UFSCar - São Carlos

30 October - 07 November 2023

Abstract booklet

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Oral presentations I

Moiré excitons in MoSe2/WS2 heterostructures

C. Serati de Brito (Universidade Federal de São Carlos), A. Chaves (Universidade Federal do Ceará), M. A. Prosnikov (High Field Magnet Laboratory (HFML–EMFL)), T. Wozniak (Wrocław University of Science and Technology), S. Guo (University of Exeter), I. D. Barcelos (Laboratório Nacional de Luz Sincrotron - LNLS), M. V. Milosevic (University of Antwerp), F. Withers (University of Exeter), A. Beer (Universität Regensburg) , J. Fuchs (Universität Regensburg), C. Schüller (Universität Regensburg), P. C. M. Christianen (High Field Magnet Laboratory (HFML–EMFL)), Y. Galvao Gobato (Universidade Federal de São Carlos)

Transition Metal Dichalcogenides heterostructures (TMD-h) with stacking angles around 0º or 60º (crystal lattice symmetry) exhibit strong emission from inter- and intra-layer excitons. The strong binding energies of these excitons, originating from a combination of quantum confinement and dielectric screening, make them robust against dissociation by temperature and external electric fields. A moiré pattern, formed by lattice mismatch and/or stacking angles, can confine exciton wave functions, enabling quantized states. This holds promise for nanophotonics and quantum information applications. For MoSe2/WS2 heterostructures, a debate surrounds the lower-energy photoluminescence (PL) emissions. Conduction bands in both constituent layers are nearly degenerate, leading to a resonant enhancement of moiré effects due to hybridization of the intra- and interlayer excitons. As a result, the observed lower-energy exciton peak in the PL spectrum was previously attributed to a hybridized intra- and interlayer exciton. However, recent reflectance contrast experiments for gated samples show that the lower-energy exciton peak lacks permanent dipole across the layers. This suggests weak hybridization and holds implications for theoretical predictions of exciton properties in heterostructures with varied stacking angles. In this work, we experimentally investigated valley Zeeman splitting in hBN/WS2/MoSe2/hBN heterostructures under magnetic fields up to 20 T. Two neutral exciton peaks were identified: the lower energy peak show a reduced g-factor compared to the higher one. Time-resolved PL experiments demonstrated short lifetimes for these peaks, implying small spatial charge separation and weak hybridization. Calculations indicate the discernible g-factor arises from exciton confinement within the moiré pattern due to lattice mismatch or interlayer twist. Thus, magneto-PL emerges as a crucial tool for understanding moiré-driven excitonic behavior in TMD-h.

Asymmetrical braneworlds and the charged lepton mass spectrum

Henrique Matheus Gauy (Universidade Federal de São Carlos), Alex E. Bernardini (Universidade Federal de São Carlos)

A braneworld mechanism for explaining the mass spectrum of the charged leptons is proposed. Based on the existence of an asymmetric warp factor for a 5+1-dimensional braneworld scenario, the proper fractions between the masses of the electron, muon and tauon are achieved. As a straightforward consequence, our results coincide with the Koide's mass formula.

Quantum computing with two independent control functions: Optimal solutions to the teleportation protocol

Emanuel F. de Lima (UFSCar), Marllos E. F. Fernandes (UFSCar), and Leonardo K. Castelano (UFSCar)

A central problem in quantum computing is the finding of an unknown target state that encodes the solution of a certain computational task. In order to accomplish this goal, the evolution from a given initial state is performed with an associated total Hamiltonian which is a time-dependent combination of two time-independent Hamiltonians: the problem-Hamiltonian, whose ground state is the unknown target, and a driving-Hamiltonian, whose ground state is the initial state. Here, we analyze this computational problem in the light of Optimal Control Theory considering each Hamiltonian modulated by an independent control function. For bounded controls, there is a minimum total evolution time beyond which the target state can be exactly prepared. We show that below this minimum time a possible optimal solution consists of both controls constantly tuned at their upper bound, provided the gradients of the associated control Hamiltonian with respect to the controls (the switching functions) are positive. We refer to this type of solution as the double-bang solution. We show that the double-bang solution is optimal for a teleportation protocol up to the minimum time. Additionally, we combine the double-bang solution and the adiabatic gate teleportation protocol to implement universal quantum computing. This approach to quantum computing is very appealing because of its simplicity and experimental feasibility. To corroborate our analytical results, we propose the use of a numerical quantum optimal control technique adapted to limit the amplitude of the controls, which converges to the double-bang solution when the final evolution time is shorter than the minimum time. We compare the fidelity of the teleported state obtained for the numerically optimized two-control functions with the usual one-control function scheme and with the quantum approximate optimization algorithm. We find that the two-control approach has a better performance than the other approaches.

Spectroscopic studies under extreme thermodynamic conditions

Ariano De Giovanni Rodrigues (Universidade Federal de São Carlos)

The non-destructive nature, speed, and versatility in data acquisition make Raman spectroscopy one of the most widely used techniques for characterizing materials and in the study of physical and chemical effects. Based on inelastic light scattering processes, this technique enables us to take direct measurements of the energies of the vibrational modes, which are determined by the interactions between the constituent atoms. Hence, the Raman spectrum is a characteristic signature of each material, which can be significantly modified as a result of compositional and structural changes, such as atomic interdiffusion, phase transitions, stress/strain, and quantum confinement, turning the Raman spectroscopy a powerful tool in the study of such properties. In this talk, in addition to dealing with the physical fundamentals involved in the inelastic scattering of light, we will discuss how Raman spectra can be measured and how the data can be interpreted to provide information about the physical characteristics of materials. Examples of the use of this technique available at the Department of Physics at UFSCar will be also presented, highlighting the possibilities of performing in situ analyses as a function of temperature and pressure, which are essential in the study of phase transitions and other properties of matter under extreme conditions.

