Condensed Matter Theory in the Metropolis

Book of Abstracts

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Talks

André Vieira - USP

Emergent dimerization and localization in disordered quantum chains

We uncover a novel mechanism for inducing a gapful phase in interacting many-body quantum chains. The mechanism is nonperturbative, being triggered only in the presence of both strong interactions and strong aperiodic (disordered) modulation. In the context of the critical antiferromagnetic spin-1/2 XXZ chain, we identify an emerging dimerization, which removes the system from criticality and stabilizes the novel phase. This mechanism is shown to be quite general in strongly interacting quantum chains in the presence of strongly modulated quasiperiodic disorder, which is, surprisingly, perturbatively irrelevant. Finally, we also characterize the associated quantum phase transition via the corresponding critical exponents and thermodynamic properties.

Eduardo Miranda - UNICAMP

Abandoned by Bloch: the dominance of disorder

Among the pillars of solid state physics is Bloch's theorem and its consequences: itinerant excitations, quasi-particles, quasi-homogeneity, unique physical properties and responses, etc. We are so accustomed to these concepts that we often do not inquire about their applicability range. Often, small amounts of disorder can be accommodated through small modifications of clean theories, but this need not always be the case. Sixty years ago, Anderson showed that single-particle states can go from extended to localized with increasing disorder. Since then, many examples have been found in which disorder has to be treated on its own terms. I will show results from recent years which illustrate this point of view. Emphasis will be given to instances where typical values of physical quantities differ by many orders of magnitude from their average values.

Jose Hoyos - USP

Cluster-glass phase in pyrochlore XY antiferromagnets with quenched disorder

We study the impact of quenched disorder (random exchange couplings or site dilution) on easy-plane pyrochlore antiferromagnets. In the clean system, order-by-disorder selects a magnetically ordered state from a classically degenerate manifold. In the presence of randomness, however, different orders can be chosen locally depending on details of the disorder configuration. Using a combination of analytical considerations and classical Monte-Carlo simulations, we argue that any long-range-ordered magnetic state is destroyed beyond a critical level of randomness where the system breaks into magnetic domains due to random exchange anisotropies, becoming, therefore, a glass of spin clusters, in accordance with the available experimental data. These random anisotropies originate from off-diagonal exchange couplings in the microscopic Hamiltonian, establishing their relevance to other magnets with strong spin-orbit coupling.

Tobias Micklitz - CBPF

On localization in Fock-space

In the talk we discuss recent field theory efforts to address many-body localization.

Francisco Rouxinol - UNICAMP

Quantum Information and Quantum Sensing Applications using Macroscopic Scale Elements

Techniques to observe non-classical behavior of micro- and nano- scale mechanical structures, which are normally well described by classical laws of physics, has received considerable attention in recent years because of the potential to use these systems as elements in quantum computing and quantum communication architectures, and for fundamental studies of the quantum-classical boundary. One important route for observing such behavior is the coupling of micro- and nanomechanical resonators to optical and microwave cavities and superconducting qubits. In this talk, we will give an overview of the field, and discuss our efforts, at UNICAMP, toward devising an electromechanical circuit to strongly couple a nanomechanical resonator to a superconducting qubit and a microwave cavity. It is expected that such hybrid systems could be an import platform to enable the production and measurement of a diversity of non-classical states of nanoscale structures; making then a potentially important element for quantum processing architectures and testing quantum behavior in new limits.

Juarez L. F. Da Silva - USP

First-Principles Investigation of Chalcogenides Materials: From Nanoflakes to 2D Solids.

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Two-dimensional chalcogenides have attracted great attention due to their unique properties and several promising applications along a wide range of fields, e.g., thin-film solar cells, CO2 reduction, biomedicine, etc. In our group, Quantum Theory of Nanomateriais - QTNano (https://www.facebook.com/QTNano/), we have focused on the study of 2D dichalcogenides [1,2,3,4], which spread from nanoflakes to 2D solids, as well as quaternary chalcogenides with the aim to tune the electronic properties. In this talk, we will report our recent highlights, which spread from the formation of 2D nanoflakes [3,4] to the stability mechanism in quaternary chalcogenides [1,2].

