

**Workshop on New Horizons in  
Quantum Correlated Materials**

**ICTP-SAIFR, Sao Paulo, Brazil**

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**List of Abstracts**

# Talks

# Hyperfine interactions and antiferroquadrupolar order: their role in PrOs<sub>4</sub>Sb<sub>12</sub>

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Many strongly correlated electron systems develop ordered phases at low temperatures that can be well understood in terms of an electronic order parameter. At ultra-low temperatures, however, the hyperfine interaction between nuclei and electrons becomes increasingly important, and we have to consider how this affects ordered phases and phase transitions close to zero temperature.

PrOs<sub>4</sub>Sb<sub>12</sub> is a superconductor below 1.85 K and 2.2 T, and develops antiferroquadrupolar (AFQ) order in magnetic fields between ~4 T and 14 T. The hyperfine constant of Pr is relatively large at 52 mK and the Pr crystal electric field levels are closely involved in both the superconducting and AFQ phases. This combination of properties makes PrOs<sub>4</sub>Sb<sub>12</sub> an ideal material to study the effects of the hyperfine interaction on multiple ordered phases [1].

I will describe magnetic susceptibility experiments as a function of magnetic field and temperature, which show that the phase boundaries in PrOs<sub>4</sub>Sb<sub>12</sub> continuously develop down to temperatures as low as a few mK.

We find that AFQ order is enhanced, whereas superconductivity is suppressed.

We explain our results in terms of a ground state composed of hybrid nuclear-electronic states with novel low energy excitations. That is, strong hyperfine interactions mean the low temperature Pr energy levels can no longer be considered as purely electronic entities, but must be described in terms of both electron and nuclear quantum numbers. The low temperature quadrupole excitations develop from these nuclear-electronic states, and are considerably modified compared to their higher temperature counterparts.

[1] A. McCollam et al., Physical Review B, 88, 075102 (2013).

## **Imaging the itinerant-to-localized transmutation of electrons across the metal-to-insulator transition in V<sub>2</sub>O<sub>3</sub>**

Andrés Santander-Syro

*Université Paris-Saclay*

**One-Sentence Summary:** This seminar will present experimental work showing how itinerant electrons localize due to increased interactions across the Mott metal-insulator transition, a puzzling fundamental phenomenon whose understanding has remained a challenge for over 50 years.

According to the “Standard Model of Condensed-Matter Physics”, the Bloch theory, metal or insulator are mutually exclusive states of matter. In insulators the highest occupied quantum-mechanical energy band is totally filled with electrons, while in metals it is partially filled. Thus, as temperature cannot change the number of electrons in a solid, it should not change either its intrinsic nature, i.e. metallic or insulating. However, V<sub>2</sub>O<sub>3</sub>, a metal at room temperature, shows a first-order metal-to-insulator transition (MIT) when cooling below, with an abrupt resistivity change of over six orders of magnitude. The very existence of a metal-to-insulator transition shakes the foundations of the well-tested Bloch model!

In fact in V<sub>2</sub>O<sub>3</sub>, as in many other transition-metal oxides, the last partially filled band is formed out of d-orbitals, which are rather localized in space. Thus, electrons in these bands can hardly avoid each other, and are subject to their strong mutual repulsion –the electron correlations, neglected in Bloch theory. The strong repulsion between electrons can inhibit their movement and result in a “Mott” metal-to-insulator transition (MIT), a fundamental phenomenon whose understanding has remained a challenge for over 50 years. A key issue is how the wave-like itinerant electrons in the metallic state change into a localized-like state in the insulator due to increased interactions. However, observing the MIT in terms of the energy- and momentum-resolved electronic structure of the system, the only direct way to probe both itinerant and localized states, has been elusive.

In this talk, I will discuss our recent experimental studies of the MIT in V<sub>2</sub>O<sub>3</sub> [1]. We used angle-resolved photoemission spectroscopy (ARPES), a technique that directly images the electronic eigen-energies of a solid. We found that in V<sub>2</sub>O<sub>3</sub> the temperature-induced MIT is characterized by the progressive disappearance of its conduction band of itinerant electrons, without any change in its energy-momentum

dispersion, and the simultaneous shift to larger binding energies of a quasi-localized state initially located near the Fermi level. Only when the state of itinerant electrons crossing the Fermi level has vanished, a complete gap of about 700 meV is observed, associated to the final energy position of the quasi-localized state. Furthermore, the spectral weights of the itinerant and quasi-localized states show a clear thermal hysteresis that tracks the one observed in resistivity data across the MIT.

**Study on the structural disorder and magnetic frustration in the QSL candidate  
Sr<sub>2</sub>Cu(W<sub>0.5</sub>Te<sub>0.5</sub>)O<sub>6</sub> perovskite under doping with Fe and Sb atoms**

Cynthia Contreras Medrano

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The properties of frustrated and low-dimensional magnetic systems are of great interest in the current physics of condensed matter. These materials can provide new and exotic states of matter, particularly the so-called “quantum spin liquids” (QSL). QSL candidate systems are mostly found in triangular networks, but recently a Cu square lattice compound Sr<sub>2</sub>Cu(W<sub>0.5</sub>Te<sub>0.5</sub>)O<sub>6</sub> has been characterized with properties that resemble a QSL state [1,2]. Moreover, this is an excellent system for studying the interplay between randomness and frustration [3]. Our study aims to better understand the effect of structural disorder by increasing disorder doping with <sup>57</sup>Fe and Sb in different percentages from 0.5% to 5%. Previous Mössbauer spectroscopy and magnetic measurements indicate that QSL state is partially preserved. Specific heat measurements have a peak near room temperature that shows a structural or electronic transition.

Daniel Carlos Cabra

*Universidad Nacional de La Plata*

**Incommensurate charge density wave vector on multiband intermetallic systems  
exhibiting competing orders**

Daniel Reyes

*Instituto Militar de Engenharia*

The appearance of an incommensurate charge density wave vector  $Q = (Q_x, Q_y)$  on multiband intermetallic systems presenting commensurate charge density wave (CDW) and superconductivity (SC) orders is investigated. We consider a two-band model in a square lattice, where the bands have distinct effective masses. The incommensurate CDW (inCDW) and CDW phases arise from an interband Coulomb repulsive interaction, while the SC emerges due to a local intraband attractive interaction. For simplicity, all the interactions, the order parameters and hybridization between bands are considered  $k$ -independent. The multiband systems that we are interested are intermetallic systems with a  $d$ -band coexisting with a large  $c$ -band, in which a mean-field approach has proved suitable. We obtain the eigenvalues and eigenvectors of the Hamiltonian numerically and minimize the free energy density with respect to the diverse parameters of the model by means of the Hellmann-Feynman theorem. We find that the inCDW phase presents a nematic-like type symmetry, which allows us to fix one of the components of  $Q = (\pi, Q_y) = (Q_x, \pi)$ . Our numerical results show that the arising of an inCDW state depends on the parameters, such as the magnitude of the inCDW and CDW interactions, band filling, hybridization and the relative depth of the bands. In general, inCDW tends to emerge at low temperatures, away from half-filling. We also show that, whether the CDW ordering commensurate or incommensurate, large values of the relative depth between bands may suppress it. We discuss how each parameter of the model affects the emergence of an inCDW phase.



## **Mott domain wall matter: a state with non-Fermi liquid behavior**

Eduardo Miranda

*UNICAMP*

Most Mott systems display a low-temperature phase coexistence region around the metal-insulator transition. The domain walls separating the respective phases have very recently been observed both in simulations and in experiments and they often cover a significant volume fraction, thus cannot be neglected. Interestingly, they resemble neither a typical metal nor a standard Mott insulator, displaying unfamiliar temperature dependence of (local) transport properties. We show that transport in this regime is dominated by the emergence of “resilient quasiparticles” with strong non-Fermi liquid features, reflecting the quantum-critical fluctuations in the vicinity of the Mott point.

## **Disorder, low-energy excitations, and topology in the Kitaev spin-liquid**

Eric C. Andrade

*USP-São Carlos*

The Kitaev model is a fascinating example of an exactly solvable model displaying a spin-liquid ground state in two dimensions. In real materials, however, deviations from the original Kitaev model are expected to appear. In this talk, I will discuss the fate of Kitaev's spin-liquid in the presence of disorder -- bond defects or vacancies -- for an extended version of the model. Considering static flux backgrounds, we observe a power-law divergence in the low-energy limit of the density of states, with a non-universal exponent. We link this power-law distribution of energy scales to weakly coupled droplets inside the bulk, in an uncanny similarity to the Griffiths phase often present in the vicinity of disordered quantum phase transitions. If time-reversal symmetry is broken, we find that power-law singularities are tied to the destruction of the topological phase of the Kitaev model in the presence of bond disorder alone. For weak to moderate site dilution, there is a transition from this topologically trivial phase with power-law singularities to a topologically non-trivial one. Therefore, diluted Kitaev materials are potential candidates to host Kitaev's chiral spin-liquid phase.