Studies of molecular Exchange rate between pores multiscale in reservoir stones

Nataly Melo Campos (Instituto de Física de São Carlos), Agide Gimenez Marassi (Instituto de Física de São Carlos), Everton Lucas de Oliveira (Centro Nacional de Pesquisa em Energia e Materiais), Arthur Gustavo de Araújo-Ferreira (Instituto de Física de São Carlos), Tito José Bonagamba (Instituto de Física de São Carlos)

In a porous medium, there is constant interaction of different fluids, for example water and oil, in addition to communication between regions of varying characteristics whose molecules are in translational movement due to self-diffusion. Therefore, there is a need to characterize the dynamics of the molecules of a confined fluid. Given this relevance, Nuclear Magnetic Resonance (NMR) presents advanced techniques and constitutes one of the most important tools in the characterization of porous media. In short, based on computational methods of reconstruction of Digital Porous Media (DPM) and NMR experiments, relaxometry theory is applied, based on the understanding of Bloch's equation. Thus, in order to analyze the connectivity between pores of different sizes in the porous medium, where the confined molecules are under diffusive effects, the T2-Filtered T2-T2 Exchange experiment [1] was implemented and computationally simulated by the Laboratory of High Resolution NMR Spectroscopy (LEAR/IFSC-USP), being an evolution of the T2-T2 Exchange experiment proposed by Lee [2]. Thus, one of the analyzes consisted of obtaining experimental data for carbonate and sandstone samples, made in the shape of 10x20 mm cylindrical plugs, to observe the exchange effects between the different pores of the samples. Another approach consisted of implementing numerical models of the exchange equations, where the maximum signal intensity to be observed by NMR was studied considering a two-pore model. These analyzes provide important elements to understand the Exchange experiment between different pores. The main challenge of the T2-T2 Exchange experiment is estimating the parameters related to exchange rates. This occurs due to the low amount of signal present in the microporosity, often being less than 5Furthermore, this signal component appears in the distribution of relaxation times varying in both amplitude and position when using the conventional Laplace transform method. However, it was found that the T2- Filtered T2-T2 Exchange experiment is faster, allowing a deeper study of the effects of exchange and relaxation in porous media, and can therefore be used in a wide range of applications, such as the study of reservoir stones in the laboratory or in connected multi-compartment systems.

References:

[1] D'EURYDICE, M.N.; MONTRAZI, E.T.; FORTULAN, C.A.; BONAGAMBA, T.J., T2-Filtered T2-T2 Exchange NMR, J. Chem. Phys. 144 (2016) 204201.

[2] LEE, J.-H.; Two-dimensional inverse laplace transform NMR: altered relaxation times allow detection of exchange correlation, J. Am. Chem. Soc. 115 (1993) 7761-7764.

Oral presentations II

Intrinsic entanglement revivals in Dirac cat states

C. F. Silva (UFSCar), A. E. Bernardini (UFSCar)

Considering the parity symmetry related to the Dirac equation, the interplay between energy localization and the temporal evolution of parity-defined quantum superpositions is investigated for fermions in a magnetic field. The unitary evolution of Dirac cat states is obtained by initializing either even or odd principal quantum numbers in the equivalent harmonic oscillator basis in relativistic Landau levels. Quantum operators feature well-defined selection rules for states thus identified, exhibiting a permanent revival structure. Our analysis is specialized for the survival probability function and for the expectation values of spinor matrix operators, which are identified as quantifiers of spin-parity correlations encoded in Dirac bispinors. In such a context, the time evolving quantum state also imprints a signature on the energy expansion. Namely, frequencies associated with revivals are doubled for each revival order, being observed up to a so-called super revival time scale. Results show that Dirac cat states exhibit a fractional revival structure, which works as a probe of suppressions and regenerations of intrinsic correlations driven by the discrete spin-parity degrees of freedom of Dirac bispinors.

Addressing the Traveling Salesman Problem through Adiabatic Quantum Computing

Gabriel Pedro L. M. Fernandes (Universidade Federal de São Carlos), Celso J. Villas-Bôas (Universidade Federal de São Carlos)

Adiabatic Quantum Computing (AQC) is a Quantum Computing model designed for solving combinatorial optimization problems. Unlike the Circuit Model of Quantum Computing, AQC utilizes the Adiabatic Theorem, relying on the interpolation between an Initial Hamiltonian, whose ground state is the state in which the quantum system is initially prepared, and a Problem Hamiltonian, which encodes the solution space of the problem to be addressed. This is done in such a way that the best solution corresponds to the state of lowest energy. If the process is performed adiabatically, the final state encodes the optimal solution.

Many optimization problems have already been tackled using AQC, including the Knapsack Problem and the Vehicle Routing Problem. These tasks are particularly challenging to solve even with advanced classical heuristics due to the explosive growth of possible solutions as the involved variables increase. In this regard, heuristics stemming from Quantum Computing provide new perspectives on the topic, albeit limited by the current state of the art.

Here, we discuss how AQC can be used to address the Traveling Salesman Problem (TSP). TSP is a combinatorial optimization problem that can be stated as follows: "A traveling salesman needs to plan a trip that passes through N cities. What is the route that minimizes the travel cost, passing through all cities exactly once before returning to the starting point?". Despite its simple formulation, the solution space of the task grows factorially with the number of cities to be visited. From an application perspective, the TSP underlies tasks of significant importance, including route planning and electronic circuit schematization.

In this presentation, we will demonstrate how the task can be approached for a set of up to 9 cities using D-Wave's cloud-based quantum devices, discussing aspects related to the current state of the art of these devices that operate based on a heuristic called Quantum Annealing.