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Helena Petrili - USP

Cedric Leao - UFABC

Caetano Miranda - USP

Leandro Seixas - Mackenzie

Edison Z. da Silva - UNICAMP

Double Rainbow and the Physics of Clusters: Computer Simulations Meets Experiments

A novel process, the formation and growth of metallic Ag nanowires (NWs) and nanoparticles (NPs) on a-Ag2WO4 upon electron beam irradiation has been discovered and was extensively investigated by different experimental techniques including transmission electron microscopy (TEM) [1-3]. Nucleation and formation of metallic Ag initiates when Ag atoms diffuse from the bulk to the surface. Ag metallic NWs grow on a-Ag2WO4, further observation showed also the formation of Ag NPs during exposition to the electron beam [4]. The present work concentrates in the study and the understanding of physical processes that occur with these new Ag NPs and their interaction. The experiments found the formation of Ag NPs of sizes from 2 to 10 nm. These NPs produced in vacuum, show very interesting behavior displaying coalescence effects [5] where two nearby NPs meet forming other large particles. Mie theory that explains the formation of the Double Rainbow is also responsible for surface plasmon resonance (SPR) effects which explains observed coalescence processes with the NPs. Associating theory and computer simulations we model this evolution process that is driven by SPR due to the electron beam, presenting new and interesting results that help the understanding of the experiments.

Work is supported by CNPq, CAPES and FAPESP. CENAPAD-SP and IFGW are acknowledged for computer time.

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Maurice de Koning - UNICAMP

Glassy Dynamics at Pre-melted Grain Boundaries in Ice Ih

Using first-principles and classical molecular dynamics simulations, we study pre-melting phenomena in pristine grain boundaries (GBs) in proton-disordered hexagonal ice Ih at temperatures just below the melting point Tm. The results are consistent with experimental estimates for the pre-melt layer thickness of low-disorder impurity-free GBs and provide key insight into the mobility of water molecules in the pre-melted layers. In particular, the translational motion of the water molecules is found to be sub-diffusive for time scales longer than 10 ns. Furthermore, it is well-described by a continuous-time random walk model characterized by a waiting-time distribution with a power-law decay, suggesting that the dynamics in the pre-melt layers at GBs in ice I is glassy in nature, even at temperatures close to Tm.

Luana Pedrosa - UFABC

Luis Gregorio Dias - USP

J. Carlos Egues - USP

Topological and non-topological edge states in quantum dots and Chern Insulators

Common wisdom has it that edge states appear only in topological systems, e.g., topological insulators and topological superconductors. In this talk I will discuss edge states in topological and non-topological InAsBi quantum dots described by a confined Bernevig-Hughes-Zhang model. Interestingly we find that these quantum dots exhibit protected helical edges states both in the topological and non-topological regimes [1]. We also investigate edge states in Chern insulators and find that they display trivial edge states not arising from band topology (Chern number) [2]. We identify the approximate chiral symmetry of the Chern insulator (exact only in the nodal semimetal) as the relevant ingredient behind the appearance of these trivial edge states. This work was supported by CNPq, CAPES, UFRN/MEC, FAPESP, PRP-USP/Q-NANO, German Science Foundation (DFG) via Grant No. SFB 1170 “ToCoTronics” and the ENB Graduate School on Topological Insulators and the Center for Emergent Materials, and NSF MRSEC under Award No. DMR-1420451.

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Belita Koiller - UFRJ

Atomically placed P in Si as quantum simulators and transport-based devices*

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Atomically precise placement of dopants in Si permits creating P nanowires by design. High- resolution images show that these wires are few atoms wide with some positioning disorder with respect to the Si structure sites, which is expected to lead to electronic localization. Experiments, however, report good transport properties in quasi-1D P nanoribbons. We investigate their electronic properties using an effective single-particle approach based on a linear combination of donor orbitals (LCDO), keeping the ground state donor orbitals' oscillatory behavior due to interference among the states at the Si conduction band minima. Our model for the P positioning errors accounts for the presently achievable placement precision [1].

For monatomic width chains, where correlation effects should be stronger than for wider chains , we show that electronic properties of donor nanowires in Si can be controlled by design to emulate Hubbard systems, even allowing for some disorder effects[2] .