## **Finding true Kugel-Khomskii systems**

Eva Pavarini

*Forschungszentrum Jülich GmbH*

About 50 years ago, in a seminal paper, Kugel and Khomskii have shown that many-body super-exchange, a purely electronic mechanism, can give rise to orbital order in the absence of lattice distortions. Since then, many materials have been claimed to host Kugel-Khomskii phenomena. Recently, one by one these claims have been proven to be incorrect, however. Modern many-body approaches have shown that orbital physics in correlated materials is rather controlled by Coulomb-enhanced crystal-field splitting, hence electron-lattice interactions. These results suggested that Kugel-Khomskii super-exchange, while very interesting in principle, it is in practice too weak to have an effect on orbital physics in real systems. In this talk I will show that this is not the case, and that materials hosting a Kugel-Khomskii transition do exist.

## **Spin excitations and electronic structure in the BaFe<sub>2</sub>As<sub>2</sub> family of materials**

Fernando Garcia

*USP-São Paulo*

To a large extent, it is accepted that magnetic excitations play a key role in promoting high temperature superconductivity in the Iron based superconductors (IBS). A major conceptual divide in the field, however, remains and concerns to which degree either low or high energy excitations are in the driver's seat of the IBS phenomenology. This divide, in turn, reflects the discussion about the description of the relevant electronic degrees of freedom in terms of either localized or itinerant electronic states.

In this talk, we shall present angle resolved photoemission spectroscopy (ARPES) and resonant inelastic X-ray scattering (RIXS) of Cr and Mn substituted Ba(Fe<sub>1-x</sub>M<sub>x</sub>)<sub>2</sub>As<sub>2</sub> (M = Cr or Mn) materials. ARPES is the standard tool to characterize the electronic structure of materials close to the Fermi level, thus probing low energy excitations, whereas RIXS is an ideal probe to high energy magnetic excitations in the IBS. In contrast to many other substitution strategies, Cr and Mn dopants cause qualitative changes in the parent compound magnetic properties but do not lead to a superconducting ground state. By comparing the electronic structure and magnetic excitations of these non-superconducting materials with the superconducting ones, we try to identify the relevant parameters and energy scales of the problem of superconductivity in the IBS materials.

**Vortex-Vortex interactions in superconductors with nematic order**

Gustavo Sergio Lozano

*Universidad de Buenos Aires*

## **Finite-time quantum quench in the extended Hubbard model**

Helena Bragança

*UnB*

Nonequilibrium dynamics of closed systems has recently received considerable attention due to advances in numerical techniques and the possibility of emulating strongly correlated chains in highly controllable experiments with ultracold atoms in optical lattices. Systems that cross quantum critical points during the quench are especially interesting. Some systems can feature a large degree of universality; in other cases, it has been observed a crossover between adiabatic and non-adiabatic stages of time evolution close to the criticality. In this work, we have investigated the formation of charge density wave (CDW) and spin density wave (SDW) ordered phases via a quantum quench. We start from a non-interacting state and use the time-dependent density matrix renormalization group to perform finite-time interacting quenches in the extended Hubbard model. We observe different regimes by varying the duration of the ramping - we go from sudden quenches to adiabatic ones. For the quenches we analyze, the adiabatic regime is reached with distinct ramping time scales depending on whether the CDW or the SDW is formed. The former needs to be slower than the latter to prevent entangled excited states from being accessed during the quench. Our findings also show that breaking the system integrability by turning on the nearest-neighbor interactions does not give rise to significant changes in the non-equilibrium behavior within the adiabatic approximation.

## **Novel subbands in electronic spectral densities of correlated systems**

Karen Astrid Hallberg

*Centro Atómico Bariloche*

In spite of important recent improvements in the theoretical handling of correlated materials, it is still difficult to obtain precise and detailed electronic structure results to compare with experiments.

We calculate and resolve with high precision the electronic spectral densities at zero temperature of one of the key models for multi-orbital strongly correlated electron materials, the Kanamori-Hubbard Hamiltonian (KH), by means of the Dynamical Mean Field Theory which uses the Density Matrix Renormalization Group (DMRG) as the effective-impurity solver. Due to the precision of this technique, we are able to observe the existence of unforeseen subbands and structure in the local density of states for finite values of the inter-orbital coupling  $V$ , which we characterize by calculating specific response functions. I will also show very recent results on the electronic densities of states of a one-dimensional version of the KH model calculated with DMRG, for which we also find in-gap subbands for finite values of  $V$ .

We expect that the results presented here together with the possibility of calculating more precise spectral functions for models of correlated materials will stimulate a closer study of the details of experimental results and, hence, will contribute to unveil the complex and elusive microscopic behavior of strongly correlated materials.

## ***IFT-Colloquium: Correlated states in magic graphene moirés***

Leni Bascones

*Instituto de Ciencias de Materiales de Madrid*

The discovery in 2018 of insulating and superconducting states in twisted bilayer graphene, at the so-called magic angle, opened a new field of research which is producing continuous surprises and amazing discoveries at an incredible pace. By twisting two or more atomically thin layers, such as graphene, or by combining layers with slightly different lattice constant a moiré pattern is formed. The properties of a moiré heterostructures are controlled by a length scale which can be several orders of magnitude larger than the atomic distance. Under certain conditions the electronic bands of moiré heterostructures close to the Fermi level are quite flat. In these cases, the kinetic energy of the electrons is small and the repulsion between the electrons controls the electronic properties. Since 2018 many different and highly tunable correlated states, with different symmetry breakings: superconducting, magnetic, nematic and topological properties have been discovered and unconventional properties show up also in the normal state of several moiré heterostructures. After a general introduction to the field I will discuss the correlated states in two of these graphene moiré systems: twisted bilayer graphene and ABC graphene trilayer on hBN, making connection to the properties of other known strongly correlated electron systems.



## **Electronic correlations in the “normal” state of twisted bilayer graphene**

Leni Bascones

*Instituto de Ciencias de Materiales de Madrid*

The discovery of superconductivity, insulating states and a plethora of symmetry breaking transitions in twisted bilayer graphene and other graphene based moiré heterostructures have opened a complete new field in the study of correlated electron systems which advances at a vertiginous pace. While the effect of correlations is more easily identifiable when they produce a phase transition to an ordered state, research in other strongly correlated electron systems has shown that the non-ordered, so-called “normal”, state can be also strongly modified by such correlations. In the talk I will discuss the strong spectral weight reorganization produced by the electronic correlations in twisted bilayer graphene.

## **Parafermionic zero modes in strongly correlated fermionic lattices**

Luis Gregório Dias

*USP-São Paulo*

The so-called "search for Majoranas" has mobilized several groups over the last decade with the goal of achieving the "holy grail" of topological quantum computation in condensed matter systems. In spite of the advances, several unanswered questions and challenges remain, as highlighted the recent events that shook the community. This begs the question of other topological excitations which could be used as non-Abelian anyons can be viewed in a different light.

In this talk, I will discuss some of these scenarios and discuss our recent proposals for modeling parafermionic zero modes, Majoranas'  $\mathbb{Z}_n$  symmetric cousins, in strongly interacting electronic systems. In particular,  $\mathbb{Z}_3$  parafermions can be, in principle, used to produce Fibonacci anyons, laying a path towards universal topological quantum computation.

In our work, we show that both  $\mathbb{Z}_4$  [1] and, more importantly,  $\mathbb{Z}_3$  [2] parafermionic modes can be realized as edge states in strongly interacting, fermionic 1D lattice models. Our DMRG calculations allow us to characterize the topological phase transition and study the effect of local operators (doping and magnetic fields) on the spatial localization of the parafermionic modes and their stability. In addition, we propose a way to detect these rather exotic quasiparticles using quantum dots.

## **Solid State Neuroscience**

Marcelo Rozenberg

*Université Paris-Saclay*

In this talk I shall introduce some basic notions of electronic neuromorphic functionalities of materials and devices. I shall first briefly describe our efforts towards implementing artificial neurons exploiting the electric Mott transition. Then, I shall describe in more detail our recent work implementing, in hardware, a new silicon-based spiking neuron.

This artificial spiking neuron is of unprecedented simplicity, thanks to the behavior of a novel memristor device that we introduced recently. This device shares the same resistive switching properties as Mott materials, however is fully built from inexpensive off-the-shelf electronic components. Importantly, the basic neuron circuit can be associated as LEGO blocks to build functional spiking neural networks that are relevant to Neuroscience, which we are beginning to explore.

# Vacancy-engineered interacting nodal-line semimetals

Mariana Malard

*UnB*

We show that lattice engineering with periodic distributions of vacancies yields a novel type of nodal-line semimetal which possess symmetry-enforced nodal lines, which are immune to arbitrarily large symmetry-preserving perturbations, and unusually robust accidental nodal lines. Both types of nodal lines arise from the structural features of the proposed vacancy-engineered lattices, as demonstrated using a minimal effective model and verified by first-principles calculations of vacancy-engineered graphene and borophene. The effect of electron-electron (e-e) interaction in graphene is addressed by quantum Monte Carlo simulations. Former studies of the pristine honeycomb lattice have demonstrated the occurrence of a quantum phase transition from a metallic to an insulating antiferromagnetic phase at a finite strength  $U_c$  of the e-e interaction. We investigate if the long-range magnetic order is preserved in vacancy-engineered graphene and, if so, how the nodal lines affect  $U_c$ .

## **Creating and Tuning Electronic states and Phases of NdNiO<sub>3</sub>**

Milan Radovic

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RENiO<sub>3</sub> (RE - Rare Earth elements) exhibit unique and multifunctional physical phenomena directly related to the spin and orbital degrees of freedom of the transition metal d-states and their interplay with the lattice. Notably, the iso-structure of RENiO<sub>3</sub> permits the realization of hetero-structures altering physical matters that are very different from their bulk form.