Optical Properties of monolayer $WSe2/\beta - Ga2O3$

Camila Cavalini (Universidade Federal de São Carlos), César Rabahi (Universidade Federal de São Carlos), Ingrid D. Barcelos (Laboratório Nacional de Luz Síncrotron), Marcelo Barbosa (Universidade de São Paulo), Mohamed Henini (University of Nottingham), Yuhao Zhang (Virginia Tech), Yara Galvão Gobato (Universidade Federal de São Carlos)

Monoclinic gallium oxide ($\beta - Ga2O3$) has attracted great attention due to its wide band gap (4.6 to 4.9 eV), high electron mobility (over 200 cm2/Vs), and a high electric field breakdown (around 8 MV/cm). Although $\beta - Ga2O3$ is not a van der Waals material, its crystalline structure allows to be exfoliated and combined with two dimensional materials (2D) such as transition metal dichalcogenide (TMD). Monolayers of TMD are direct gap semiconductor materials at two inequivalent $\pm$ K valleys and have strong exciton binding energy.

In this study, we have investigated the optical and magneto-optical properties of monolayer tungsten diselenide (WSe2) on exfoliated/large crystals of Ga2O3. Remarkably, we have obtained high optical quality samples with stable emissions and exciton photoluminescence linewidth comparable to WSe2/h-BN samples. At low temperature, the emission spectrum evidences several sharp peaks that are promissing candidates for single photon emitters. Here, we have investigated in detail their optical and magneto-optical properties.

Our results suggest that $\beta - Ga2O3$ is indeed a promising diecletric material to protect the surface of ML transition-metal dichalcogenide materials and also to explore fundamental physics in view of applications in opto-electronic and quantum information technology.

Quantum dots as an active reservoir for longer effective lifetimes in GaAs bulk

G. M. Jacobsen (Universidade Federal de São Carlos), H. Bragança (Universidade de Brasília), G. E. Marques (Universidade Federal de São Carlos), Yu. I. Mazur (Universidade de Arkansas), G. J. Salamo (Universidade de Arkansas), B. Liang (Universidade da Califórnia), V. Lopez-Richard (Universidade Federal de São Carlos) e M. D. Teodoro (Universidade Federal de São Carlos)

AlInAs/AlGaAs quantum dots (QDs) are good emitters along the visible region and their electronic transitions are still controversial, being either assigned as the optical transition between an electron and a S or P polarized hole, or by the emission coming from different families of quantum dots with different geometries. Here, we demonstrate that the QD emission is composed by two major contributions of dot families with distinct sizes and, as a consequence of quantum-confinement effects, different band alignments. Their temperature dependence shows clear signs of lateral coupling, i.e., carrier transfer between the dots and the lifetimes extracted from the transients confirm the coexistence of type-I and type-II QDs. A second interesting effect also appears for the GaAs bulk emission when the excitation energy is chosen to be above (2.82 eV) and below (1.69 eV) the QD peak energy. The bulk transient associated to the GaAs band gap at 10 K is eleven times longer when the higher excitation energy is employed compared to the lower value regime. As the temperature increases above 50 K, this ratio sets at 2.5 times. These observations have been explained by a theoretical framework with a set of coupled rate equations considering the QDs as carrier reservoirs for the bulk, demonstrating that the optical transition dynamics along the GaAs layer can be effectively controlled by the presence of the quantum dot layer and the excitation energy.

Optimizing the directions of the high-frequency fields of the continuous dynamic decoupling

Paulo Eduardo Zanni Junior (Universidade Federal de São Carlos), Leonardo Kleber Castelano (Universidade Federal de São Carlos)

In this research project, we are engaged in making an investigation of the methodology recognized as "continuous dynamic decoupling". This method is based on the application of continuous high-frequency external fields to maximize the fidelity of quantum logical operations performed on a decohering qubit. Assuming a known error vector and an environment represented by a scalar boson field at a finite temperature, this method allows effectively reduced decoherence during logical operations through the application of continuous external fields orthogonal to the error vector. The principal objective of this project is to enhance this methodology by finding the optimized directions for the application of external fields that maximize the fidelity in logical operations performed on a qubit. Since we must have the protective field orthogonal to the error vector, the optimization of the directions of the protection field application will be restricted to a plane. We illustrate these findings numerically for a Hadamard quantum gate and an environment with ohmic spectral density.

Oral presentations III

Excitonic Complexes in MoSe2/Clinochlore heterostructures

Alessandra Ames (Universidade Federal de São Carlos), Raphaela de Oliveira (Universidade Federal de Minas Gerais), Ingrid D. Barcelos (Laboratório Nacional de Luz Síncrotron), Alisson R. Cadore (Laboratório Nacional de Nanotecnologia), Marcio Daldin Teodoro (Universidade Federal de São Carlos)

Layered materials (LMs) have garnered considerable attention since the exfoliation of graphite to obtain single layers of graphene. Among the LMs, the study of the class of transition metal dichalcogenides (TMDs) is prominent. The TMDs belongs to the semiconductors category and mostly operate in the visible spectrum range. Such materials exhibit a generic lamellar structure following the formula MX2 (M=metal and X=chalcogen) and can be combined with various other materials, without the restriction of lattice matching, to form van der Waals heterostructures (vdWHs). Yet, these materials need to be exfoliated onto flat substrates with minimal impurities, leading to the exploration of insulators such as hexagonal boron nitride (hBN) as a solution to this problem. However, much of the researches have focused on synthetic materials, which can be expensive. To address this issue, investigations are underway to explore naturally occurring LMs, such as phyllosilicates. Phyllosilicates, which includes micas, chlorites and clays, can be exfoliated into monolayer and few-layer flakes and are naturally occurring wide bandgap insulators. Among the chlorites, the clinochlore is poorly explored and shows a flat surface and a bandgap of 4.35 eV, characteristics that make it promising for substrate applications. In this study, samples of MoSe2 monolayers deposited onto exfoliated clinochlore were investigated by photoluminescence and magneto-photoluminescence, where we focused on the excitonic complexes that naturally occurs due to the charge imbalance of the clinochlore, favoring bi-exciton and trion emissions with strong and narrow lines emissions, showing that the optical quality of this nanostructures are compared to the hBN counterparts.

