Magnetic moments and non-Fermi-liquid behavior in quasicrystals

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Motivated by the intrinsic non-Fermi-liquid behavior observed in the heavy-fermion quasicrystal Au51Al34Yb15, we study the low-temperature behavior of dilute magnetic impurities placed in metallic quasicrystals. We find that a large fraction of the magnetic moments are not quenched down to very low temperatures, leading to a power-law distribution of Kondo temperatures, accompanied by a non-Fermi-liquid behavior, in a remarkable similarity to the Kondo-disorder scenario found in disordered heavy-fermion metals.

Unveiling a crystalline topological insulator in a Weyl semimetal with time-reversal symmetry

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Unlike topological insulators, which have a gap in the spectrum, Weyl semimetals are characterized by gapless points (Weyl nodes) in the Brillouin zone. Close to these nodes, the effective Hamiltonian is that of a 3D Weyl fermion. This phase provides the scenario for several exotic phenomena, like the so called chiral anomaly in the presence of electric and magnetic fields and the existence of topologically protected surfaces with Fermi arcs in slab configurations.
The band touching at the nodes in these 3D systems is possible when inversion symmetry or time reversal symmetry is broken. In this talk I will review different mechanisms to generate the Weyl semimetal phase and the topological characterization. I will also discuss, in particular, a lattice model for a periodic array of two layers of spinless electrons, which has time-reversal symmetry and broken inversion symmetry. This model supports a Weyl semimetal phase for a wide range of the parameters in addition to topological crystalline insulating phases. By mapping to an effective Weyl Hamiltonian, it is possible to derive some analytical results for the phase diagram as well as for the structure of the nodes in the spectrum of the Weyl semimetal.

Simplicity vs. complexity in thermoelectric quantum materials: the cases of $FeGa_3$ and RT_2Zn_{20}

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Photoelectrons Unveil Topological Transitions in Graphene like Systems

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The topological structure of the wave functions of particles in periodic potentials are characterized by the Berry curvature Ω_{kn} whose integral on the Brillouin zone are topological invariants known as the Chern numbers. The bulk-boundary correspondence states that these numbers define the number of edge or surface topologically protected states. It is then of primary interest to find experimental techniques able to measure the Berry curvature. However, up to now, there are no spectroscopic experiments that proved to be capable to obtain information on Ω_{kn} to distinguish different topological structures of the $\it{bulk}$ wave functions. Based on experimental results of the dipolar matrix element of graphene, here we show that ARPES experiments with the appropriate x-ray energies can unambiguously detect changes of the Chern numbers in graphene and graphene-like materials opening new routes towards the experimental study of topological properties of condensed matter systems.

$GaTa_4Se_8$: a new prototype of 3D Mott-Hubbard physics

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Mott predicted in the 40s that as a function of density a solid state system may undergo a dramatic transition between a metallic and an insulator state. This follows from the competition between the potential energy due to the Coulomb repulsion between electrons and their kinetic energy. Eventually, this metal-insulator transition (MIT) became the celebrated Mott transition and is now a paradigmatic example of strongly correlated electron physics. In the 90s theoretical work on the Hubbard model predicted that the Mott transition in magnetically disorder systems should occur along a first order line and end in a finite temperature second order critical point. We study the correlation-driven insulator-to-metal transition in the 3D Mott system GaTa_{4}Se_{8}, as a function of temperature and applied pressure. We report novel experiments on single crystals, which demonstrate that the transition is of first order and follows from the coexistence of two states, one insulating and one metallic that we toggle with a small bias current. Our experiments and theoretical results have demonstrated that the GTS phase diagram is in excellent agreement with the theoretical expectations for the Mott transition.

Superconductivity in Complex Electronic Systems under Pressure

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Study on superconductivity in complex electronic systems is an active project in the China's newly established high-pressure research center. Here we overview the progress in the past two years in the search and discovery of superconductivity in materials with highly efficient thermoelectric performance and topological order. We also present experimental results for the new understanding of the interplay of superconductivity and competing electronic phases in cuprates, iron-based superconductors, and transition-metal dichalcogenides. Specifically, we report our discovery of pressure-induced charge density wave (about 1/7 of the in-plane reciprocal vector) in optimally doped $Tl_2Ba_2Ca_2Cu_3O_{10+\delta}$ at high pressures and room temperature and its competition with superconductivity. We show how pressure is used to identify the essential interactions that give rise to high T_c superconductivity. Experimental clues are provided for enhancing T_c based on the route to synthesize superconductors with such higher T_c's at ambient conditions.