The talk will overview the electronic structure of differently strained NdNiO<sub>3</sub> (NNO) films grown solely and in proximity to magnetically ordered manganite layers. It will be shown that substrate-induced strain tunes the crystal field splitting, consequently changing the Fermi Surface (FS) properties, nesting conditions, and spin-fluctuation strength, and thereby controls the Metal-Insulator Transition (MIT) [1]. Furthermore, the comprehensive experimental study combined with theoretical calculation reveals the direct magnetic coupling between the NNO film and the manganite layer in proximity, altering magnetic ordering and electronic structure in the nickelate layer and suppressing the MIT. [2].

Overall, our studies establish different approaches to manipulating the properties and electronic phases in NNO, signifying perspectives of TMOs, in general, for novel applications.

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## **The role of electron-phonon interactions in quasi-2D compounds**

Natanael de Carvalho Costa

*UFRJ*

Over the past decades, a great deal of interest has been given to quasi-2D materials, with a large experimental effort being invested to unveil their electronic correlation properties. Some novel compounds exhibit complex phase diagrams, with the emergence of charge-density wave (CDW) or superconductivity, whose nature is still not clear, although being associated with strong electron-phonon (el-ph) interactions. These findings have raised issues about the relevance of the el-ph coupling for correlated materials, rather than just the electron-electron one. Given this motivation, here we present an overview of recent results about the role of the el-ph interaction with these compounds -- from transition-metal dichalcogenides to the twisted bilayer graphene. We add our contribution to this discussion, from a theoretical point of view, by developing and performing state-of-the-art quantum Monte Carlo simulations for the Hubbard-Holstein Hamiltonian, the "standard model" for this kind of system. Starting with simple geometries, such as the square lattice, we study the competition and interplay between antiferromagnetism (AFM) and CDW, establishing rich phase diagrams. Interestingly, in the region between AFM and CDW phases, we have found an enhancement of superconductivity, with favored unconventional pairing. Similarly, we also determine semimetal-to-insulator quantum critical points in the honeycomb lattice, the same geometry as the graphene. Dealing with interacting Dirac fermions leads to quite different results: the critical points are very susceptible to changes in the phonon frequencies, drastically affecting the phase diagram. On the other hand, we show that the el-ph interaction does not change the AFM universality class of the phase transitions. Indeed, understanding how to control and manipulate these many-body states remains a challenge for experimental physicists, and it is the bottleneck for eventual applications on semiconducting devices. As a step towards this end, our theoretical findings may shed light on the emergence of correlated properties in these quasi-2D materials.

## **The optical response of the quantum material family BaCoS<sub>2</sub>-BaNiS<sub>2</sub>**

Ricardo Lobo

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BaCoS<sub>2</sub> and BaNiS<sub>2</sub> are the end members of a solid solution that shows a vast array of quantum properties. The Co material is a strongly correlated insulator with an antiferromagnetic transition, as well as a structural phase transition, around room temperature. At 28% Ni doping the solution undergoes an electronic metal-insulator phase transition to a Drude metal. The metallicity persists all the way to the pure Ni compound, where in addition to the Drude metal, we observe a strong contribution from bands with linear dispersion at the Fermi level. These will give origin to dispersive Dirac nodal lines. We performed optical conductivity measurements combined with ab-initio calculations to reverse engineer the role of each band in the physical response of these materials. We explained uncommon features in their optical response such as a linear dispersion of the optical conductivity and the existence of an isosbestic line separating a spectral-weight transfer across Dirac nodal states.

## **Orbital anisotropy in Kondo lattice materials**

Ricardo Urbano

*UNICAMP*

Heavy-fermion (HF) metals are described by strong electron-electron interactions that can be tuned across a quantum phase transition between localized f-electron magnetism and itinerant heavy-mass Fermi liquid behavior. Therefore, the overlap between neighboring atomic wave functions is a central feature and gives rise to a range of emergent phenomena, including AFM, unconventional superconductivity, and the ability to tune from one ground state to the other in this class of materials. Nevertheless, measuring the degree of this hybridization by conventional methods is challenging and indirect. We, thus, provide an approach using NMR to determine the magnetic couplings between the f-electrons and neighboring nuclear spins in a series of Kondo lattice materials and find that the hybridization is strongly direction dependent in this significant class of superconducting HF materials. The experimental data are discussed in terms of a change in Ce's 4f orbitals that arises from evolution of crystal-electric field (CEF) energy levels upon doping/pressure. We demonstrate that the hyperfine coupling probed by NMR provides a quantitative measure of orbital anisotropy.



## **Spontaneous spin chirality versus magnetization in a zigzag chain**

Rodrigo Pereira

*International Institute of Physics-UFRN*

Quantum spin systems can break time reversal symmetry without breaking spin rotation symmetries by developing a spontaneous spin chirality. In general, a continuous transition from a chiral spin state to a magnetically ordered phase would be unconventional because these phases break different symmetries. To investigate the competition between the two types of order, we construct an anisotropic spin chain model that exhibits a stable chiral phase whose excitations correspond to Majorana fermions coupled to a  $Z_2$  gauge field. Using a combination of exact solutions, effective field theories and numerical simulations, we characterize the unconventional phase transitions from the chiral phase to other (magnetic or non-magnetic) phases in this model. We interpret these transitions in analogy with deconfined quantum criticality in higher dimensions.

## Exploring thermal transport in complex oxides

Valentina Martelli

*USP-São Paulo*

Perovskite-type complex oxides are a family of compounds that have attracted growing interest because of the variety of tunable physical properties making them attractive for technological applications in different areas [1]. One prominent representative of this class of materials is the cubic SrTiO<sub>3</sub> that has gathered fundamental research efforts across different topics, as, for instance, superconductivity, thermoelectricity, ferroelectricity [2-3]. Recently, we investigated thermal transport in single crystalline SrTiO<sub>3</sub>, a less explored property that revealed the presence of the Poiseuille flow of phonons at low temperature, possibly phonon localization and a high-temperature diffusivity approaching the Planckian limit ( $\tau=\hbar/kBT$ ) [4]. The findings pointed to the role of the lattice degrees of freedom and of specific phonon modes in setting and manipulating the heat conduction profile. In this context, we have very recently started the investigation of thermal transport in BaBiO<sub>3</sub>, another perovskite with a crystal structure undergoing multiple phase transitions as a function of temperature and displaying emerging phenomena [5]. In this talk, I will present and discuss the perspectives on our current investigations.

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## Emergence of superconductivity at the onset of nematic order

Vanuildo Silva de Carvalho

*Universidade Federal de Goiás*

We study the pairing instability of a two-dimensional metallic system induced by Ising-nematic quantum fluctuations in the presence of an unavoidable relevant coupling of the nematic order parameter to the elastic modes (acoustic phonons) of the lattice. We find that this nematic coupling  $\lambda_{\text{latt}}$  leads to a decrease of both the superconducting (SC) critical temperature  $T_c$  and the gap function  $\Delta$ , regardless of the gap symmetry. Interestingly, we show that  $\lambda_{\text{latt}}$  provides a knob that allows us to investigate the emergence of the SC phase at low temperatures, as an instability from either a non-Fermi liquid or a Fermi liquid normal state. The phase transitions between the SC and these normal states are characterized by different critical exponents, which may also vary for each gap symmetry. Finally, we argue that these results might explain the dependence of  $T_c$  in the vicinity of the nematic quantum critical point exhibited by the compound  $\text{FeSe}_{1-x}\text{S}_x$ .

## **Entanglement as a witness of metal-insulator transitions in 1D systems**

Vivian França

*UNESP-Araraquara*

We investigate the average single-site entanglement as a probe for quantum phase transitions in interacting one-dimensional systems described by the Hubbard model. In particular metal-insulator transitions are investigated in the presence of electrical field and also in disordered chains via density-functional theory calculations. We show that the minimum disorder strength required to the so-called full Anderson localization – characterized by the real-space localization of pairs – is strongly dependent on the interaction regime. The degree of localization is found to be intrinsically related to the interplay between the correlations and the disorder potential. In magnetized systems, the minimum entanglement characteristic of the full Anderson localization is split into two, one for each of the spin species. We show that although all types of localization eventually disappear with the increasing of temperature, the full Anderson localization persists for higher temperatures than the Mott-like localization.

## **S=3/2 Kitaev Spin Liquids**

Willian Natori

*Institute Laue Langevin*

The Kitaev honeycomb model (KHM) has a unique place in quantum magnetism due to its importance in the theory of quantum spin liquids, topological computation and material science. Routes to implement higher spin KHMs in solid-state platforms revived the interest in theoretical studies on this model's characterization for  $S > 1/2$ , which do not possess an exact solution. We constructed a parton mean-field theory (PMFT) to unveil the ground state of the  $S=3/2$  KHM that displayed a remarkable quantitative agreement with the results of DMRG simulations. Such an unusual result is explained by an exact mapping between an extensive number of conserved quantities and a static  $Z_2$  gauge field. This mapping allows the exact evaluation of expectation values for a number of operators within mean-field theory by extending theorems for integrable spin-orbital models. We showed that the ground state of the spin-3/2 KHM corresponds to the lowest energy Majorana spin liquid that preserve all the symmetries of the model. Based on this result, we propose a mechanism to obtain a spontaneous time-reversal symmetry breaking from an out-of-plane single ion anisotropy, which displays interesting similarities to a magnetic field on the  $S=1/2$  KHM. The single-ion anisotropy on a fixed sector leads to a three-spin-orbital interaction that induces an octupolar order related to the introduction of second-nearest neighbor hoppings of Majorana particles. Possible implementations of this CSL on van der Waals monolayers are discussed by the end of the talk.