Quantum Inspired Recommendation System

Amanda G. Valério (UFSCar), Alexandre Cesar Ricardo (UFSCar), Gabriel P. L. Fernandes (UFSCar), Nicolas A. C. Carpio (UFSCar), Matheus da Silva Fonseca (USP), Celso Jorge Villas Boas (UFSCar)

Recommendation algorithms are built on the assumption that you can generate a valid recommendation on a topic by searching for patterns or subsets in a database. In other words, it is possible to recommend films not yet seen by a user based on what other users with similar tastes have seen. The purpose of this work is to implement the (quantum-inspired) recommendation algorithm proposed by Ewin Tang (2019), inspired by the quantum recommendation algorithm of Kerendis and Prakash (2016). One problem encountered in generating recommendations is dealing with the large volume of data that needs to be analysed. One way of reducing the complexity of generating recommendations, and thus the processing time, is to employ matrix sampling techniques, using Singular Value Decomposition ($A = U\Sigma V^T$) and reducing the resulting matrices U , Σ and V^T by the rank of the matrix A (database). An important point is that the state preparation of the quantum algorithm has been replaced by a set of sampling assumptions of norm $\ell 2$, (Euclidean norm), which makes singular value estimation possible in time independent of m and n. This leads us to use a data structure formed by a set of binary trees storing the input data matrix. This was crucial for the quantum-inspired algorithm to achieve a complexity similar to that of the quantum algorithm, with a small polynomial slowdown, and remain efficient. At the end of the implementation, this inspired algorithm will be applied and tested on a business optimization problem and its results will be compared with other classical and quantum algorithms tested by the research group.

Microstructural, surface, and electrical properties of nanostructured W1-xMnxO3 gas sensor

João Victor Nascimento de Palma (Departamento de Física - Universidade Federal de São Carlos), Waldir Avansi Jr (Departamento de Física - Universidade Federal de São Carlos), Luís Fernando da Silva (Departamento de Física - Universidade Federal de São Carlos)

Semiconducting metal oxides (SMOx) are an important class of materials in the physics of materials. Among them, tungsten trioxide (WO3) is a wide band-gap n-type semiconductor. This SMOx has been widely used as resistive gas sensors (chemiresistors). Using light stimulation in sensors has been an efficient way to induce chemical reactions at room temperature; commercial gas sensors have worked at temperatures around 200°C. Also, gas sensing performance of WO3 can be improved by adding certain dopants. In the case of manganese (Mn), the introduction of such dopant into the WO3 lattice can be favorable in the sensing performance. In this work, we present an experimental investigation of the influence of annealing temperature and Mn content on the microstructural and surface properties of nanostructured WO3 films prepared by a soft chemical method. The samples were characterized by XRD, Raman, UV-Vis, XPS and FE-SEM techniques. Regarding the sensing performance, DC electrical measurements were performed under UV illumination, and exposing the samples to different nitrogen dioxide (NO2) levels. XRD and Raman measurements revealed the crystallization of the samples with annealing temperature and with Mn content, where we obtained the monoclinic structure for the W1-xMnxO3 nanoparticles. SEM images showed that W1-xMnxO3 crystals exhibit an irregular shape with a size of ca. 110 nm. UV-Vis spectroscopy analysis showed that Mn ions did not affect significantly the energy gap of the WO3 films. Also, XPS spectroscopy revealed the presence of Mn2+ in all tested samples. Regarding to oxygen O 1s XPS spectra, oxygen-metal ratio decreased with Mn content, and three oxygen components belonging to Metal-O bonds, oxygen defects and Metal-OH bonds were found presenting an increase in the adsorption component for with Mn content. Electrical measurements revealed that the samples were sensitive to UV light stimulation, detecting ppb NO2 levels at room temperature under UV illumination.

From classical to quantum loss of light coherence

Mateus Antonio Fernandes Biscassi (Universidade Federal de São Carlos), Romain Bachelard (Universidade Federal de São Carlos), Mathilde Hugbart (Université Côte d'Azur)

Light is a precious tool to probe matter, as it captures microscopic and macroscopic information on the system. We here report on the transition from a thermal (classical) to a spontaneous emission (quantum) mechanism for the loss of light coherence from a macroscopic atomic cloud. The coherence is probed by intensity-intensity correlation measurements realized on the light scattered by the atomic sample, and the transition is explored by tuning the balance between thermal coherence loss and spontaneous emission via the pump strength. Numerical simulations are realized in parallel with the experimental measurements , which allow to identify the critical role of the low temperature in the observation of the transition. Furthermore, the simultaneous measurement of the field-field correlations allows us to verify that the Siegert relation is valid for both regimes. The Siegert relation establishes an equivalence between the (loss of) coherence for the field and for the intensity, thus, we can conclude that the field does not suffer extra loss of coherence compared to the intensity. Our results illustrate the potential of cold atom setups to investigate the classical-to-quantum transition in macroscopic systems.

Critical Phenomena in Rock-Paper-Scissors Model

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We conducted an investigation into the influence of variations in a control parameter on the emergence of spatial patterns in the Rock-Paper-Scissors model, as well as how these patterns dissipate as we approach the critical value. The Rock-Paper-Scissors model consists of three species and an empty site, initially randomly distributed on a square lattice, wherein an active cell interacts with only one of its four neighbors. The possible interactions are categorized as motion (where active and passive entities swap positions), reproduction (active reproduces filling an empty site), or predation (active predates the passive generating an empty site). In summary, this model represents a cyclic interaction system devoid of any preferred orientation. However, it exhibits signatures of a continuous phase transition from diversity (the symmetric phase) to uniformity (the non-symmetric phase). Thus, we were motivated to study this type of system and analyze how changes in one of its control parameters, namely the motion parameter, influence the system as the critical value is approached. Through a series of numerical experiments, our aim is to verify the specific universality class to which the Rock-Paper-Scissors model with three species and an empty site belongs.

