Workshop on Heavy Fermion Materials and Quantum Phase Transitions

December 9-11, 2013
Rice University, Houston TX

Rice BioScience Research Collaborative (BRC)
6500 Main St., Houston TX 77005, Room 280

http://kondo.rice.edu
Workshop on Heavy Fermion Materials and Quantum Phase Transitions

Organized by

Quantum Magnetism Laboratory, Rice University
Department of Physics & Astronomy, Rice University

Sponsored by

U. S. Army Research Office
Rice University

Topics

• Heavy Fermion Materials
• Quantum Phase Transitions
• Unconventional Superconductivity
• Spin-orbit Coupling and Topological States
• Connection to d-electron Systems
• Non-equilibrium Physics, Cold Atoms

Organizers

Qimiao Si *                              Elihu Abrahams (UCLA)
Matthew Foster *                          Emilia Morosan *
Douglas Natelson *                        Andriy Nevidomskyy *
Barbara Braun and Umbe Cantu **
* Rice University  ** Rice University (Administration)

http://kondo.rice.edu
Scope

The workshop will address frontier topics on the Kondo effect and quantum phase transitions in heavy fermion materials and related systems, a broad area which lies at the intersection of some of the most important phenomena in quantum condensed matter physics. The workshop will gather a small group of top experts to discuss the status of the field, and to assess the opportunities for new physics.

Presentation Guidance

Oral sessions

All oral sessions will be held in Lecture Hall 280 on the second floor of the BRC building. Each talk includes 5 minutes of discussion time.

Poster sessions

The poster sessions will be held in the Exhibition Hall, on the first floor of the BRC building.

The poster board size is 4 x 4'.

If you have additional questions regarding the poster session, please contact Professor Emilia Morosan (emorosan@rice.edu).

Wireless Internet Access

Wireless access is available through the wireless network 'Rice Guest.' Simply select this network, agree to the terms and conditions, and you should have full access, including electronic journals supported by the Rice library.
Program
Monday, December 9

Arrival
6:00pm - 8:00pm Buffet Dinner for Speakers
Hilton Hotel, Travis A (8th floor)

Tuesday, December 10

7:30 - 8:15am Breakfast (outside Lecture Hall 280)

Opening - Welcome Remarks
(Chair: Qimiao Si)

8:30 - 8:35am George L. McLendon, Provost & Professor of Chemistry, Rice University
8:35 - 8:40am Tom Killian, Chair, Department of Physics & Astronomy, Rice University
8:40 - 8:50am Marc Ulrich, Physics Division Chief & Condensed Matter Physics, U.S. Army Research Office

Session 1 - Experimental and Theoretical Perspectives
(Chair: Qimiao Si)

8:50 - 9:25am Frank Steglich
“Mott type physics in lanthanide-based intermetallics”
9:25 - 10:00am Piers Coleman
“Strange metals, beta YbAlB4 and the heavy fermion quasi-crystal YbAlAu”

10:00 - 10:30am Group photo and coffee break (outside Lecture Hall 280)

Session 2 - Quantum Criticality
(Chair: Elihu Abrahams)

10:30 - 11:00am Hilbert von Lohneysen
“Quantum phase transition in the partially frustrated heavy-fermion system CePdAl”
11:00 - 11:30am Silke Paschen
“Quantum criticality in cubic heavy fermion compounds”
11:30 - noon Meigan Aronson
“Yb2Pt2Pb: Emergent criticality on the Shastry-Sutherland lattice”

Session 3 - Poster Preview
(Chair: Emilia Morosan)
12:00 - 12:15pm One minute per poster
12:15 - 2:15pm Lunch (Exhibition Hall, 1st floor)
Poster session (Chair: Emilia Morosan)

Session 4 - Discussion I
2:15 - 3:15pm Elihu Abrahams
leading discussions on quantum criticality

Session 5 - Heavy Fermion Materials by Design
(Chair: Emilia Morosan)
3:15 - 3:45pm Gabriel Kotliar
“Towards theory assisted material design with f and d electron systems”
3:45 - 4:15pm M. Brian Maple
“Routes to heavy fermion behavior in correlated electron materials”
4:15 - 4:45pm Coffee break (outside Lecture Hall 280)

Session 6 - Discussion II
4:45 - 5:30pm Emilia Morosan
leading discussions on heavy fermion materials

Session 7 - Kondo Physics in Cold Atoms
(Chair: Tom Killian)
5:30 - 6:00pm Han Pu
“Single impurity in quantum gases”
6:00 - 6:30pm Eugene Demler
“Quantum impurities in ultracold atoms: From polarons to orthogonality catastrophe to Kondo effect”
7:00pm Organized Dinner for Speakers
Wednesday, December 11