Why are the Co-based 115 compounds different?: The case study of GdMIn5 (M=Co,Rh,Ir)

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In this work, we analyze an interesting regularity that is experimentally observed in the RMIn5 (R=4f or 5f elements; M=Co, Rh, Ir) family of compounds, where the lowest Néel temperatures are obtained in the Co-based materials. We focus our analysis on the GdMIn5 compounds and perform density-functional-theory-based total-energy calculations to obtain the parameters for the exchange coupling interactions between the magnetic moments located at the Gd3+ ions. Our calculations indicate that the ground state of the three compounds is a C-type antiferromagnet determined by the competition between the first- and second-neighbor exchange couplings inside GdIn3 planes and stabilized by the couplings across MIn2 planes. We then solve a model with these magnetic interactions using a mean-field approximation and quantum Monte Carlo simulations. The results obtained for the calculated Néel and Curie-Weiss temperatures, the specific heat, and the magnetic susceptibility are in very good agreement with the published experimental data. Remarkably, we show that the first-neighbor interplane exchange coupling in the Co-based material is much smaller than in the Rh and Ir analogs which leads to a more two-dimensional magnetic behavior in the former. This result help explain the observed lower Néel temperature in Co-115 systems and may shed light on the fact that the Co-based 115 superconductors present the highest TC. We also explore the effect of a uniaxial pressure along the c axis and find that the magnetic coupling between planes can be strongly reduced by both positive and negative stresses.

How to distinguish between Majorana and Kondo signals in a quantum dot-topological quantum wire junction?

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Predictions of the appearance of zero-energy Majorana bound states at the ends of a topological quantum wire [1] have spurred a significant amount of research in recent years. Although measurements [2] of zero-bias peaks in the transport properties of quantum wires with induced topological superconductivity are consistent with these predictions, there has been some controversy as a number of Majorana-unrelated alternative possibilities (such as the Kondo effect) can account for these experimental features.

Motivated by these findings, we investigate the low-temperature transport properties of an interacting quantum dot (QD) coupled to a topological quantum wire [3]. We explore the interplay of Kondo and Majorana modes in this system by mapping a realistic description of the dot+quantum wire set-up to an effective Anderson impurity model coupled to a local Majorana modes. The low-temperature regime is investigated using the numerical renormalization group (NRG). We find evidence of a strong interplay between Majorana and Kondo physics. Our results show a strong renormalization of the Kondo temperature by the QD-Majorana interaction, which can drive the system from a Kondo-dominated to a Majorana-dominated ground state. By quenching the Kondo effect with Zeeman fields, we found a persistent $0.5e^2/h$ conductance coming from the Majorana mode leaking into the QD. These properties can be used for the experimental distinction of Majorana and Kondo modes in topological quantum wires.

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NMR evidence for inhomogeneous nematic uctuations in BaFe2(As1-xPx)2

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We present evidence for nuclear spin-lattice relaxation driven by glassy nematic fluctuations in isovalent P-doped BaFe2As2 single crystals. Both the 75As and 31P sites exhibit stretched-exponential relaxation similar to the electron-doped systems. By comparing the hyperfine fields and the relaxation rates at these sites we find that the As relaxation cannot be explained solely in terms of magnetic spin fluctuations. We demonstrate that nematic fluctuations couple to the As nuclear quadrupolar moment and can explain the excess relaxation. These results suggest that glassy nematic dynamics are a universal phenomenon in the iron-based superconductors.