Poster sessions I

Applications of Quantum Neural Network in Fluid Dynamics

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The increasing demand for Machine Learning (ML) techniques to address fluid dynamics problems arises from the challenges posed by the spatial and temporal complexities of solving Differential Equations (DEs). In literature, the use of ML to tackle DEs and seek solutions is evident, as exemplified in a fluid dynamics simulation governed by the Navier-Stokes equations. In this scenario, the application of Machine Learning has led to a remarkable improvement, with gains of up to 40-80 times in simulation speed and 8 to 10 times in resolution compared to traditional numerical methods. This advancement offers promising prospects to address complex fluid dynamics challenges and enhance traditional methods of analysis and simulation.

Quantum algorithms hold the potential to surpass their classical counterparts through the capabilities of quantum computer processing. Specifically, Quantum Neural Networks (QNNs) encode classical neural network algorithms into quantum systems, aiming to leverage the benefits of quantum processing. The aim of this presentation is to discuss a doctoral project focused on the application of classical and Quantum Neural Networks to solve fluid dynamics problems governed by Differential Equations, utilizing the Physics Informed Neural Network approach.

Analytical Methods for Deriving Effective Hamiltonians: Focusing on the Method of Small Nonlinear Rotations

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Effective Hamiltonians play a pivotal role in the realm of optical quantum and quantum information systems, often manifesting in scenarios involving multiphoton processes and nonlinear optical phenomena. Broadly, an effective Hamiltonian is a modification of the original Hamiltonian, tailored to describe the quantum system with the purpose of simplifying calculations and obtaining approximate eigenvalues and eigenstates. To achieve this objective, a certain portion of the system is intentionally neglected, allowing us to focus on the specific phenomena of interest. In this work, we present a comprehensive review of the most common methods employed to derive Effective Hamiltonians, including the Rotating Wave Approximation (RWA) and Generalized Rotating Wave Approximation (GRWA), the James-Jerke's method, adiabatic elimination, and the method of small nonlinear rotations. We offer a formalized presentation of each method, detailing their application, advantages, disadvantages, applicable regimes, and exemplifying their use through application scenarios. Notably, we place a primary emphasis on the Method of Small Nonlinear Rotations (MSNR). This approach revolves around identifying a parameter, substantially smaller than unity, or even a unitary transformation that permits the description of the entire system through an effective Hamiltonian with diagonalized form. We analyzed higher orders of approximation and demonstrated that the method should be applied recursively when terms off the principal diagonal remains in Hamiltonian. The removal of terms situated off the principal diagonal enhanced the precision of the original system's approximation. This study aims to compile and elucidate the analytical methods routinely employed in quantum optics and quantum information, shedding light on their characteristics and limitations. This endeavor is poised to facilitate forthcoming research in these domains.

Neural networks over continuous variables of a single trapped ion

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Quantum computing in continuous variables is an alternative approach to quantum computing based on qubits - enumerable and finite units of information. Instead of using discrete qubits, quantum computing in continuous variables employs continuous quantum states to store and process information. These continuous states can be represented by variables such as position and momentum, or amplitude and phase. One of the advantages of quantum computing in continuous variables is its ability to handle and process a potentially infinite number of quantum states. This can make certain tasks, such as simulating complex quantum systems, more efficient than the traditional approach, also known as digital quantum computing.

Quantum computing in continuous variables has also proven to be a promising approach for implementing quantum communication protocols, such as quantum cryptography and quantum teleportation algorithms. Furthermore, this approach may have applications in areas like optimization and machine learning.

Recently J. M. Arrazola et al. [Phys. Rev. A 100, 032306 (2019)] proposed a quantum algorithm for solving nonhomogeneous linear partial differential equations of the form $A\psi(r) = f(r)$ in the continuous variables model of quantum computing. Its nonhomogeneous solution is obtained by inverting the operator A along with the preparation and measurement of special ancillary modes. In this work we suggest modifications in its structure to reduce the costs of preparing the initial ancillary states and improve the precision of the algorithm for semi-definite operators. These achievements enable easier experimental implementation of the quantum algorithm.

Optimizing resetting of superconducting qubits

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In this presentation, we conduct an examination of models concerning information resetting in superconducting qubits. Our focus centers on a main qubit linked with distinct auxiliary dissipative systems, which are used to erase the information stored in the main qubit. Our investigation underscores the importance of determining a optimum set of parameters for each approach. This strategic facilitates a notable reduction in the reset duration for the models under consideration.

Trapped ion quantum simulator applied to chemistry: obtaining the ground state of a hydrogen atom

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Since a quantum computer was first conceptualized by Richard Feynman in 1982, quantum computing research has become prominent in both industry and academia, especially in recent years. Due to its numerous potential applications, quantum simulation is an area of great interest to fields such as chemistry, pharmacy, and material science. These simulations involve simulating a challenging-to-control and -prepare system of interest (the simulated system) using a more manageable system (the simulator), by mapping the features of the former onto the latter. There are many methods available to conduct such simulations, each with its own objectives. In this work, we intend to study the Variational Quantum Eigensolver (VQE), an algorithm that has demonstrated great efficiency in computing the ground state of atoms and molecules. We will use this method to obtain the ground state energy of a hydrogen atom. The obtained results can be experimentally tested using a trapped ion platform from the group of Prof. Dr. Thomas Monz at the University of Innsbruck, as well as IBM quantum computers, which are freely accessible. Ultimately, we expect this work to lay the foundation for our group to apply the VQE to more complex systems.