Transport properties are inferred from the calculated localization length ξ at the half-filling. For 1 to 3 atoms thick wires, ξ shows a rich non-monotonic behavior with respect to placement target parameters. We consider different systems widths and disorder scenarios, we explore how transverse and longitudinal aimed interdonor distances can be chosen to optimize and control the ξ for specific device applications.

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Marcio Varella - USP

Positronic Molecules

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The development of experimental techniques has allowed for the production and manipulation of antiparticles at extremely low energies. A wealth of new science arose from the interactions of such low-energy antiparticles, most notably antiprotons [1], muons [2] and positrons [3], with electrons, atoms and molecules.

One of the most interesting aspects of the research on positrons would be the formation of positronic compounds, i.e., bound states formed in scattering experiments in which a positron attaches to a vibrationally excited molecular core. The formation of about 60 positronic molecules has been reported [4], and theoretical models [5, 6] have also been proposed to describe the attachment and vibrational dynamics underlying the formation of such compounds. New possibilities for low-energy positron Physics and Chemistry also arise from positronium (Ps) manipulation advances. Ps2 molecules [7], Ps−anions [8], as well as laser spectroscopy of Ps and Ps2 [9] are now experimental facts, and even control over annihilation in excited Ps atoms has been achieved [10], among other breakthroughs.

We report on a fundamentally new kind of positronic compounds, which are not formed by positron attachment to stable molecules. Two otherwise repelling atomic anions are bound together by a positron, and the formation of positronic covalent bonds is discussed [11]. The calculations were performed with the Any-Particle Molecular Orbital (APMO) approach [12] implemented in the Lowdin [13] computer code, which has been previously employed to obtain positron binding energies to ordinary molecules [14, 15]. Our results were obtained at different levels of theory and always indicate the existence of stable positron-bonded diatomic molecules. Finally, we will also briefly discuss ongoing studies of solvated Ps atoms.

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Kaline Coutinho - USP

Caio Lewenkopf - UFF

Quantum thermodynamics: Entropy evolution in strongly coupled mesoscopic systems

We develop a theory of the entropy evolution in time-dependent, strongly coupled electron systems [1]. The formalism naturally avoids the problem of the system-bath distinction by defining the entropy current in the attached leads. This current can then be used to infer changes of the entropy of the system which we refer to as the inside-outside duality. We carry out this program in an adiabatic expansion up to first order beyond the quasistatic limit. When combined with particle and energy currents, as well as the work required to change an external potential, our formalism provides a full thermodynamic description, applicable to arbitrary noninteracting electron systems in contact with reservoirs. This provides a clear understanding of the relation between heat and entropy currents generated by time-dependent potentials and their connection to the occurring dissipation.

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Eric Andrade - USP

Uncovering novel phases in j=3/2 Mott insulators

Mott insulators with strong spin-orbit coupling are promising candidates for realizing novel phases of matter, for instance, quantum spin liquids. One of the best examples is the effective model for materials with local j=1/2 moments on the honeycomb lattice, the Kitaev-Heisenberg model, whose phase diagram contains a quantum spin liquid with a Dirac spectrum of Majorana fermion excitations. In this talk, I will present phase diagrams of effective models describing j=3/2 local moments, which are relevant, for instance, to Mott insulators with heavy magnetic ions in 4d^1 or 5d^1 configuration. The additional pseudo-orbital degree of freedom contained in this model can potentially enhance quantum fluctuations, via frustrating compass-type interactions or even unexpected SU(4)-symmetric interactions. As an example, I will discuss a possible quantum spin-orbital liquid on the hyperhoneycomb lattice and in the recently synthesized twisted bylayer graphene.

Posters

Rui Aquino dos Santos da Silva - UERJ

Dynamical phase transitions in two-dimensional Fermi liquids with quadrupolar interactions