Exotic magnetism in 5d ordered double perovskites

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UNICAMP

5d transition-metal atoms, mostly Re, Os and Ir, have been employed in the synthesis of novel materials with exotic magnetic and electronic properties. The rich physical behavior of many of such systems arises from a fine balance of physical ingredients such as the large spatial extension of magnetically ative 5d orbitals (leading to strong hybridization with neighboring magnetic or non-magnetic ions), strong spin-orbit coupling and intermediate on-site Coulomb interaction. The fairly simple double perovskite crystal structure provides a convenient network to investigate such physics, also allowing for either ordered or disordered mixing of 5d and 3d transition-metal ions. In this context, the electronic and magnetic properties of the ordered double perovskites Ca2FeReO6 and Ba2FeReO6 have been investigated by means of X-ray absorption spectroscopies (XAS and XMCD), neutron and synchrotron x-ray diffraction, and Raman scattering. Amongst our findings, we highlight an incipient orbitally-ordered metallic state [1] and the discovery of a novel excitation, namely the spin-electron-phonon, in half-metallic Ba2FeReO6 [2], a transition from non-colinear to colinear magnetism at the metal-insulator transition of Ca2FeReO6 [3,4], and a large orbital magnetic moment in oxygen 2p orbitals due to hybridization with Re 5d electrons [4] in both compounds. In this talk, the remarkable electronic and magnetic properties of the Re and Fe-based double perovskites will be reviewed and interpreted in terms of the coexisting and sometimes competing interactions found in this system.

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Solutions of the Two Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms

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Numerical results for ground state and excited state properties (energies, double occupancies, and Matsubara-axis self energies) of the single-orbital Hubbard model on a two-dimensional square lattice are presented, in order to provide an assessment of our ability to compute accurate results in the thermodynamic limit. Many methods are employed, including auxiliary field quantum Monte Carlo, bare and bold-line diagrammatic Monte Carlo, method of dual fermions, density matrix embedding theory, density matrix renormalization group, dynamical cluster approximation, diffusion Monte Carlo within a fixed node approximation, unrestricted coupled cluster theory, and multi-reference projected Hartree-Fock. Comparison of results obtained by different methods allows for the identification of uncertainties and systematic errors. The importance of extrapolation to converged thermodynamic limit values is emphasized. Cases where agreement between different methods is obtained establish benchmark results that may be useful in the validation of new approaches and the improvement of existing methods.

Criticality and quenched disorder: rare regions vs. Harris criterion

Jose Abel Hoyos Neto
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We combine scaling arguments and optimal fluctuation theory to establish a general relation between quantum Griffiths singularities and the Harris criterion for quantum phase transitions in disordered systems. If a clean critical point violates the Harris criterion, it is destabilized by weak disorder. The Griffiths singularities are quantified and consequences to the new critical theory are discussed. In contrast, if the Harris criterion is fulfilled, Griffiths singularities are of power-law type and can coexist with clean critical behavior. We present applications of our theory to a variety of systems including quantum spin chains, classical reaction-diffusion systems and metallic magnets. Based on these results we propose a unified classification of phase transitions in disordered systems.

Excitonic magnetism in models and materials

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Excitonic magnetism, also called van Vleck magnetism, has been theoretically proposed in some strongly correlated materials with non-magnetic atomic ground states. I will describe the strong-coupling approach to this phenomenon and explain its connection to Bose-Einstein condensation of spinful bosons. Next, I will show numerical results obtained for excitonic magnets with dynamical mean-field theory and present doping of exitonic insulators as a new way to states of matter with unusual properties such a dynamically generated spin-orbit coupling.

Transport properties of three-dimensional Weyl semimetals near a Weyl node

Bruno Rizzo (UFF), Alexis Hernandez (UFRJ), and Caio Lewenkopf (UFF)

We present a numerical method to compute the Landauer conductance in disordered there-dimensional Weyl semimetals. The method allows for the introduction of boundary conditions at the system surfaces and accounts for an external magnetic field. By construction, the proposed discretization scheme avoids the fermion doubling problem. Three-dimensional Dirac and Weyl semimetals exhibit a disorder-induced quantum phase transition between a semimetallic phase at weak disorder and a diffusive-metallic phase at strong disorder. Using a minimal single-Weyl node model and a finite-size scaling analysis of conductance, we analyse the transport properties close to the quantum phase transition.