Quantum iSWAP gate in superconducting qubits

Bruno A. Veloso (UFSCar), Alan C. dos Santos (UFSCar), Romain Bachelard (UFSCar), Celso J. Villas-Bôas (UFSCar)

The field of quantum computation has gained significant attention in recent years due to the promise of significantly speeding up certain computational tasks. Among the various systems proposed for implementing these computers, artificial atoms built using superconducting circuits are one of the most promising frameworks. In these systems, quantum information is encoded and processed using devices constructed within superconducting circuits using lithography techniques, the so-called superconducting qubits (1). The main advantage of this method is the ability to incorporate multiple qubits into a single circuit. In our work, we present a system of three superconducting qubits in which we can coherently transfer information from the first qubit (Q_1) to a second qubit (Q_2), conditioned on the state of a control qubit (Q_c) in a behavior analogous to that of a transistor. By deriving the effective Hamiltonian of this system, we demonstrated that it implements the quantum iSWAP gate. Furthermore, despite the conventional treatment of the system as a perfect two-level system, we have shown that assuming a third energy level significantly modifies the system's dynamics in specific cases, a result that was experimentally verified (2). Our results emphasize that, even when not populated, the higher energy levels of superconducting qubits play a substantial role in the functioning of these devices. A role that must be considered when developing and controlling such superconducting systems.

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Open Quantum Generalization of Boltzmann Machine

Nicolás Armando Cabrera Carpio(Universidade Federal de São Carlos), Celso Jorge Villas Boas(Universidade Federal de São Carlos)

The junction between physics and machine learning models is not unknown to researchers in these fields, for example, Hopfield networks, a type of recurrent neural networks (RNN), are based on the Ising model. They are of significant importance because of the connection they make between artificial neural network research, physics and brain research. We can understand Restricted Boltzmann Machines (RBM) as a stochastic generalization of Hopfield networks. Which is formed by N binary variables (Vertices in t graph) S = S1,...,SN, where, Si E -1,1. In the context of Ising models these binary variables represent Spins, where Si personifies the state of the microscopic magnetic moment whether it is pointing up(1) or down(-1). For the RBM Si represents the state of the neuron whether it is transmitting(1) or not(-1) a neuronal signal. We will then have, with the RBM, data represented as a thermal state in a energy function of an Ising model, this energy function is defined in a graph where the vertices are the neurons and the edges are the connections between them. We distinguish two sets of neurons in the RBM: The visible layer, which is the neuron layer that we will have access to, for example, to insert data or to read the outputs of the network, and the hidden layer that provides extra degrees of freedom for the model, and there are no connections between neurons in the same layer. In this work, we introduce a generalization based on Open Quantum Systems (OQS) of the Restricted Boltzmann Machine, in particular, in terms of the time evolution of the density matrix described by the Markovian Lindblad equation. This description allows us to treat quantum coherent effects and classical dissipative dynamics on the same page, which in principle would be impossible due to the incompatibility between the unitary time evolution of closed quantum systems and the dissipative evolution characteristic of neural networks.

Characterizing memristors and other nonlinear semiconductors out of equilibrium

Rafael Schio Wengenroth Silva (UFSCar); Fabian Hatmann (Universität Würzburg); Ovidiu Lipan (University of RIchmond); Victor Lopez-Richard (UFSCar)

Memcomputing is a computational paradigm that combines information processing and storage on the same physical platform. Key elements for this topic are devices with inherent memory such as memristors. Yet, despite the widespread emergence of memory effects in various solid systems, a clear understanding of the basic microscopic mechanisms that trigger them is still a puzzling task. We report basic ingredients of the theory of solid state transport, intrinsic to a wide range of mechanisms, as sufficient conditions for a memristive response that points to the natural emergence of memory. This emergence should be discernible under adequate set of driving inputs, as highlighted by our theoretical prediction and general common trends can be thus listed that become a rule and not the exception, with contrasting signatures according to symmetry constraints, either built-in or induced by external factors at the microscopic level. We unveil very concise and accessible correlations between general intrinsic microscopic parameters such as relaxation times, activation energies, and efficiencies with external drives: voltage pulses, temperature, illumination, etc. Its simplicity has also allowed a direct correlation with reported experimental observations with the potential of pointing out the optimal driving configurations. We also demonstrate how the availability of nonequilibrium charge carriers and their retarded path towards equilibrium, which are pervasive during the charge transport through metamaterials, photo-diodes, solar cells, memristive devices, sensors, electrochemical processes on surfaces, among others, affect the impedance response in very peculiar ways. The emergence of counterintuitive features such as negative capacitances can be proven to be a metaphoric construction with shallow physical meaning. This analytical approach creates a paradigm for impedance spectroscopy studies with impact in physics, electrochemistry, nanotechnology, and engineering.

Laser induced metals on glass surface

Juliana Mara Pinto Almeida (Universidade Federal de São Carlos); João Victor Lemes Marsola (Universidade Federal de São Carlos); Antonio Carlos Hernandes (Universidade de São Paulo)

The widespread use of the laser as an instrument for processing materials has provided a significant advance in studies on local changes in the structure and properties of glasses. These areas allow the application of these concepts in care for the development of photonic devices and in microfluidics. The evolution of laser techniques has made possible processes such as 3D fabrication and glass surface crystallization. Furthermore, laser-induced crystallization is relevant to functionalize glass matrices by mixing different micro/nanocrystals, such as LiNbO3 and $\beta - BaB2O4$with second harmonic generation [1]. , it is important to look for materials with significant third-order susceptibility, and for this purpose, heavy metal oxide glasses have great prominence due to their hyperpolarizability. Previous results on 50-BO1.5-50PbO glass surprised that the femtosecond laser associated with etching in KOH solution resulted in the architecture of lead oxide microcrystals [2]. In this work, to determine the influence of pulse duration on the crystallization process, a nanosecond laser was used to irradiate 50-BO1.5-50PbO glass. For the parameters of the laser, focused on the surface of the sample, pulses of 10 ns, at 1064 nm, repetition rate of 10 Hz, and scanning speed 0.2-7 mm/s, the results, boosted the crystalline phase in the bottom surface of the sample. The formation of metallic lead (Pb) was identified by X-ray diffraction, being responsible for alterations in the crystallization process in KOH solution previously investigated. The authors are grateful for the support of FAPESP, CAPES and CNPq.