7:30 - 8:15am  Breakfast (outside Lecture Hall 280)

Session 8 - Spin-Orbit Coupling
(Chair: Andriy Nevidomskyy)

8:30 - 9:00am  Zachary Fisk  
“Kondo Insulators”

9:00 - 9:30am  Yong Baek Kim  
“Topological phases and non-Fermi liquid in 5d electron systems with strong spin-orbit coupling”

Session 9 - Discussion III

9:30 - 10:00am  Andriy Nevidomskyy  
leading discussions on spin-orbit physics in heavy fermions

10:00 - 10:30am  Coffee Break (outside Lecture Hall 280)

Session 10 - Low-dimensional Systems
(Chair: Matt Foster)

10:30 - 11:00am  Gleb Finkelstein  
“Majorana quantum critical behavior in a resonant level coupled to a dissipative environment”

11:00 - 11:30am  Doug Natelson  
“Nanoscale junctions to examine Kondo systems out of equilibrium”

Session 11 - Discussion IV

11:30 - noon  Matt Foster  
leading discussions on low-D and non-equilibrium Kondo physics

12:00 - 2:15pm  Lunch (Exhibition Hall, 1st floor)  
Poster session (Chair: Emilia Morosan)

Session 12 - Quantum Criticality and Superconductivity
(Chair: Pengcheng Dai)

2:15 - 2:45pm  Stefan Kirchner  
“Condensation energy of CeCu2Si2 and theoretical implications”
2:45 - 3:15pm  Collin Broholm  
“From incommensurate correlations to mesoscopic spin resonance in YbRh2Si2”

3:15 - 3:45pm  J. C. Seamus Davis  
“Quasiparticle interference imaging of heavy-fermion formation and Cooper pairing”

3:45 - 4:15pm  Coffee Break (outside Lecture Hall 280)

**Session 13 - Connections between f- and d-Electron Systems**  
(Chair: Ilya Vekhter)

4:15 - 4:45pm  Joe D. Thompson  
“Building Bridges between Correlated f- and d-Electron Systems”

**Session 14 - Summary and Outlook**

4:45 - 5:45pm  Qimiao Si  
leading discussions

7:00pm  Organized Dinner for Speakers

**Thursday, December 12**

Departure
Abstracts I:  
Invited talks  
Tuesday, Dec. 10
Frank Steglich, MPI CPfS

“Mott type physics in lanthanide-based intermetallics”

In this talk, experimental evidence of a Kondo destroying quantum critical point in antiferromagnetic (AF) heavy-fermion metals will be provided (see, F. Steglich et al., arXiv: 1309.7260). For these materials, the detachment of the electronic (“Mott type”) and AF instabilities as well as the interplay of unconventional superconductivity and quantum criticality will also be discussed.

Piers Coleman, Center for Materials Theory, Rutgers University

“Strange Metals, beta YbAlB4 and the heavy fermion quasi-crystal YbAlAu”

In the antiferromagnetic (AF) heavy-fermion (HF) compound CePdAl (TN = 2.7 K), Ce atoms occupy a geometrically frustrated distorted kagom lattice. Neutron scattering data (Donni et al., 1996) indicate that only two thirds of the Ce moments participate in long-range AF order. Hence we investigate the effect of frustration on the quantum phase transition (QPT) between AF and paramagnetic ground states, which in HF systems arises from the competition between RKKY interaction and Kondo effect. In CePdAl, a QPT can be induced by Ni substitution. TN(x) of CePd(1-x)NixAl decreases roughly linearly with x, with TN \rightarrow 0 at xc \sim 0.144. The low-T specific heat C(T) evolves toward C/T \sim \ln(T_0/T) when approaching xc. Both features are compatible with the Hertz-Millis scenario for 2D quantum-critical fluctuations, which might arise from decoupling the AF planes by planes of frustrated Ce atoms. Neutron scattering data of CePdAl single crystals suggest that the frustrated Ce moments develop below TN short-range order. Thermal-expansion and magnetostriction measurements are used to establish the magnetic phase diagram and to clarify whether a structural distortion can lift the frustration.