(New?) Low dimensional systems: richness and diversity of their electronic properties

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The properties of low dimensional systems strongly depend on their size, width, composition and environment. This applies, both, to quasi zero and quasi one dimensional systems as well as to ultrathin films or 2D nano-objects and nanostructured surfaces. In this talk I am going to present a brief overview on the electronic and magnetic properties of some low dimensional systems which have been obtained or isolated in the last decade. The focus will be put on systems which have been studied or are being studied within our group. In particular, the attention will be set on the polarity driven mechanisms responsible for the structural transitions which take place in dichalcogenide nanoribbons of small width and on the emergence of a 2D electron gas, by breaking of the charge disproportionation, at the surface of charge ordered semiconductors.

Haldane phase and magnetic end-states in 1D topological Kondo insulators

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A topological Kondo insulator (TKI) is a special state of matter that arises from the combination of strong correlations in localized f-bands, and topological band theory. While TKIs are well understood in two and three spatial dimensions, little is known about their one-dimensional counterpart. In this work, we focused on a particular model, the p-wave Kondo-Heisenberg model in 1D, which has been proposed recently as a model Hamiltonian exhibiting a TKI groundstate. We study this model by means of Abelian bosonization and the density matrix renormalization group (DMRG), and show that, at half-filling, the system is insulating and supports topogically-protected spin-1/2 end-states. Moreover, we unveiled an interesting connection to the physics of the spin-1 Haldane chain, which is a prototypical example of a strongly correlated topological system. A possible realization of this model in systems of ultracold atoms is discussed.

Using idealized models and basic concepts to guide and interpret quantitative calculations

Richard Martin
UIUC and Stanford University

Emergent symmetries in disordered quantum spin chains

Eduardo Miranda
UNICAMP

A common theme in low- or high-energy physics is the fact that a state may have a symmetry lower than its underlying Hamiltonian/Lagrangian. Behind this feature is the phenomenon of spontaneous symmetry breaking. A far less common situation corresponds to a low-energy state whose symmetry is *greater* than its underlying Lagrangian. The most famous example is the critical 2D Ising model in a small magnetic field, which has an emergent (and ill-understood) E_8 symmetry. Other examples have been found in the last few years. We have uncovered one such case is the context of strongly disordered spin chains. Indeed, in the limit of very strong disorder, where exact results can be obtained, we have shown that spin-1 chains with underlying SU(2) symmetry show emergent SU(3)-symmetric behavior in two different phases. Interestingly, the constituents of each phase can be viewed as bound states of either three SU(3) quarks (baryons) or a quark and an antiquark pair (a meson). Chains with higher spin sizes also show emergent SU(N) phases but only mesonic phases exist. In the search for more exotic examples, we will show results of ongoing work on disordered SO(N)-symmetric chains with possible “baryonic” phases.

Combined external pressure and chemical substitution studies on $BaFe_2As_2$ single crystals

Pascoal Pagliuso
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Unparticles and Anomalous Dimensions in the Strange Metal Phase of the Cuprates

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Cuprate superconductivity remains an unsolved problem because no knock-down experiment has revealed unambiguously the nature of the charge carriers in the normal state. As a window into laying plain what is strange about the normal state in the cuprates, I will focus on the power-law optical conductivity in the mid-infrared frequency range. I will show that a consistent story of the ac and dc transport properties can be obtained if the current acquires an anomalous dimension.

I will then show how the anomalous dimension can be measured by experimental detection of the fractional Aharonov-Bohm (AB) phase in the strange metal regime of the cuprates. In the presence of an anomalous dimension, the AB phase deviates strikingly from the standard result and hence offers a precise diagnostic as to what is strange about the strange metal.

Spin-Orbit Coupling, Strong Interactions, and Topological Character

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In recent years the electronic structure of crystalline solids has come under close scrutiny because of the various types of topological characters that may arise. Most of the work is done at the one-electron (non-interacting) level, and most innovations have arisen from model tight-binding Hamiltonians and their eigenvectors. This talk will focus on a few examples of discoveries made computationally through DFT studies of actual materials, thus providing a physical realization as the discovery was made. Competition and partnership between strong interactions and spin-orbit coupling will be emphasized. Examples will include (1) the 'semi-Dirac' point Fermi surface phase in VO2 thin films, the first member of a class now called multi-Weyl: massive in some direction, massless in other direction; (2) a nodal loop semimetal phase found in computational studies of thin SrVO3 films, realized more recently in NbP etc.; (3) the buckled honeycomb lattice of a (111) bilayer of LaMnO3 encased on LaAlO3, which is a Chern insulator and may be a realization of the Weyl-Mott insulator proposed recently by Morimoto and Nagaosa.