Quantum nematic phases of Fermi liquids have been observed in several highly correlated systems, such as high Tc superconductors, heavy fermions and quantum Hall systems. The isotropic-nematic quantum phase transition can be understood as a Fermi surface instability, driven by attractive quadrupolar interactions. Using bosonization, the non-Fermi liquid character of this transition has been explicitly shown. In this work, we focus on the dynamics of the isotropic phase when the isotropic-nematic transition is approached. For this purpose, we study collective excitations of a two-dimensional Fermi surface considering density-density, as well as quadrupolar interactions.Using a semiclassical approximation in the bosonized theory, we write an evolution equation for Fermi surface fluctuations, analog to the Landau Fermi liquid formalism. By expanding the Fermi surface deformations in an angular momentum basis, the system is reduced to a set of infinitely coupled harmonic oscillators. Each oscillator describes a Fermi surface deformation mode with a specific symmetry. Focussing on the isotropic and the quadrupolar modes, we integrate out all other higher angular momentum components to compute the exact Green's functions. To do this, we use a "decimation" technique. Truncating the system to n modes, we are able to compute a recurrence relation in which the order Green's function is written in terms of the order one. Then, by carefully taking the limit , we compute the exact Green's function. The normal frequencies are computed from .The dispersion relation of the normal modes depends on two Landau parameters, and , that codify the density and the quadrupolar interactions respectively. We compute the dynamical fase diagram, where we display the normal modes in the plane. We show that, in specific regions of the plane, the dynamics of the Fermi surface fluctuations changes abruptly, signalling a dynamical phase transition.

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L. Cabral - USP

Azobenzene Adsorption on the MoS2(0001) Surface: A Density Functional Investigation within van der Waals Corrections

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Light sensitive organic molecules, such as azobenzene, has attracted the attention due to their ability to functionalize two-dimensional layered systems and to engineer their electronic structure. Azobenzene is an organic molecule formed by the functional group azo, {N{{ N{ , and two aromatic benzene rings. Here, we study the adsorption properties of the cis- and trans-azobenzene conformations on the molybdenum disulde MoS2(0001) layer [1]. Our investigations are based on density functional theory within the van der Waals corrections to improve the description of the weak molecule-surface interactions. By performing total energy calculations, the stability of the azobenzene in gas-phase and placed on the surface is discussed. We found that the lowest energy configurations are the trans-isomer in gas-phase and the conformations located horizontally on the MoS2(0001) substrate. We observed an increase in the relative total energy among the azobenzene isomers (trans and cis) in the gas-phase and the azobenzene supported on the MoS2(0001) surface, which can be explained by the contact of the two rings of the trans-isomer with the surface. We also analyzed the adsorption energy and work function for each configuration. Thus, our results establish how the azobenzene changes the local environment on the MoS2(0001) monolayer.

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Denis R. Candido - USP

Edge states across the topological phase transition due to approximate chiral symmetry in quantum anomalous and spin Hall systems

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In this work [1] we demonstrate that a quantum anomalous Hall system [2] (Chern insulator) always exhibits edge states right at the phase transition (except when the system becomes charge-conjugation symmetric), where the Hamiltonian is gapless, and in the vicinity of the topologically trivial and non-trivial gapped phases. We show that the origin of these edge states can be attributed to the approximate chiral symmetry of the Hamiltonian. Additionally, we demonstrate that while the non-trivial quantum Hall topology is responsible only for the existence of these edge states within the energy gap region, the approximate chiral symmetry is the ingredient responsible for the edge state existence in the remaining energy range in both topological and trivial phases. This behavior is described by the realistic one block of the BHZ model [3] of a quantum spin Hall system, which was already noticed [4] but remained unexplained. This work was supported by German Science Foundation (DFG) via Grant No. SFB 1170 “ToCoTronics”, the ENB Graduate School on Topological Insulators, CNPq, Capes, FAPESP and PRP-USP/Q-NANO.

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Denis R. Candido - USP

Blurring the boundaries between topological and non-topological phenomena in dots

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In this work [1] we first predict using the k.p method and the valence band anti-crossing theory that the common III-V InAs0.85Bi0.15/AlSb quantum well becomes a room temperature 2D topological insulator for well thickness dc>6.9nm. Second, we analytically solve the correspondent BHZ model [2] for our TI by introducing a cylindrical confinement defining cylindrical quantum dots (QDs). Surprisingly, we find for the non-topological QDs “geometrically protected” discrete helical edge states, i.e., Kramers pairs with spin-angular- momentum locking, similar to the topological protected helical edge states within the gap in the topological QDs. We calculate the circulating currents associated to both trivial and topological edge states and find no substantial difference between them. The two terminal conductance calculation for two pairs of edge states as a function of the QD radius and the gate controlling its levels with respect to the Fermi energy of the leads shows a double peak at 2e2/h for both topological and trivial QDs. In conclusion, our results blur the boundaries between topological and non-topological QDs as for the protection of the helical edge states, their calculated circulating currents and their two terminal conductance measurements. This work was supported by CNPq, CAPES, UFRN/MEC, FAPESP, PRP-USP/Q-NANO and the Center for Emergent Materials, an NSF MRSEC under Award No. DMR-1420451.