Silke Paschen, Vienna University of Technology

“Quantum criticality in cubic heavy fermion compounds”

Meigan Aronson, Stony Brook University and Brookhaven National Laboratory

“Yb2Pt2Pb: Emergent criticality on the Shastry-Sutherland lattice”

A generic phase diagram has been proposed for the heavy fermions, where the interplay of magnetic order and electronic localization are controlled by the f-electron/conduction electron coupling and by magnetic frustration. Quantum fluctuations that suppress magnetic order are found in systems with reduced dimensionality, geometrically frustrated lattices, or dimerization. There are few heavy fermion compounds where this frustration is decisive, and so there are unexplored regions of the generic phase diagram. We report experimental results on metallic Yb2Pt2Pb, where Ising-like Yb ions dimerize on the Shastry-Sutherland lattice (SSL), forming the rungs of orthogonal spin ladders. Yb2Pt2Pb orders AF at 2.06 K, with a SDW-type modulation of the dimer moments in the SSL planes. Definitive evidence for the one-dimensional character of Yb2Pt2Pb comes from neutron scattering experiments that find spinon excitations that disperse along the ladders. Yb2Pt2Pb is the first metal where 1D physics can be explored, and we discuss related compounds where the interplay of the Kondo effect and dimerization may also be present.

Gabriel Kotliar, Rutgers University

“Towards theory assisted material design with f and d electron systems”

We will review the state of the art of electronic structure highlighting successes in the area of f electron materials. Connections with d electron materials will be made highlighting research opportunities in theory assisted material design.
Brian Maple, University of California, San Diego

“Routes to heavy fermion behavior in correlated electron materials”

Different scenarios for heavy fermion behavior and possible underlying mechanisms in correlated electron metallic systems are discussed in this talk. Heavy fermion behavior has been observed in a wide range of f-electron materials and some d-electron materials. Examples of f-electron materials that exhibit heavy fermion behavior include many intermetallic compounds based on Ce, Pr, Sm, Yb, U, and Pu and several cuprates containing Pr and Nd. An example of a d-electron material that displays heavy fermion behavior is the compound LiV2O4. The relation between heavy fermion behavior in dense f-electron compounds and Kondo and valence fluctuation behavior in dilute f-electron systems in the normal and superconducting states is considered.

Han Pu, Rice University

“Single impurity in quantum gases”

The system of cold atoms is intrinsically clean. However, impurities and disorder can be artificially engineered which allows one to investigate their effects in a controlled manner. I will describe two types of localized impurities. The first represents a classical impurity in the form of a localized external potential. I will show how a superfluid Fermi gas, topological or nontopological, responds to such an impurity. The second represents a quantum impurity in the form of an extra atom. We study the collision dynamics of such an impurity atom with a quantum gas.
Eugene Demler, Harvard University

“Quantum impurities in ultracold atoms: From polarons to orthogonality catastrophe to Kondo effect”

In this talk I will review recent theoretical and experimental progress in exploring dynamical quantum impurities in ultracold bosonic and fermionic systems. I will discuss several novel phenomena, including universal RF spectra, quantum flutter, and Bloch-type oscillations arising from $2k_F$ scattering in one dimensional systems. I will show how tools of ultracold atoms can be used to explore open questions of Kondo physics.
Abstracts II:
Invited talks
Wednesday, Dec. 11
Zachary Fisk, UC Irvine

“Kondo insulators”

Experiment finds that the Kondo insulator SmB6 has a robust conducting surface state at low temperatures, as expected for a topological insulator. The temperature dependent properties of SmB6 will be discussed in the context of those of Kondo insulators in general.

Yong-Baek Kim, University of Toronto

“Topological phases and non-Fermi liquid in 5d electron systems with strong spin-orbit coupling”

We discuss recent developments in physics of 5d transition metal oxides, where the interplay between electron interactions and strong spin-orbit coupling may lead to a plethora of novel quantum ground states. In particular, we explain how the topological phases such as topological insulator, Weyl semi-metal, and quantum spin liquid may arise in these systems. Emergence of a three-dimensional non-Fermi liquid phase with quadratic band-touching and interactions with f-electron local moments are also discussed. We would make connections between these theoretical ideas and existing/future experiments.
Gleb Finkelstein, Duke University

“Majorana quantum critical behavior in a resonant level coupled to a dissipative environment”

We investigate tunneling through a resonant level embedded in a dissipative environment, which suppresses tunneling rates at low temperatures. Specifically, the resonant level is formed in a carbon nanotube quantum dot, and the dissipative environment is realized by fabricating resistive leads. For the symmetric coupling of the resonant level to the two leads, we find that the resonant peak reaches the unitary conductance $e^2/h$ despite the presence of dissipative modes. Simultaneously, the width of the resonance tends to zero as a non-trivial power of temperature. We draw a connection between our system and a resonant tunneling in a Luttinger liquid and interpret the observed unitary resonance of vanishing width in terms of a quantum critical point (QCP). We further investigate an exotic state of electronic matter obtained by fine-tuning the system exactly to the QCP. We report on several transport scaling laws both near and far from equilibrium, including a non-Fermi-liquid quasi-linear scattering rate at the QCP, interpreted in terms of a Majorana mode localized at the resonant level.

