based on Majorana zero modes, which is a theoretical particle that does not occur in nature. In this thesis, a review of topological superconducting qubits, Majorana fermions, and recent developments will be presented.

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Rabi oscillations and measurement of the rotating frame spin relaxation time $T_{1\rho}$ of atomic hydrogen
The conventional longitudinal (T_1) and transverse (T_2) spin relaxation times do not fully characterize the relaxation behavior of *dressed spins* under resonant microwave (mw) irradiation. In the rotating frame at resonance, the quantization axis of dressed spins aligns along the x-axis, distinguishing it from the y-axis. Consequently, relaxation rates along these directions differ, typically following the relation: $T_2/2 < T_{1\rho} < T_1$. This thesis focuses on measuring the spin-lattice relaxation time in the rotating frame ($T_{1\rho}$) of atomic hydrogen encapsulated in polyhedral oligomeric silsesquioxane (POSS) cages (H@POSS). The study will determine the spectral density function $J(\omega_1)$ at the nutation frequency ω_1. To achieve this, the student will employ various pulse sequences that include high-turning-angle (HTA) pulses combined with free induction decay (FID) or spin echo detection. The results will provide, for the first time, a detailed understanding of the spin relaxation behavior of H@POSS during the application of quantum gates based on long, resonant microwave pulses.

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Spin clock transitions of atomic hydrogen

Electron spins in molecular spin systems are promising candidates for qubits; however, protecting them from environmental noise that leads to decoherence remains a critical challenge for practical applications. In such systems, decoherence primarily arises from fluctuations in electron–nuclear interactions. A common strategy to mitigate this effect is the reduction or elimination of magnetic nuclei within the host material. An alternative and increasingly attractive approach involves the use of *clock transitions*—specific points at which the electron paramagnetic resonance (EPR) frequency becomes insensitive to variations in the local magnetic field, thereby decoupling the spin system from environmental magnetic noise. In atomic hydrogen, such clock transitions occur when the static magnetic field (B_0) is aligned parallel to the microwave field (B_1), a configuration known as the *parallel mode*. In this thesis, the student will investigate this system by analyzing transition probabilities for both hydrogen (^1H, I = 1/2) and deuterium (^2H, I = 1) isotopes. The work will include the characterization of clock transition properties and simulations to predict the expected enhancement in spin coherence time (T_2).

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Design and fabrication of Quantum Bolometers based on 2D Materials
Quantum bolometers are highly sensitive detectors used to measure the energy of incoming radiation, particularly microwave photons, by detecting the heat generated when the radiation is absorbed. They are crucial for advancing quantum technologies, especially in the development of superconducting quantum computers and other systems that rely on the interaction of qubits via microwaves. These bolometers can be constructed from materials like graphene and are capable of detecting very massless and/or very light particles, offering improved sensitivity and readout speeds compared to traditional detectors. The thesis will focus on specific topologies and circuits used in for the integration of these quantum sensors, circuit analysis, frequency tuning and read out methods will be explored. Optimization of noise is also an issue for investigation.

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Meta analysis of transcriptomic data of a disease

Transcriptomic data (e.g. single cell RNA-seq, etc) could provide information about the effect of a disease into the transcriptional profile of the genes of the organism. The aim of the thesis would be to perform a meta-analysis of publicly available transcriptomic data, in order to unveil the effect of the disease into the expression profile of the genes, by combing and integrating data from various studies.

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