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Pedro M. Cônsoli - USP

Stability of ordered phases of the Heisenberg-Kitaev model in a magnetic field

In 2006, A. Kitaev presented the exact solution of an anisotropic spin-1/2 model with bond dependent interactions on the honeycomb lattice. His work and the following realization that such a system consists of a quantum spin liquid spurred an intense search for materials properly described by this hamiltonian. Once its generating mechanism was understood, it became clear that the Kitaev interaction complements the Heisenberg term in Mott insulators with strong spin-orbit coupling. While the properties of the resulting Heisenberg-Kitaev model have been extensively studied, several questions related to the effects introduced by an external magnetic field remain unanswered. Thus, we apply here spin-wave analyses in order to study the canted zigzag and canted stripy phases subject to a [100]-oriented magnetic field. Besides showing dispersions for both cases, we present a modified phase diagram which includes magnetically disordered phases originated by quantum fluctuations. Finally, we suggest that the same framework be applied to investigate more complex phases which arise in a [111]-oriented field. In particular, interesting candidates for future studies are two vortex phases whose chiral classical configurations might indicate the existence of edge modes, a typical topological signature.

Joao Carlos Gatelina - USP

Scaling of correlation functions of the random XX spin-1/2 chain

We study the spin-spin correlation functions of the random XX spin-$1/2$ chain via an exact numerical diagonalization of the Hamiltonian. Using higher numerical precision, we verified a universal power-law decay of the average correlation function, as predicted by the strong-disorder renormalization-group method. Therefore, recent claims of logarithmic corrections to the scaling are not consistent with our data. We have verified that the typical correlation function decays as a stretched exponential with the distance when measured with respect to the associated localization length. In addition, the associated exponent prefactor of the respective scaling function does not vary significantly with disorder. Finally, we also show that the universal correlation function distribution weakly violates the single-parameter scaling theory.

Michel Miranda - USP

Phase Transitions in Frustrated Magnets

Classical Monte Carlo simulations indicate that the Palmer-Chalker--Paramagnet phase transition in easy-plane pyrochlores is of fluctuation-driven first order. This is in striking contrast with experiments which indicates a continuous phase transition. Since the experiments are performed near the quantum phase transition between the Palmer-Chalker and the order-by-disorder ψ_2 phase, we intend to investigate the role played by the quantum fluctuations. Our strategy is to study the effective action for the transition incorporating quantum fluctuations via a $1/S$ (spin-wave) approximation. In this way, we hope to better understand the interplay between quantum and thermal fluctuations in frustrated magnets.

Willian Natori - USP

The search for exotic states of matter induced by the combined effects of strong correlation and spin-orbit coupling has stimulated the study of transition metal oxides with 4d and 5d elements. We have developed theoretical tools to describe the magnetism of these compounds when the heavy ion is in the d1 configuration in previous works (PRL 117, 017204; PRB 96, 125109). In the present work, we study the effective spin-orbital model that describes the magnetism of 4d1 or 5d1 Mott insulators in ideal tricoordinated lattices (arXiv:1802.00044). The model is displays anisotropic and bond-dependent interactions between multipoles of j=3/2 angular moment operators. However, in the limit of vanishing Hund's coupling, the model has an emergent SU(4) symmetry. We demonstrate that this large symmetry can be made explicit by means of a Klein transformation on pseudospin degrees of freedom. A geometrical criterion for the emergence of this SU(4)-invariance was proposed. Taking the hyperhoneycomb lattice as an example, we employ parton constructions with fermionic representations of the pseudospin operators to investigate possible quantum spin-orbital liquid states. The energies of the projected wave functions were computed using variational Monte Carlo methods. Our numerical results show that the lowest-energy quantum liquid corresponds to a zero-flux state with a Fermi surface of four-color fermionic partons. We also show that this quantum spin-orbital liquid is stable against tetramerization and has a much lower energy than the simplest ordered states even when Hund`s coupling induced perturbations are included.