Douglas Natelson, Rice University

“Nanoscale junctions to examine Kondo systems out of equilibrium”

Over the last 15 years quantum impurity problems have been examined using semiconductor quantum dots and nanoscale junctions as tunable model systems. Transport through these devices allows access to regimes far from equilibrium, and nanoscale junctions incorporating nontrivial electrodes (e.g., ferromagnetic metals) can further the examination of previously unexplored cases of quantum impurities coupled to baths of excitations. I will summarize recent progress in these experiments, discussing universality expected in the nonequilibrium Kondo response, observations of unusual Kondo physics in junctions between ferromagnetic metals, and noise measurements as a probe of correlation physics. The prospects for insights into other material systems and devices will also be discussed.
Unconventional superconductivity occurs in a broad range of strongly correlated electron systems. The only unifying characteristic features seems that unconventional superconductivity occurs in close vicinity of zero-temperature. Heavy fermion compounds represent prototype systems to address the interplay between quantum criticality and unconventional superconductivity. Based on an in depth study of the magnetic excitation spectrum of CeCu2Si2, a prototypical heavy fermion compound, we obtain a lower bound for the change in exchange energy. The comparison with the superconducting condensation energy demonstrates that the build-up of magnetic correlations near the quantum critical point drives superconductivity in CeCu2Si2. In addition, our comparison establishes a huge kinetic energy. We argue that the recent advances in scanning probe methods applied to heavy fermions may allow to directly probe this kinetic energy loss and elucidate the relation between kinetic energy loss and the nature of the underlying quantum critical point.

Spin fluctuations are reported near the magnetic field driven quantum critical point in YbRh2Si2 [1]. On cooling, ferromagnetic fluctuations evolve into incommensurate correlations with a characteristic in-plane wave vector of $q_m = (d, d)$ with $d = 0.14 \pm 0.04$ r.l.u. At low temperatures, an in plane magnetic field induces a sharp intra doublet resonant excitation at an energy $g\mu_B\mu_0 H$ with $g = 3.8 \pm 0.2$. The intensity is localized at the zone center and has a width in momentum space indicating precession of spin density extending $\chi = 6 \pm 2$Å beyond the 4f site. [1] C. Stock, C. Broholm, F. Demmel, J. Van Duijn, J. W. Taylor, H.J. Kang, R. Hu, and C. Petrovic, Phys. Rev. Lett. 109, 127201 (2012).
Millikelvin spectroscopic imaging STM is a new approach for heavy fermion studies. Using quasiparticle interference imaging (QPI), we achieved the first visualization of heavy fermion formation [1] via splitting of a light k-space band into the two heavy fermion bands. Imaging of a Kondo-hole [2] then revealed its nanoscale heterogeneity of hybridization. The first QPI imaging of the k-space electronic structure for a heavy fermion superconductor [3] revealed the multi-band energy gaps $\Delta(k)$ of CeCoIn$_5$. Now, the heavy band-structure is used to measure the f-electron magnetic interactions. Solving the gap equations and hypothesizing these interactions as mediating Cooper pairing, yields numerous quantitative predictions. Their impressive agreement with the measured characteristics of CeCoIn$_5$ provides strong direct evidence that its pairing is mediated by the f-electron magnetism [4].


Joe Thompson, Los Alamos National Laboratory

“Building bridges between correlated f- and d-electron systems”