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# Posters

# Thickness dependent heat transport experiments in complex oxides

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BaBiO<sub>3</sub> is a complex oxide that displays superconductivity when hole doped [1]. It undergoes to several structural transitions between 100K and 800K, opening a major challenge in understanding the role of phonons in the emergence of collective quantum states. BaBiO<sub>3</sub> was predicted to host topologically protected surface states when the cubic symmetry is considered [2, 3]; however, bulk BaBiO<sub>3</sub> is monoclinic and it could possibly approach a cubic structure only when 2D limit is achieved and, thus, breathing and tilting distortions are suppressed [4]. The study of heat transport  $\kappa(T)$  in bulk and thin films of BaBiO<sub>3</sub> can contribute to this debate as it was shown in another complex oxide [5] that thermal conductivity can reveal exotic phonon regimes related to specific phonon modes.

Steady-state methods (one-heater-two-thermometers) are commonly employed to investigate thermal transport in bulk samples, whereas  $3\omega$  technique can be applied to study heat transport in thin films.  $3\omega$  method is an advanced non-commercial method [6] based on the determination of the thermal response of a specimen as a consequence of an AC excitation supplied to an appropriate heater-thermometer deposited on the sample. In this work, we present and discuss a home-made  $3\omega$  setup developed to study thermal transport in the complex oxide BaBiO<sub>3</sub> as a function of thickness and temperature.

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# **Magnetic and transport properties of interacting fermions on nodal line semimetals**

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Nodal line semimetals (NLSMs) have been attracting a great deal of interest for their topological properties. These systems exhibit crossing bands forming lines with linear dispersion, which are robust to any perturbation that preserves some particular symmetries of the Hamiltonian. Recently, it has been suggested that NLSMs may be created by vacancy-engineering graphene-like compounds, which enforce the symmetries by taking into account just geometrical aspects. Similar to the honeycomb lattice, it is important to understand the properties of interacting Dirac fermions in these symmetry-enforced geometries. For the former, previous studies of the Hubbard model have shown the occurrence of a quantum phase transition from a metallic phase to an insulating antiferromagnetic one for a finite value of  $U_c$ . Therefore, investigating if long-range order emerges in NLSMs, and how  $U_c$  changes as a function of external parameters may shed light on future studies in graphene. In view of this, here we investigate the properties of the Hubbard model in a honeycomb lattice, with sites depleted in such a way that preserves glide symmetries. We analyze it at half-filling through (i) tight-binding calculations: to determine the occurrence of nodal lines; (ii) Quantum Monte Carlo simulations: to examine how the magnetic and transport properties of our system are affected by these nodal lines, comparing the results with those of the honeycomb lattice.



# **Can Caroli-de Gennes-Matricon and Majorana vortex states be distinguished in the presence of impurities?**

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Majorana zero modes states (MZMs) are predicted to appear as bound states in vortices of topological superconductors. MZMs are pinned at zero energy and have zero charge due to particle-hole symmetry. MZMs in vortices of topological superconductors tend to coexist with other subgap states, named Caroli-de Gennes-Matricon (CdGM) states. The distinction between MZMs and CdGM is limited since current experiments rely on zero-bias peak measurements obtained via scanning tunneling spectroscopy. In this work, we show that a local impurity potential can push CdGM states to zero energy. Furthermore, the finite charge in CdGM states can also drop to zero under the same mechanism. We establish, through exploration of the impurity parameter space, that these two phenomena generally happen in consonance. This means that energy and charge shifts in CdGM may be enough to imitate spectroscopic signatures of MZMs.

# Growth and structural characterization of the quasi-one-dimensional $\alpha$ and $\beta$ -Bi<sub>4</sub>I<sub>4</sub> single crystals

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The quasi-one-dimensional Bi<sub>4</sub>I<sub>4</sub> compound presents two stable phases at room temperature:  $\alpha$  and  $\beta$ -Bi<sub>4</sub>I<sub>4</sub>. They share the same molecular chains, which are kept together by Van der Waals interactions, and differ for the way those chains are stacked [1]. Recently,  $\alpha$  and  $\beta$ -Bi<sub>4</sub>I<sub>4</sub> have been predicted to host a trivial and non-trivial band structure, respectively [2]. ARPES experiments support this picture [3, 4], but a thorough study of transport coefficients in the two phases is still lacking. With this motivation, we have grown single crystalline Bi<sub>4</sub>I<sub>4</sub> ( $\alpha$ ,  $\beta$ ) and here we present the investigation of the crystals by X-ray diffraction. Finally, we discuss the structure analysis obtained by Rietveld refinement.

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## **Electronic and magnetic properties of FeO: A DFT+U approach**

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Metal oxides are materials of great interest in the scientific community. They can be used as high-temperature superconductors, catalysts, or even in magnetic data storage. The bulk FeO and its (111) surface shows fascinating phenomena both from theoretical and practical points of view. This oriented surface has a great potential to be used as a substrate to grow two-dimensional materials, like graphene, and has shown a great capability of Hydrogen adsorption. From the theoretical standpoint, the focus of this paper, FeO is a prototypical system to investigate the physics of strongly correlated systems and Mott insulators. Those materials present a band-gap due to the strong electron-electron correlation interactions, which appear due to the presence of localized d electrons. Therefore, calculating its fundamental properties, specially the electronic structure, via DFT is a great computational and physical challenge. In this work, we applied the DFT+U functional, developed by Matteo Cococcioni and inspired by the Hubbard model hamiltonian, to the bulk FeO and its (111) surface to recreate theoretically its electronic and magnetic properties. The (111) surface was chosen because of the [111] spin oriented atoms. The proposed model successfully describes the bulk structural, magnetic and electronic properties. Furthermore, the model predicts that even in ambient temperature the ground state is anti-ferromagnetic, which agrees with experiments. For the (111) surface, interesting results were obtained. The antiferromagnetic state is still predicted as the ground state and the surface presents metallic states.

# Transport investigation in doped SmB6 single crystals

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In Topological Kondo Insulators (TKI), both topologically protected surface states and insulating bulk stem from strong electronic correlations [1]. In these systems, exploring the interplay between transport coefficients, non-trivial topology and electronic correlations requires to carry out experiments under multiple external parameters on candidate materials. In this context, we selected the compound SmB6 which was recently classified as a KTI [1] [2], in order to study the behavior of the transport coefficients (electrical, thermal, thermoelectric) when the protected surface state is suppressed through magnetic doping. Here, we present our recent investigation of electrical transport at low temperature in pure and doped (Gd, Y) SmB6 single crystals. We discuss our results in the context of spectroscopic experiments in a similar series of samples [3]. Finally, we introduce the experimental setup designed at LQMEC to carry out thermal and thermoelectric measurements under multiple extreme conditions and we discuss the application in SmB6 samples, whose typical geometric dimensions are lower than 5 mm.

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# **Chiral spin liquid with spinon Fermi surface protected by symmetry**

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The complete understanding of the ground state for a certain Hamiltonian in strongly correlated quantum spin systems is a big challenge in theoretical physics. Among the novel phases in this framework, quantum spin liquids have been studied extensively. Quantum spin liquids are systems with localized spins on the lattice, where the ground state is highly entangled and does not present magnetic order. Our focus in this work is the chiral spin liquid, which breaks time-reversal symmetry and some reflection symmetries of the lattice. We use Y junctions of spin-1/2 Heisenberg chains as building blocks for the honeycomb lattice, where using non-Abelian bosonization we probe the low energy excitations of the bulk in the spin chains. In that picture, the problem is gluing spin currents by imposing chiral boundary conditions. In addition to that, we want to study the instability of the chiral spin liquid phase in the presence of perturbations, such as backscattering processes that may occur at the junctions. We expect that our exact construction may be related to others parton mean-field states with spinon Fermi surfaces.

# First Principle Study of the Surface 2DEG on Perovskite Alkaline Stanates

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The study of conducting transparent oxides has attracted increasing attention in the latest years given their potential technological applications on the field of optoelectronics and their physical properties related with the electron-phonon coupling. The properties that are most desirable on these materials are wide band gaps, which are responsible for the transparency, and high electronic mobility. Recent reports have shown that these properties can be achieved by the perovskite alkaline stanates  $\text{BaSnO}_3$  (BSO)[1] and  $\text{SrSnO}_3$  (SSO)[2]. Moreover, perovskites are well known to show interesting emerging phenomena on their surfaces and interfaces, which does not appear naturally on their bulk form, such as, the two dimensional electron gas (2DEG) at the interface of  $\text{SrTiO}_3/\text{LaAlO}_3$ . More recently, photoemission measurements observe the formation of a 2DEG on the surface of a 1% La-doped BSO thin film [3], where the corresponding electron gas was reported to have a very high mobility.