Acknowledgments: R. Pentcheva, V. Pardo, K.-W. Lee, S. Gangopadhyay.

Real-Space Calculation of the Conductivity Tensor for Disordered Topological Matter

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Although the transverse conductivity can be easily calculated in pure systems in momentum space, its calculation in real space, allowing for the non-perturbative introduction of disorder, is very computationally consuming. As a result, there are very few numerical approaches for this task and most of them are limited to very small systems. We describe a novel approach, based on a little-known formulation of the Kubo formula, that allows the calculation of the conductivity tensor for large systems, of the order of 10^6 sites [1]. It also has the advantage of obtaining both conductivities in a single calculation step and for various values of temperature and chemical potential, capturing the topology of the band-structure. Our method is also highly parallelizable and can be ported to GPUs, eliminating the need for supercomputers.

We believe our method can be useful in the study of topological matter and for that purpose, we illustrate its power by looking at systems with non-trivial topology where the effects of disorder have been, up to now, mostly unknown. We analyze the interplay between disorder and inversion symmetry-breaking in a Chern insulator[1], the spin Hall conductivity of graphene with adsorbed atoms[2] and the effect of an external magnetic field in the Quantum Hall effect of a Chern insulator.

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Magnetism and phase transitions in compressed Oxygen

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Among the diatomic molecules O2 stands out for its magnetic moment (S=1) caused by the exchange interaction between electrons in the two-fold degenerate highest-occupied molecular orbitals. Being one of the most common and important elements in nature, Oxygen has an exceedingly well-explored phase diagram under pressure, up to and beyond 100 GPa. At low temperatures and pressures below 8 GPa Oxygen crystallises in antiferromagnetic phases where the O2 molecules retain the gas-phase spin S = 1 character. At higher pressure a broad insulating ε phase has been reported from about 8 to 96 GPa. In this phase molecules group structurally together to form quartets while switching, as believed by most, to a nonmagnetic state [1]. Here we present theoretical results strongly connecting with existing vibrational and optical evidence, showing that this is true only above 20 GPa, whereas the S = 1 molecular state survives up to about 20 GPa [2]. The ε phase thus breaks up into two: a spinless ε0 (20-96 GPa), and another ε1 (8-20 GPa) where the molecules have S = 1 but possess only short-range antiferromagnetic correlations. The first-order phase transition extends at finite temperature and most likely terminates into a crossover with a critical point near 30 GPa and 200 K.

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Signatures of correlation: from excitons to satellites

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One of the simplest, yet most striking, outcomes of electron correlation is the exciton. The creation of electron-hole pair(s), under external perturbation, is an intrinsic collective excitation of the system and, from the theoretical point of view, is defined in terms of 'beyond single-particle'. In this contribution I will first illustrate the importance of excitonic effects in the optical spectrum of solids, taking Vanadium dioxide as an example, underlying some general (local fields, de-polarization effects) and technical aspects (starting point of perturbative approaches, self-consistency). In a second part, I will focus on the generality of the screening concepts, and the interchange among theoretical approaches (Bethe-Salpeter equation, Time Dependent Density Functional Theory, GW approximation) as well as spectroscopy techniques (optical, Inelastic X-ray scattering, Electron Energy Loss and Photo-emission spectroscopy).

Floquet topological insulators: materials engineering by driving…

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The study of out of equilibrium systems opens the possibility to observe new phenomena absence in equilibrium. In recent years the topic has been revitalize due to the development of new ideas and theoretical concepts as well as the exquisite control reached experimentally in different systems (like graphene, superconducting quits, cold atoms and photonics crystals, for instance). A particular area of research is the study of how the presence of (periodic) time dependent potentials can induced topological properties in an otherwise topologically trivial material. These systems are called Floquet topological insulators and, as the ordinary topological insulators (TI), present a bulk gap in their (quasi-) energy spectrum and chiral states at their edges/surfaces or at the interfaces with other materials. In this talk I will present some recent results for the case of massless Dirac fermions (electrons in graphene or and ordinary TI, for instance) in the presence of circularly polarized laser radiation where we characterized the bulk topological properties and the chiral states that appear at the border or around defects and adatoms. We also evaluate the effect on the charge transport and show how they lead to a Hall signal.