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Poster sessions II

Universal Quantum Computation Using Atoms in Cross-Cavity Systems

Luiz Otavio Ribeiro Solak (UFSCar), Daniel Zini Rossatto (UNESP) e Celso Jorge Villas-Bôas (UFSCar)

Quantum gates are the building blocks of quantum circuits, which in turn are the cornerstones of quantum information processing. In this work we theoretically investigate a single-step implementation of both a universal two- (CNOT) and three-qubit (quantum Fredkin) gates in a cross-cavity setup coupled to a Λ-type three-level atom. Within a high-cooperativity regime, the system exhibits an atomic-state-dependent quantum interference involving the two-mode single-photon bright and dark states of the input light pulses. This allows for the controlled manipulation of light states by the atom and vice versa. Our results indicate these quantum gates can be implemented with high probability of success using the state-of-the-art parameters, either for the weak- or strong-coupling regime, where the quantum interference is due to an electromagnetically-induced-transparency-like phenomenon and the Autler-Townes splitting, respectively. This work not only paves the way for implementing quantum gates in a single step using simple resources, thus avoiding the need to chain basic gates together in a circuit, but it also endorses the potential of cross-cavity systems for realizing universal quantum computation.

Subradiance and Superradiance of a dense ensemble of cold, isotropic atoms

Felipe Carvalho Brambila (UFSCar), Raul Celistrino Teixeira (UFSCar), Pablo Gabriel Santos Dias (UFSCar), Ana Cipris (IFSC-USP)

The phenomenon of light scattering by an atomic cloud has two well-known effects in the literature called subradiance and superradiance, in which the decay of the fluorescence observed after a rapid excitation pulse has its characteristic curve altered. The present study aims to monitor the consequent modifications of the universal power decay curves emitted by the cloud in a dense regime after turning off the incident excitation laser light. For this, numerical simulations are carried out which, using a certain geometry for the atomic cloud, obtain the eigenvalues of the eigenmodes of the cloud and thus its average decay curve, enabling the analysis of sub- and superradiance phenomena for different values of density and optical depth of the sample.

Experimental classes for the Physics Degree: Adaptation of furniture and materials for use by people with disabilities

Samuel Harb Cerqueira Leite (Universidade Federal de São Carlos), Profa. Dra. Tatiane Cosentino Rodrigues (Universidade Federal de São Carlos)

In the context of experimental practices within undergraduate physics courses, accommodating the needs of individuals with disabilities, or People With Disabilities (PWD), is crucial. This work is dedicated to highlighting the essential adaptations undertaken by a student with both physical and visual impairments. Throughout this study, the student participated in classes as an observer, enabling the identification of necessary adaptations required for their participation in experimental classes in subsequent semesters. Several experimental procedures had to be adjusted to facilitate one-handed experimentation, while visual impairment necessitated the use of enlarged photographs for improved data observation. Furthermore, the student utilized their feet for making measurements. In essence, this work details the development of personalized approaches that empowered the student to engage fully in these experiments according to their unique needs.

Role of sulfur vacancy on the adsorption properties of small molecules on MoS2

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The in-lab isolation of a single graphene layer with Scotch tape promotes a breakthrough in materials science due to its intriguing properties. However, graphene has a metallic behavior, motivating the search for novel semiconducting 2D materials. In this scenario, the semiconducting MoS2 monolayer attracted great deal of attention. It belongs to the class of Transition Metal Dichalcogenide (TMD) materials and demonstrated potential for applications in several fields, including molecular sensors with high selectivity. In this work, we investigate the adsorption of 12 small molecules of interest for energy on the MoS2 surface. Our investigation was performed within the Density Functional Theory framework using the Vienna Ab initio Simulation Package (VASP). The adsorption on undecorated MoS2 considers several adsorption sites and molecular orientations. However, the geometries for systems with sulfur vacancies were generated by removing one sulfur atom from the lowest energy configurations of molecules on undecorated MoS2. Our results show that the molecules interact mainly via van der Waals bonds with the monolayer, except for NO. Moreover, the molecular adsorptions have three different behaviors: (1) The NO molecule promotes a change of 1.25 eV of the work function on undecorated MoS2 due to the change in the Fermi level induced by the addition of states inside the bandgap, and it passives the Sulfur vacancy on vacancy MoS2 suggesting a possible application of the material in sensing application of the NO. (2) The Sulfur vacancy induced changes in the work function of the molecules H2O, N2, CO, O2, NO, and SO2 adsorbed on MoS2, mainly due to the effect of the electrical dipole. (3) NO2 and SO2 promote changes in the electronic structure close to the valence and conduction bands. Our results also show that a macroscopic quantity (work function) depends on a microscopic quantity (electric dipole) highlighting mechanisms of censoring in the MoS2 monolayer.