In order to better understand the electronic structure of the surface of the doped stanates we have performed density functional theory (DFT) calculations for different terminations. For the pristine case (without dopants) we find that the  $\text{SnO}_2$  termination is required to obtain the correct electronic states associated with the 2DEG, where the lowest conduction band comes from the Sn-5s states at surface. This indicates that upon electron doping these states will be filled, giving rise to a surface 2DEG, in good agreement with photoemission data. On the other hand, for the BaO and SrO terminations the opposite occurs. In this case the bottom of the conduction band comes from the bulk, indicating that in these terminations a 2DEG will not appear. The calculated theoretical effective masses of the surface states of BSO and SSO were found to be in good agreement with previous theoretical and experimental results for the bulk values, but our calculations were unable to reproduce the significant smaller values observed by the photo-emission spectroscopy, suggesting that other detailed studies must be carried out in order to better understand the renormalization of the 2DEG effective mass. Finally, for the doped materials we find the most stable configurations lead to the appearance of the 2DEG, without any significant modification of the sub-bands.

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## Generalized symmetries and fractons

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In recent years a new phase of matter named fractons has been discovered. This is a topological phase with very exotic physical properties. One imprint is the presence of excitations with severe restrictions of mobility: isolated quasiparticles are completely immobile, whereas certain bound states can eventually be mobile. This kind of excitation first arose in the context of spin liquids and now is known to appear also in different contexts like elasticity theory and linearized gravity. One approach to studying this unusual state is to use field theoretical models exhibiting generalized symmetries that can lead to conservation laws in agreement with fracton physics. In certain situations these generalized symmetries are so-called higher-form symmetries, namely, symmetries that imply conservation of charges that are  $n$ -forms ( $n$  is bigger than zero, which would be the usual case). Field theories with generalized symmetries exhibit many interesting properties. One can also construct a gauge theory that exhibits this exotic phenomenology. This can be done by using a tensor gauge theory that ultimately describes gapless fracton phases. Such gauge theories have a close connection with gravitational physics and this is a subject of great interest since its discovery. In this work, we present a field theoretical description of generalized symmetries to describe this new state of matter.

## **Kondo screening across a disordered metal-insulator transition**

Igor César de Almeida

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Disorder is always present in real materials, and it may lead to inserting new physics as we break translational invariance. We are motivated by the phosphorous doped silicon (Si:P) semiconductor in this work. Each phosphorus atom contributes one extra electron to the conduction band, which moves to an impurity band close to the bottom of the conduction band. As the density of dopants increases, we observe a metal-insulator transition (MIT). Interestingly, this MIT coexists with the formation of local magnetic moments, leading to a non-trivial thermodynamic response. In this work, we model this impurity band by a tight-binding model with randomly placed sites on a cubic lattice, with the hopping mediated by the insulating silicon background. We characterize the non-interacting MIT via a finite size scaling of the two-point conductance. Then, we add diluted local moments to the problem and investigate their contribution to the thermodynamics as we cross the MIT. The coupling between these magnetic moments and the impurity electrons screen this moment below the Kondo temperature  $T_K$ . Due to disorder, we have a distribution  $P(T_K)$ , with a power-law tail at low energies, which we follow across the MIT. Then, we investigate the screening of two impurities, which also have a direct coupling, via the RKKY interaction and how the random singlet formation competes with the Kondo effect. We construct a  $T=0$  phase diagram as a function of the magnetic couplings, Kondo and RKKY. We follow the thermodynamic responses across the MIT, connecting our results to the phenomenology of Si:P.



# **Formation of spin and charge ordering in the extended Hubbard model during a finite-time quantum quench**

Isaac Martins Carvalho

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We investigate the formation of charge (CDW) and spin (SDW) density waves by starting from a non-interaction state and studying how it evolves in time under a Hamiltonian with finite electronic interactions. We consider the one-dimensional, half-filled extended Hubbard model (EHM) featuring these insulating phases for repulsive interaction, which we solve within time-dependent density matrix renormalization group. By employing linear finite-time quenches in the on-site and nearest-neighbor interactions, we find the existence of impulse, intermediate, and adiabatic regimes of time evolution. In the impulse case, the system remains frozen at its initial state. In the opposite limit of adiabatic evolution, the system follows closely the ground state of the corresponding equilibrium Hamiltonian. Our results indicate that this adiabatic regime is reached with distinct ramping time scales depending on whether the CDW or the SDW is formed: the latter requires smaller times than the former. More interestingly, for the quench towards the CDW ordering, in the intermediate regime that precedes the adiabatic one, we observe that the evolved state includes more entangled states, which correspond to excited states of the equilibrium Hamiltonian. These entangled states are avoided if the quench happens slowly, contributing to the larger time scale observed for the formation of the CDW ordering as compared to the SDW one. Our findings also show that the breaking of the system integrability, by turning on the nearest-neighbor interactions, does not give rise to any significant change in the non-equilibrium behavior within the adiabatic approximation.

# **The phase diagram of the t-t' Hubbard model: a variational auxiliary-field quantum Monte Carlo approach**

Jadson Lucas

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Strong electronic interactions may lead to many phenomena in condensed matter physics, such as the emergence of magnetism, superconductivity, and spin liquid phases. Analyzing their occurrence and eventual effects from unbiased methodologies still is a challenge to theoretical physicists, usually requiring numerical analysis. Within this context, in this work we investigate the Hubbard model on the square lattice, with nearest ( $t$ ) and next-nearest neighbour hopping ( $t'$ ) terms, which is the “standard model” to understand the role of frustration in electronic materials. To this end, we perform state-of-the-art simulations using the Variational Auxiliary Field quantum Monte Carlo (VAFQMC) method. It is a recent methodology that improves the trial variational wave function by systematically adding auxiliary fields to the interaction term, e.g. as done by the Hubbard-Stratonovich transform. Given this, we examine the spin, charge, and pair correlation functions, providing the phase diagram at the half-filling. In particular, we provide details about the competition between the staggered and striped antiferromagnetic phases, as well as the emergence of a spin liquid one at strong coupling.

## Study of CDW suppression of BaBiO<sub>3</sub> in BBO/BTO heterostructures

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Heterostructures and interfaces can be used to tune the balance between the competing orders presented in numerous quantum materials, such as complex perovskite oxides. The perovskite structure is ubiquitous in nature and has a large number of candidates that possess interesting properties, such as superconductivity and magnetoresistance. Two other examples are the BaBiO<sub>3</sub> (BBO) and BaTiO<sub>3</sub> (BTO), with the latter being a well studied ferroelectric, whereas the former is known as a Peierl's insulator which upon hole doping manifests superconductivity.

In this work, we have studied the lattice distortions and electronic properties of BBO/BTO superlattices in the ultrafin limit. By means of density functional theory calculations we have investigated the properties of BBO( $X$  u.c.)/BTO ( $Y$  u.c.) superlattices, with  $X, Y = 2$  and  $4$ . Our results show that the most stable energetic configuration is obtained when BBO has a Glazer's distortion  $a_0a_0c^-$ , followed by a configuration where the BBO exhibits a  $a_0a_0c^+$  distortion. More important, we find that the confinement of BBO does not lead to a suppression of the CDW phase. Furthermore, we do not find any considerable charge transfer between BTO and BBO, which partially explains the robustness of the breathing distortions in the ultrathin limit. Regarding the BTO structure, our results indicate that for  $2$  u.c. there is no spontaneous ferroelectricity. Finally, our calculated bandstructures indicate that the observed distortions lead to the stabilization of the insulating bond-disproportionated phase.

## **Entanglement on the Hubbard model on a ladder**

João Pedro Gama D'Elia

(Universidade Federal do Rio de Janeiro)

The study of entanglement on condensed matter systems has become an important tool for understanding the properties and evolution of quantum states, in particular for the identification of quantum phase transitions (QPT). Different entanglement quantifiers such as the Von Neumann entropy and the concurrence are being extensively studied for their ability to correctly identify those transitions. Other quantities like the fidelity susceptibility, have been shown to identify infinite order phase transitions in the XXZ Heisenberg model, and thus proven a useful tool for the study of quantum phase transitions.

We use the Lanczos method to calculate the ground state of the Hubbard model on ladders at half filling. We consider different values for the hopping along ( $t$ ) and perpendicular ( $t_{\text{perp}}$ ) to the rungs and study the effect of varying the ratio  $t/t_{\text{perp}}$ , as well as the interaction strength. We study QPT probing the entanglement between different subsystems of the ladder by calculating the Von Neumann entropy and concurrence as well as the fidelity susceptibility. We also calculate spin-spin and charge-charge correlation function to identify the different phases.

# RKKY interaction mediated by Weyl Fermi arcs

João Victor Ferreira Alves

(IFUSP)

The interest in unconventional quasi-particles in condensed matter systems has been renewed in the last decade, fueled by the avalanche of experimental data on topological semimetals, also referred to as Weyl semimetals [1]. These states refer to topological 3D band-crossings characterized by the degeneracy and the functional form of these crossings. Surface states known as Fermi arcs may appear connecting pairs of these so called “topological nodes”, Fermi arcs have deep penetration to the bulk, in contrast with surface states of other topological systems.

By inserting magnetic impurities in these systems, we expect a long-range coupling between the impurities in the form of the famous Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction [2, 3]. In this work, we theoretically study how the Fermi arcs in Weyl systems can mediate (and perhaps enhance) RKKY interactions between impurities located on surfaces (even opposite surfaces) and in the bulk of Weyl semimetals.