Spin density wave instabilities in the NbS_2 monolayer

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In this pesentation, we will talk about the magnetic properties of the NbS$_2$ monolayer studied by first-principles calculations. The transition metal dichalcogenides (TMDC) are a family of laminar materials presenting exciting properties such as charge density waves (CDW), superconductivity and metal-insulating transitions among others. 2H-NbS$_2$ is a particular case within the family, because it is the only one that is superconductor without exhibiting a CDW order. Although no long range magnetic order was experimentally observed in the TMDC, we show here that the single monolayer of NbS$_2$ is on the verge of a spin density wave (SDW) phase. Our calculations indicate that a wave-like magnetic order is stabilized in the NbS$_2$ monolayer in the presence of magnetic defects or within zig-zag nanoribbons, due to the presence of unpaired electrons. We calculate the real part of the bare electronic susceptibilty and the corresponding nesting function of the clean NbS$_2$ monolayer, showing that there are strong electronic instabilities at the same wavevector associated with the calculated SDWs, also corresponding with one of the main nesting vectors of the Fermi surface. We conclude that the physical mechanism behind the spin-wave instabilities are the nesting properties, accentuated by the quasi 2D character of this system, and the rather strong Coulomb interactions of the 4d band of the Nb atom. We also estimate the amplitude of the spin-fluctuations and find that they are rather large, as expected for a system on the verge of a quantum critical transition.

Ab initio quantum Monte Carlo for strongly correlated systems

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One of the largest challenges in condensed matter physics is the description of emergent materials physics when electron correlation is important. Quantum Monte Carlo offers a unique opportunity to make progress on this challenge because it allows us to simulate the electron correlation directly at a high but scalable computational cost. In recent years, there has been quite a bit of progress in using first principles quantum Monte Carlo calculations to simulate electrons in so-called strongly correlated materials; materials in which the interactions between electrons change the qualitative ground state.

I will summarize some of the work underway in my group to develop and apply quantum Monte Carlo calculations for the description of strongly correlated systems. This work can largely be divided into two tracks: developing new capabilities and applications to strongly correlated materials. For the first track, I will discuss a new method to use ab-initio QMC data to downfold onto effective Hamiltonians. This method can give insight and allow us to compare correlated materials, in addition to using the effective Hamiltonian for more coarse-grained simulations. It is implemented in the open-source package QWalk (http://qwalk.org). For the second track, I will discuss the metal-insulator transition in vanadium dioxide. By simulating the electron interactions directly, the physics in these challenging materials becomes much more clear.

Spin crossover in iron bearing mantle minerals: some geophysical consequences

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Strange metals, fermion signs and entanglement.

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The strange metals as observed in high Tc superconductors and other correlated electron systems are arguably the greatest enigma of condensed matter physics. The difficulties are rooted in the fundamentals of physics: the lack of a general mathematical mathematical framework to deal with strongly interacting fermions at finite density, the “fermion sign problem”. The holographic duality as discovered in string theory is the first method yielding a precise description of non-Fermi liquids [1]. These holographic strange metals are suggestively similar to the laboratory variety, at the same defeating the basic principles of bosonic field theory. These are quantum critical phases with scaling properties alien to those computable with conventional methods. Remarkably their entanglement entropies demonstrate that their ground states are more densely entangled than deemed possible. I will present some first indications that this is rooted in the sign structure. Using the so-called nodal surface (zero’s of the wave-function) as a measure, this fermionic entanglement structure can be addressed in a geometrical language. The nodal surface of a Fermi liquid is characterized by a scale but using a particular Ansatz a quantum critical state can be described characterized by a fractal nodal surface. We show that such states are characterized by entanglement entropies bearing similarity to those of the holographic strange metals.

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