Signatures of light-induced interactions between atoms

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Often seen as complex problems, atomic systems with high spatial density are natural. The complexity includes the challenging task of accounting for the interactions between the atoms, such as light-induced interactions. Some effects of these interactions include the saturation of the index of refraction, increased transmission for dense systems, absence of light localization, and others. High-density samples are difficult to probe since the majority of light becomes trapped inside. However, it is still expected that the light that leaks out carries information about the interactions. To achieve this, we will measure the correlation functions (g(1) and g(2)) for the light scattered under different regimes of spatial interaction. The system under inspection is a dense cloud of strontium atoms trapped in an Optical Dipole Trap (ODT). With this setup, we can achieve densities up to $10^14 atoms/cm^3$, a regime in which the so-called near-field interactions are expected to contribute to the overall scattering cross-section. Different possibilities for excitation and light collection will be explored. For example, excitation can be localized in a specific portion of the cloud, leading to more multiple scattering. Alternatively, a constant intensity excitation can be achieved using a much larger beam, inducing more single scattering. The collection of light can also be performed in the forward direction or perpendicular to it.

Control of the classical dynamics of a particle in the Morse-Coulomb potential

Gabriel Amici (Universidade Federal de São Carlos) Orientador: Emanuel Fernandes de Lima (Universidade Federal de São Carlos)

In this project, we propose the study of the classical dynamics of a particle in the forced Morse-Coulomb potential. This is an unprecedented potential in the literature of Coulomb behavior in the long range linked to a repulsive barrier of the Morse potential type. This potential asymptotically describes the Coulomb potential and is continuous and differentiable up to second order. The potential also has a parameter that makes it possible to adjust the degree of hardness of the repulsive part along with the depth of the potential well. In the presence of time-dependent external fields, this model presents chaotic dynamics associated with the anharmonicity of the potential and the coupling with the external field. In this project, we intend to use the Optimal Control Theory (OCT) to find control fields for this system. In the OCT formalism, the external field is considered the control function of the system, which must be determined by maximizing a performance criterion. We will seek to find optimized fields for various performance criteria, numerically solving the Euler-Lagrange equations associated with the control problem. The central point of the project will be to verify to what extent the control fields of the Morse-Coulomb potential are effective for controlling dynamics in the Coulomb potential, thus providing an alternative non-singular potential for the study of the hydrogen atom. In this way, the research project will allow the development of theoretical and computational skills of the candidate, as well as providing an investigation of an unprecedented system with the potential for new discoveries.

Implementation Of An Optical Accordion For Bosonic Strontium Atoms

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Studies on collective effects of light scattering can be categorized into two groups based on the density regime of the atomic sample, which can be either dilute or dense. The dilute regime is characterized by the condition $\rho/k^3 \ll 1$, where ρ is the spatial density and $\lambda = 2\pi/k$ is the wavelength of the atomic transition. On the other hand, the dense regime is defined by the condition $\rho/k^3 \geq 0.1 - 1$. In this work, a way to achieve a 2D geometry is proposed so that it is possible to study light scattering in a dense regime in this condition.

The role of Jahn-Teller distortion in the relative stability between the black and yellow phases of transition metal doped CsSnI3 perovskites

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Halide perovskites hold great potential as low-cost materials for efficient photovoltaic applications[1]. However, their widespread use still encounters two main challenges: (i) toxicity, as lead (Pb) is present in the most high-efficiency devices, and (ii) inherent structural instabilities[2,3]. While the $CsSnI3$ perovskite offers a lead-free alternative, overcoming the toxicity issue, it still perpetuates the issue of instability[4]. Specifically, a photo-inactive yellow phase has a lower formation enthalpy than the photo-active black phase, leading to an undesirable phase transition that serves as a source of inherent instability[5,6]. This study employs ab initio density functional theory calculations to explore the influence of substitutional doping in CsSnI3 at the Sn-site with 3d transition metals on the relative interphase stability between the yellow and black phases. Our investigation reveals a significant reversal in the stability between these phases through doping with Co, Cu, and Zn. This stability exchange is attributed to Jahn-Teller distortions within the doped octahedra, taking into consideration the distinctive octahedral interconnections in the black and yellow phases. In the black phase, there are corner-shared octahedra, contrasting with the edge-shared octahedra in the yellow phase. Of particular significance is the impact of Zn ion doping, which not only alters the relative stability but also maintains a pristine bandgap region devoid of defect states. These findings carry substantial implications for the development of stable, non-toxic photovoltaic materials with improved performance.

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Fundamental Limit To a Cavity Linewidth Narrowing With Single Atoms

Lucas Ribeiro da Silva Santos (Universidade Federal de São Carlos), Murilo Henrique de Oliveira e Celso Jorge Villas-Bôas (Universidade Federal de São Carlos)

Optical cavities in the Fabry-Perot configuration (two parallel mirrors) work out as resonators for the electromagnetic field. Their natural transmission linewidth depends on the natural properties of the mirrors involved (transmission and reflection coefficients, and absorption rates) and the distance between them. However, one can modify and control this linewidth using the electromagnetically induced transparency (EIT) phenomenon. The EIT is a quantum interference phenomenon capable of altering the optical response of a medium, turning an initially opaque atomic sample into transparent for a given radiation field (probe field) upon the incidence of a second field (control field). Once an atomic system is trapped inside the optical cavity, its linewidth can be altered by adjusting the control field strength. This allows one to reach much narrower cavity linewidths when compared to the natural ones. This narrowing has an immediate application, which is the manufacture of frequency filters adjustable by external fields. However, in the single-atom regime, there is a fundamental limitation to this narrowing of the linewidth, since in this regime quantum fluctuations cannot be disregarded. With this in mind, in this work we focus on how the linewidth of an optical cavity behaves for different numbers of atoms trapped inside of it. In addition, we also investigate how the other system parameters, such as the atom-cavity coupling and the intensities of the probe and control fields, affect the linewidth. To this end, we numerically simulate the quantum system using Python and QuTip, interested in the stationary characteristic EIT transmission spectrum, from which we can measure the linewidth for each set of parameters. Ultimately, this work focuses on important unanswered questions and could show whether it is possible to observe a quantum signature in the transmission of these systems, shedding a light on both fundamental and practical gaps.