Based on the description of long-range coupling between magnetic impurities in a metallic nanowire [4], we analytically study the generalized case for an 3D Dirac Hamiltonian in the form  $H\mathbf{k} = \epsilon_0\sigma_0 + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}$ , where  $\epsilon_0$  is the Fermi energy,  $\mathbf{d}$  is an arbitrary 3D vector field in  $\mathbf{k}$ -space and  $(\sigma_0, \boldsymbol{\sigma})$  is the 4-vector of Pauli matrices. This choice gives a Dirac-like spectrum  $E_{\mathbf{k}} = \epsilon_0 \pm |\mathbf{d}(\mathbf{k})|$ , with Weyl nodes at the points where and a linear dispersion around these points. We consider coupling between our system and two magnetic impurities, using a interaction term inspired by [4].

By writing the interaction operators in the basis that diagonalizes the Hamiltonian, we have found that, in second order perturbation theory, there are complex interaction terms between all 3 spin directions of both impurities (9 terms, in total). These terms can be classified as generalizations of RKKY, Ising and Dzyaloshinskii–Moriya interactions. In addition, we compared these analytical results with numerical calculations for a minimal Weyl model with only two Weyl nodes, which can be written in a tight-binding form as :

$$\mathbf{d}(\mathbf{k}) = \{2t_x(\cos(k_x a) - \cos(k_0 a)) + m(2 - \cos(k_y a) - \cos(k_z a)), 2t_y \sin(k_y a), 2t_z \sin(k_z a)\} .$$

By discretizing the model and placing magnetic impurities at opposite surfaces, we can numerically obtain the leading contribution of the effective RKKY long-range interaction through the bulk and Fermi arc states as a function of the surface separation.

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## **Subsystem trace distances of random states**

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Imagine one of two known random pure states composed of  $N$  qubits has been randomly selected. What is the probability that performing an optimally chosen experiment on  $N_A$  of the qubits we correctly identify the selected state? In this work we give an answer to this question calculating the average subsystem trace distances of random pure states. Employing a replica trick we derive analytical results which we check against numerical simulations.

# **Magnetic fluctuations and superconducting order in magic angle twisted bilayer graphene**

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Recently, the exploration of 2D materials has called the attention of the strong correlated matter community, specially graphene-derived 2D systems, such as monolayers, bilayers, trilayers, and double-bilayers. They are very controllable platforms in which one can produce very rich phase diagrams changing doping without produce new samples. Specifically, twisted bilayer graphene (TBG) was observed to present correlated insulating and even superconducting ground states at the so called twist magic angles, which can be used to tune superconductivity applying a current in the bilayer. In this ongoing work, we model TBG studying its background magnetic fluctuations aiming to describe the superconducting pairing mechanism of the system. We calculate spin and charge susceptibilities making use of the RPA approach. The pairing mechanism will be determined studying the pair vertex elements. As already observed in experiment, we expect to describe the consequences of the chiral d-wave Cooper pairs present in TBG at the lowest magic angle, and give a step further numerically describing the phase diagram of the system through a calculation of the interaction matrix elements using a recently developed atomistic model.



## Entanglement studies of the Heisenberg J1-J2

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The one-dimensional Heisenberg model with competing nearest and next-nearest-neighbor interactions (denoted by  $J_1$  and  $J_2$ , respectively) display several quantum critical points (QCP's) in the ground state, depending on the ratio  $\alpha = J_2/J_1$ , with  $J_2 > 0$ . These QCP's separate different kinds of magnetically ordered, or quasi-ordered, phases, which have been theoretically studied with the aid of several methods; In addition, the possibility of experimentally probing these unusual magnetic phases have also boosted the interest in the synthesis and characterization of related materials.

Further insight into the nature of these phases, as well as into the nature of the QCP's may be obtained by examining the amount of entanglement as a function of  $\alpha$ . To this end, we may use entanglement entropy, which has proved to be a powerful tool to discuss quantum phase transitions.

In what follows, we first discuss exact diagonalization for the Heisenberg model with nearest-neighbor (NN) interactions as well as we present correlation function and entanglement entropy calculations.

## **DFT calculations applied to one-dimensional superlattices**

Lucas Gimenes

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Technological devices involving nanostructured materials, such as superlattices, have become a reality, especially due to the advance of experimental control in the deposition of atoms or molecules for composing such nanostructures. However, for an optimal use of these nanostructured devices, theoretical investigation of their properties is necessary requiring undoubtedly the quantum treatment of complex systems. In this context, the Density Functional Theory (DFT) stands out as a powerful tool for the study of the interacting and inhomogeneous nanostructures. In this project, we investigate the physical properties of superlattices described by the Hubbard Model via DFT calculations. Among the properties that will be analyzed as a function of the several parameters of the superlattices are the energy, the density profile and the entanglement entropy.

# Magnetism and metal-to-insulator transitions in the anisotropic Kagome lattice

Lucas Oliveira Lima

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In the study of magnetism, the occurrence of flat bands is of particular interest due to the enhancement of spin correlations. Amongst these systems, the Lieb and Kagome lattices have interesting features. Both exhibit three bands, but differing in the energy of the flat band relative to the dispersive ones: in-between (Lieb) or at the top (Kagome). Such difference for the noninteracting electronic structure leads to stark distinct physical responses when taking into account electron-electron interactions. Indeed, while the ground state of the Hubbard model on the Lieb lattice exhibits an ordered ferrimagnetic phase at the half-filling, frustration effects in the Kagome lattice lead to a disordered magnetic phase at the same filling, with the occurrence of a metal-to-insulator Mott transition at a finite interaction strength,  $U_c$ . Interestingly, both geometries are topologically connected, i.e. we are able to generate the Lieb lattice from the Kagome one, and vice versa, simply by adjusting an anisotropy hopping parameter  $t'/t$ , such that  $t'/t = 0$  corresponds to Lieb's lattice and  $t'/t = 1$  to Kagome. Despite the properties of both geometries having been individually and extensively scrutinised, the “transition” between them has barely been examined, particularly away from half-filling. In view of this, here we investigate the Hubbard model in the anisotropic “Lieb-Kagome” lattice at different fillings using two different methodologies: (i) mean-field Hartree-Fock approximations, and (ii) Determinant Quantum Monte Carlo (DQMC) simulations. Through the latter, we investigate the nature of the spin correlations and probe long-range order through the structure factor analysis; we also examine unequal-time current-current correlation functions, as well as density of states and spectral functions, in order to discuss the metal-insulator transitions. The DQMC data are supplemented by analyses through the Hartree-Fock approximation, especially at those fillings in which the infamous “minus-sign problem” precludes conclusions to be drawn at very low temperatures. In so doing we have been able to propose phase diagrams for the magnetic and transport properties on both sides of this “transition”, for different fermionic densities.

# **Continued fractions method for 1D quantum scattering by periodic building blocks**

Luna Rhaine Nascimento Oliveira

(UFPR)

Nonrelativistic quantum scattering in one-dimensional networks is an essential problem in physics, not just due to the several mathematical techniques that emerged intending to solve the issue like the transfer matrix method, the most used one, but due to the variety of applications, like those in condensed matter and quantum computation. In this work, we propose an analytic method that uses the exact Green function to obtain recurrence relations for the scattering coefficients of a block of compact support potentials. With it, we show that is possible to employ continued fractions to determine the transmission and reflection coefficients for any barrier formed by a sequence of  $N$  building blocks, where  $N$  can be a large number, larger than any previous method. Furthermore, our approach enables the shaping of building blocks formed by any combination of potentials in a very intuitive way. Once they are exact and analytically solved potentials we use Dirac delta, square wall, and trapezoidal wall as a basis, and we study the scattering effects of the possible combinations between them, especially the behavior of the transmission probability for different potential parameters and incident wavenumbers.

## **Exploring via density functional theory calculations cold atoms properties**

Marina Sanino

(UNESP)

Technological devices involving nanostructured materials have become reality, especially due to advances in experimental control, both in cold atom systems and in the deposition of atoms or molecules to compose nanostructures. Theoretically, one finds the challenges of realizing the quantum treatment of complex systems. In this context, Density Functional Theory (DFT) stands out as one of the powerful computational methods for the study of nanostructures. In this project, we propose to investigate the physical properties of cold atoms described by the Hubbard model with harmonical confinement via DFT calculations. Among the properties that will be analyzed are the energy, density profile, and entanglement entropy. The latter, in particular, is a fundamental ingredient in Quantum Information Theory and, therefore, essential for the development of new devices for processing quantum information.

## **Continuous measurement dynamics of a single q-bit**

Matheus Monteiro

(Centro Brasileiro de Pesquisas Físicas (CBPF))

In nature, there is no quantum system perfectly isolated from its surrounding, neither instantaneous measurements in time: those arise only as idealizations and meanings to understand nature on its principles. In this work, we investigate the dynamics of a fairly simple measured quantum system, that is, of a single q-bit continuously measured in time. We derive the dynamical equation for the measured q-bit, a stochastic Schrodinger equation (SSE), from coupling the system to ancilla q-bits which are projectively measured. We then calculate the q-bit's purity as a function of time from numerical solutions of the SSE. We compare results for average and typical purities, where averages are done over different measurement histories, for purifications from continuous and projective measurements on  $N$  decoupled q-bits.

## The two-dimensional $t$ - $t'$ Holstein model

Maykon Vinicius Monteiro de Araujo

(Federal University of Piauí)

The competition and interplay between charge-density wave and superconductivity have become a central subject for quasi-two-dimensional compounds. Some of these materials, such as the transition-metal dichalcogenides, exhibit strong electron-phonon coupling, an interaction that may favor both phases, depending on the external parameters, such as hydrostatic pressure. In view of this, here we analyze the single-band  $t$ - $t'$  Holstein model in the square lattice, adding a next-nearest neighbor hopping  $t'$  in order to play the role of the external pressure. To this end, we perform unbiased quantum Monte Carlo simulations with an efficient inversion sampling technique appropriately devised for this model. Such a methodology drastically reduces the autocorrelation time and increases the efficiency of the Monte Carlo approach. By investigating the charge-charge correlation functions, we obtain the behavior of the critical temperature as a function of  $t'$  and, from compressibility analysis, we show that a first-order metal-to-insulator phase transition occurs. We also provide a low-temperature phase diagram for the model. A variety of interesting phenomena, such as metal-to-insulator transitions, superconductivity, or spinliquid phases. With the advent of optical lattices, in which ultracold atoms emulate fermionic interacting systems, the Hubbard model has been experimentally studied in an unprecedented way, opening an avenue to investigate these phenomena. By adjusting the parameters of the counterpropagating laser beams one may be able to control the hopping amplitude, allowing one to interpolate from a square lattice to a triangular one, and, in turn, to further examine the nature of the phases emerging in frustrated systems. However, since reducing temperature is an experimental challenge, theoretical analyses by unbiased methodologies may provide further insights into these systems, and shed light on experimental features of ultracold atoms. In view of this, in the present work, we investigate the repulsive Hubbard model on the anisotropic triangular lattice by unbiased quantum Monte Carlo simulations. We examine its thermodynamic properties, as well as the magnetic and transport properties of the system at finite temperatures. From these results, we discuss the possible occurrence of metal-to-insulator transitions and spin liquid phases.

# **Magneto-transport and Shubnikov-de Haas oscillations in the layered ternary telluride topological semimetal candidate Ta<sub>3</sub>SiTe<sub>6</sub>**

Muhammad Naveed

(University of São Paulo)

Topological semimetals characterize a unique class of quantum materials hosting Dirac/Weyl fermions. The important features of topological fermions can be exhibited by quantum oscillations. Here, we report the magnetoresistance and Shubnikov-de Haas (SdH) quantum oscillation of longitudinal resistance in the single crystal of topological semimetal candidate Ta<sub>3</sub>SiTe<sub>6</sub> with a magnetic field up to 38 T. The periodic amplitude of the oscillations shows related information about the Fermi surface. The fast Fourier transformation spectra represent a single oscillatory frequency. The analysis of the oscillations shows the Fermi pocket with a cross sectional area of  $0.13 \text{ \AA}^2$ . Combining magneto-transport measurements and the first-principles calculation, we find that these oscillations come from the hole pocket. Hall resistivity and the SdH oscillations recommend that Ta<sub>3</sub>SiTe<sub>6</sub> is a hole dominated system.



## **Quantum Phase Transitions in distinct disordered landscapes**

Murilo Alexandre Garcia Silva

(São Paulo State University)

Entanglement is a well established tool for detecting and characterizing quantum phase transitions. In disordered and interacting nanostructures, the Mott and Anderson localization have been explored via the linear entropy, a proper measure for quantifying bipartite entanglement of pure states. Here we compare different disorder landscapes commonly used to simulate disordered nanosystems and their connections to the Mott-Anderson physics. We quantify the linear entropy via density-functional theory (DFT) calculations for the one-dimensional Hubbard model.

## Surface thermal transport in PbTe: 3-omega technique

Murilo Balhester de Andrade

(USP)

Tin telluride (SnTe) has recently received growing interest as a thermoelectric material because of its potential to substitute the toxic PbTe [1]. Interestingly, SnTe has been also classified as topological crystalline insulator [2], bringing a fresh view on this class of monochalcogenides. In order to identify the role of non-trivial topology in determining the thermoelectric performance, a comparative investigation of surface thermal transport in PbTe and SnTe might be insightful. Surface thermal conductivity can be experimentally studied by using the  $3\omega$ -technique [3], a method based on an AC excitation supplied to an appropriate heater/sensor deposited on a specimen's surface, allowing for the determination of thin films and bulk thermal conductivity. This method presents the advantage of low dependence on black-body radiation and sample geometry, unlike the standard steady-state two-thermometers/one-heater method, which requires higher precision on samples size and preparation, control of the temperature gradient across it and is highly sensible to black-body radiation at higher temperatures [3]. On the other hand, the challenge in the  $3\omega$  technique resides on the heater previous design, study and deposition, and on the settings of the electronic circuitry. In this context, we discuss the feasibility of the  $3\omega$  method applied to monochalcogenides and we present our last results in a measurement of thermal transport of single crystalline PbTe at room temperature.

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# **Interaction effects on the spinless one-dimensional Su-Schrieffer-Heeger model via exact diagonalization**

Pedro Barreto

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The one-dimensional spinless Su-Schrieffer-Heeger model (SSH 1d) is the simplest system to exhibit a topological insulator phase. It consists of a chain with staggered hopping, mediated by a modulation of the hopping integral.

As probes of the topological transition, the SSH 1d model shows excitation gap closing process, concomitant with a change in the Zak phase, which is a gauge invariant cumulant, from trivial (zero) to topological (non-zero).

Regarding topological insulators, there is an open question concerning the effects of interactions on the robustness of topological phases. In this work, we investigate the SSH 1d model with nearest-neighbours coulomb repulsion.

To investigate this, we use exact diagonalization methods to solve the SSH model on finite size chains. We calculate the excitation gap, the charge density wave structure factor, the nearest-neighbour correlation functions, the Zak phase and the fidelity metric. The results are compiled on a phase diagram.

# DIMENSIONAL CROSSOVER IN THE THREE-DIMENSIONAL ATTRACTIVE HUBBARD MODEL

RODRIGO ALVES FONTENELE

(UFRJ)

The attractive Hubbard model (AHM) describes superconductivity driven by on-site pairing interactions. At half filling, the critical temperature,  $T_c$ , is zero for the square lattice by virtue of the Mermin-Wagner theorem, while it is finite in three dimensions. With the continuing development of optical lattices experiments, in which ultracold fermionic atoms are loaded and the interaction amongst them is controlled through an external magnetic field, the attractive Hubbard model has been experimentally studied in an unprecedented way. By adjusting the parameters of the counterpropagating laser beams one may be able to control the hopping amplitude between square planes, so that the crossover between two and three-dimensional behaviours could be followed. In solid state materials this could be achieved by applying uniaxial pressure, which would similarly introduce anisotropy in the hopping parameters. In view of this, a systematic study of the critical temperature as a function of the interplane hopping,  $t_{\perp}$ , is certainly of interest, especially due to the fact that the lowest temperatures achieved in the experiments are still somewhat higher than those predicted theoretically for the isotropic model. Any indication of routes towards increasing critical temperatures should therefore be of great help to experimentalists. With this in mind we have performed Quantum Monte Carlo simulations on the three-dimensional model with axially anisotropic hopping; we allow the ratio  $\alpha \equiv t_{\perp}/t$ , where  $t$  is the planar hopping amplitude, to vary between  $\alpha < 1$  and  $\alpha > 1$ . We discuss the behaviour of  $T_c$  thus obtained, as well as the thermal behaviour of correlation functions, double occupancy, and other experimentally measurable quantities.

## **Magnetic order and RKKY interaction in metallic quasicrystals**

Ronaldo Araújo

(Universidade de São Paulo)

Motivated by the non-Fermi-liquid behavior observed in quasicrystals and their approximants, we study a simple model for magnetic impurities placed at sites with different local environments coupled by the RKKY interaction. We use the tight-binding model for different sizes of Ammann-Beenker tiling to calculate these interactions. We find that the magnetic interaction strongly depends on the distance between the impurities and the local environment. The spin relaxation rate  $T_1$  decreases with the size of the quasicrystal approximant, as expected from the experimental results. In second, we study Ising spins coupled with RKKY interactions using Monte Carlo simulations. Despite the frustrated interaction, the spins in the octagonal tiling freeze in an antiferromagnetic-like state, but a spin-glass behavior has been found in icosahedral quasicrystals in experiments.

# Exceptional Points in Fermi Liquids with multipolar interactions

Rui Aquino dos Santos da Silva

(UERJ)

The Landau Theory of Fermi liquids describes the dynamics of quasi-particles, with energy very close to the Fermi energy, interacting with coherent particle-hole states. Collective modes are not a closed system, since they can exchange energy with individual quasi-particles. In this way, damped modes appear in the spectrum. This mechanism, known as “Landau damping”, trigger non-Hermitian degeneracies, called exceptional points.

Exceptional points are singularities of the Hilbert space characterized by a level degeneracy where not only the energy eigenvalues coalesce but also the eigenvectors. Therefore, at these special points of the parameter space, the Hamiltonian cannot be diagonalized.

Quasi-particle interactions are parametrized by a set of Landau parameters  $\{F_0, F_1, F_2, \dots\}$ , that codify different angular momentum channels. Most of the results on thermodynamic and transport properties of Fermi liquids are based in the simplest model where only density ( $F_0$ ) interactions are considered. Usually, in Galilean invariant Fermi Liquids, dipolar interactions ( $F_1$ ) renormalizes the effective mass,  $m^* = (1+F_1)m$ . So, systems with electron mass enhancement, as GaAs/AlGaAs quantum

wells or MgZnO/ZnO heterojunctions could have  $F_1 = 0$ . In addition, Fermi liquids quadrupolar interactions ( $F_2$ ) began to call the attention of the condensed matter community because it is the simplest model supporting an isotropic-nematic transition. Nematic fluctuations play a crucial role in several strongly correlated systems, such as cuprates and Fe-based superconductors and a variety of Quantum Hall Effects.

In this work, we show the existence of exceptional points in the collective mode spectrum of Fermi liquids with multipolar interactions. Using multidimensional bosonization and a real space renormalization group approach we compute the dynamic quadrupolar susceptibility. Through a careful analysis of its analytical properties, we show that, in the weak attractive region, two stable collective modes coalesce to an exceptional point. We completely characterize this singularity, explicitly showing its

topological properties. Experimental signatures are discussed in two different set-ups: pump-probe spectroscopy, to observe the dynamic response in the time domain; and in the AC conductivity of Fermi liquids with dipolar and quadrupolar interactions in a narrow slab. We show that the finite size of the slab imprints clear signatures of the collective mode spectrum in the conductivity as well as in the dephasing between the electric field and the current density.

# **An auxiliary field Quantum Monte Carlo approach to the extended Hubbard model**

Sebastião Sousa

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The Hubbard model is one of the simplest models describing interactions between electrons in strongly correlated systems, and despite dominance of the on-site term,  $U$ , Hubbard's original paper already discussed weaker longer ranged interactions between electrons. In this hierarchy, the nearest neighbour coupling,  $V$ , gives rise to interesting effects due to the competition with  $U$ . When  $U, V > 0$ , the on-site term favours antiferromagnetism (AFM) while the extended interaction favours the formation of a charge density wave (CDW). The cases with at least one of the interactions being attractive leads to superconductivity competing with the above phases. Actually, one of the proposals to describe high temperature superconductivity (SUC) is based on this extended Hubbard model (EHM) with  $U > 0$  and  $V < 0$ . In the present work we use Determinantal Quantum Monte Carlo (DQMC) simulations to analyse some properties of the EHM on a square lattice. The cases where  $U$  and  $V$  can be positive/negative are analysed, displaying phase separation and SUC, in addition to the AFM and CDW phases. We determine the leading pairing symmetries within the SUC phases, and discuss the  $U$  vs  $V$  phase diagram for the model. We also report on the use of the infamous 'minus-sign problem' as an additional tool to pinpoint some of the quantum phase transitions of the model.

# **Analysis of entanglement measures for probing quantum phase transitions in superlattices**

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Superlattices are systems in which materials of different compositions or structures share the same interface and present a periodic alternation between them. Quantum phase transitions are expected to emerge in such superlattices, driven for example by the periodic potential. Entanglement — one of the most intriguing phenomena in quantum mechanics — has played an important role in detecting and characterizing quantum phase transitions. Here we investigate the quantum phase transitions via entanglement measures in superlattices described by the one-dimensional Hubbard model. The periodicity is simulated through the periodic variation of the external potential. We perform density-matrix renormalization group calculations to quantify average single-site entanglement: the bipartite entanglement between a single site with respect to the remaining lattice sites averaged over the sites in the ground state. In particular we calculate the von Neumann entropy and the linear entropy. Both measures are related to each other, since the linear entropy corresponds to the linear term of the expansion of the von Neumann measure. However our results reveal that in some cases they may differ even qualitatively. We find that linear entropy is, in some cases, much less sensitive to quantum phase transitions in homogeneous, superlattice, and disordered systems than the von Neumann entropy.



## Effect of Mn concentration on vibrational modes in CdMnTe alloys

Thamires Cordeiro Soares

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The diluted magnetic semiconductors (DMS) are a class of materials obtained by introducing magnetic impurities into semiconductor structures. This assigns magnetic properties as well as allows the proper control of the energy gap of these materials [1]. Such modifications make the SMDs promising materials for various applications in optoelectronics. An example of this kind of material is the  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  (CMT), which is obtained by replacing the cadmium atom for manganese, where  $x$  represents the molar fraction of Mn. The pure CdTe is a group II-VI compound that has a direct energy bandgap of  $\approx 1,5$  eV, which allows for this material to absorb photons in the visible spectrum region of light and makes it a widely used option in technologies such as photovoltaic cells and infrared detectors. The introduction of manganese ions allows new applications for this structure, such as in gamma-ray detectors, magnetic field sensors and spin-based memories [2-4]. In the present work, we investigated the dependence of the main CMT longitudinal Raman active optical modes on the manganese concentration. For measurements of lattice parameters and manganese concentration it was applied, respectively, energy dispersive X-Ray spectroscopy (EDS) and X-rays diffraction (XRD) techniques. It was possible to show that Vegard's law is obeyed very closely, for manganese concentration ranging from  $x = 0$  (pristine CdTe) up to  $x = 0.65$ . A pronounced redshift and blueshift occur, respectively, for the CdTe-like and MnTe-like longitudinal-optical phonon modes, as the concentration of Mn increases. Such dependence is linear when the energy of the incident photons is higher than the optical bandgap, in agreement with previous works [4]. However, when the incident photon energy approaches from the optical band gap, this linear behavior is not observed. This result suggests that the polarization of the medium does not vary linearly with  $x$  at low frequencies, and we show that it may be associated with an increase in the screening effect of the dipole moments as the manganese concentration increases.

# Scanning tunneling spectroscopy of Ising anyons in Kitaev materials

Tim Bauer

(Heinrich-Heine-Universität Düsseldorf and IIP UFRN)

Recent and widely discussed measurements in Kitaev materials indicate the existence of a non-Abelian spin liquid phase that is expected to arise in spin-orbit assisted Mott insulators with orbital degeneracy. The candidate materials can be exfoliated down to monolayer thickness and thus possibly studied using spin-polarized tunneling probes. Here, we derive the effective cotunneling Hamiltonian from the microscopic Hubbard-Kanamori model that gives rise to the Kitaev interactions at low energies. The effective exchange coupling reveals that a measurement of the tunneling conductance gives access to the dynamical spin structure factor (DSSF). We use exact results for the DSSF in the pure Kitaev model to probe signatures of Majorana zero modes in a scanning tunneling spectroscopy experiment.

## Interface and confinement effects in YBCO/LSMO heterostructures

Vitor Assunção

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Oxide heterostructures have attracted increasing attention due to the emergence of new phenomena at interfaces and also due to the new ability to control the different interactions and engineering new electronic phases in strongly correlated oxides. More recently, it was demonstrated that the number of manganite layers of YBCO(YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub> )/LCMO(La<sub>1-x</sub>Ca<sub>x</sub>MnO<sub>3</sub>) superlattices can be used to control the strength of correlations in the cuprate, leading to superconductor-to-insulator transitions [1].

In this work we have studied the structural, magnetic, and electronic properties of YBCO(YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub> )/LSMO(La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub>) heterostructures by means of density functional theory (DFT) calculations and its DFT+U extension. We find that LSMO transfer electrons to YBCO and gives rise to residual local moments ( $\sim 0.06$  mb/Cu atom) on the copper atoms near the interface. These local moments couple ferromagnetically within the CuO<sub>2</sub> planes. Our calculations indicate that the induced local moments depends on the local structure of the interface and on the amount of charge which is transferred between the oxides. The obtained density of states indicates a suppression of spectral weight of Cu-3d states around the Fermi energy as a result of residual ferromagnetism, charge transfer, and structural distortions. The interface Cu-O-Mn bond distance is affected by changing the termination of YBCO from the CuO<sub>2</sub> planes to the CuO chains which we believe is connected with the changes in charge transfer. Moreover, we find a magnetic 'dead layer' configuration at LSMO near the interface for both terminations, though its existence does not change the in-plane ferromagnetism induced in the copper atoms.

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# **Vortices in a parity-invariant Maxwell-Chern-Simons model**

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In this work we propose a parity-invariant Maxwell-Chern-Simons  $U(1) \times U(1)$  model coupled with two charged scalar fields in 2+1 dimensions, and show that it admits finite-energy topological vortices. We describe the main features of the model and find explicit numerical solutions for the equations of motion, considering different sets of parameters and analyzing some interesting particular regimes. We remark that the structure of the theory follows naturally from the requirement of parity invariance, a symmetry that is rarely envisaged in the context of Chern-Simons theories. Another distinctive aspect is that the vortices found here are characterized by two integer numbers.

## **Thermoelectric properties in the 2D Hubbard Model**

Willdauany Cristina

(Universidade Federal do Rio de Janeiro -UFRJ)

Thermoelectric effects are responsible for the direct conversion of thermal energy into electrical energy and vice versa and have a wide range of technological applications. The thermoelectric performance of a material reflects its ability to convert voltage into temperature gradients while minimizing the irreversible effects of Joule heating and thermal conduction and is directly related to the Seebeck coefficient or thermopower. We here calculate the Seebeck coefficient for the two-dimensional Hubbard model on a square lattice for different temperatures, densities and values of the interaction strength. We also calculate the conductivity for the same set of parameters and probe how the thermopower and charge transport are related in the presence of strong correlations.