The heavy-fermion state that emerges at low temperatures arises from the Kondo-derived entanglement of itinerant and localized electrons in compounds based on a lattice of 4f-elements. This strongly correlated state is susceptible to instabilities, such as magnetic order and superconductivity, that have analogies in correlated 3d-electron compounds. Though the Kondo effect was discovered from the study of dilute 3d-elements in a metallic host, there are no 3d-based heavy-fermion compounds. Presumably their absence is the result of the more spatially extended wavefunctions of 3d-electrons relative to the 4fs. The 5f-electrons of Pu, which are more localized than the 3ds but more extended than the 4fs, offer the opportunity of finding electronically correlated compounds based on Pu that bridge 4f- and 3d-electron physics. The recently discovered heavy-fermion superconductors PuCoIn$_5$ and PuRhIn$_5$ and their isostructural derivatives PuCoGa$_5$ and PuRhGa$_5$ may be providing that bridge. Properties of these compounds suggest that they are near a quantum-phase transition. Like their Ce-counterparts, PuCoIn$_5$ and PuRhIn$_5$ appear to be close to a T=0 antiferromagnetic instability; whereas, the smaller effective masses and much smaller unit cell volumes of PuCoGa$_5$ and PuRhGa$_5$ suggest that they may be near a T=0 valence instability. * In collaboration with E. D. Bauer, G. Koutroulakis and H. Yasuoka. Work at Los Alamos was
performed under the auspices of the US DOE and supported by the Los Alamos LDRD program.
Abstracts III:
Poster session
Ireneusz Bulik, Rice University

1. “Density Matrix Embedding Theory from Broken Symmetry Lattice Mean-Fields”

The problem of computationally efficient treatment of strongly-correlated electronic materials remains open. Despite the plethora of available approximations, the search for more accurate and computationally affordable theoretical schemes remains unabated. In particular, the Density Matrix Embedding Theory- DMET (Phys. Rev. Lett. 109, 186404, (2012)) is a novel and promising tool that casts the problem of the correlated lattice models into an effective, frequency independent impurity model. The algorithm to find optimal bath environment is straightforward, though depends on the mean-field solution of the entire lattice model. In the present work, we investigate the performance of DMET procedure with impurity model derived from the spin-symmetry broken formalism. Moreover, we propose further approximations to DMET procedure that greatly improves convergence properties while delivering high-quality results as benchmarked for the 1D Hubbard model.

Wenxin Ding, Rice University

2. “Topological Characteristics and Anomalous Hall Effect in Frustrated Kondo Lattice Systems”

Topological characteristics of electronic states have been the focus of studies in the context of spin-orbit-coupled insulators. Pr2Ir2O7 is a frustrated Kondo system that has a large zero field anomalous Hall Effect that hints for a chiral spin liquid ground state of the local moments. Recently, thermodynamic measurements reveal a divergent Grüneisen ratio, which indicates a nearby quantum critical point. Motivated by these findings, we study the prototype chiral spin liquid state on the J1-J2 square lattice with Kondo coupling, and use it as a probe of the Kondo destruction transition. For the Kondo screened phase, we study the topological properties of the hybridized heavy quasi-particle bands, and show that they yield a zero-field anomalous Hall effect. For the Kondo destroyed phase, the chiral spin liquids state mediates an effective chiral interaction among the electrons that also give rise to a zero field anomalous Hall Effect. The behavior of the Hall response on approach, and across, the quantum critical point is discussed based on these calculations. This work has been supported by ARO and the Welch Foundation.
Shayan Hemmatiyan, Texas A&M University

3. “Quantum phase transitions in the Kondo-necklace model”

We present the results of perturbative unitary transformations for the Kondo-necklace model in the magnetic low-energy limit of strongly correlated heavy fermion materials. We study quantum phase transitions between these different phases, and show the effect of anisotropies in terms of quantum information properties and the vanishing of the energy gap. We employ the perturbative unitary transformations to calculate the energy gap and spin-spin correlations for the model in spatial dimensions $d = 1, 2, \text{and } 3$ as well as for the spin ladders. In particular, we show that the method, although being perturbative, can detect the phase transition point by imposing the spontaneous symmetry breaking, in good agreement with numerical and Green’s function methods. We also use concurrence, a bipartite entanglement measure, to probe the criticality of the model.

Leonid Isaev, Louisiana State University

4. “Orbital order and Hund’s rule frustration in Kondo lattices”

We analyze a microscopic origin of the Kondo effect-assisted orbital order in heavy-fermion materials. By studying the periodic two-orbital Anderson model with two local electrons, we show that frustration of Hund’s rule coupling due to the Kondo effect leads to an incommensurate spiral orbital and magnetic order, which exists only inside the Kondo screened (heavy-electron) phase. This spiral state can be observed in neutron and resonant X-ray scattering measurements in U- and Pr-based heavy-fermion compounds, and realized in cold atomic gases, e.g. fermionic $^{173}\text{Yb}$. 
Rayner Roberto Rodriguez Guzman and Carlos Jimenez-Hoyos, Rice University

5. “Symmetry-projected variational approaches for fermionic Hubbard systems”

We present the application of a multi-component, symmetry-projected variational ansatz to half-filled and doped 1D Hubbard systems. We provide numerical evidence that the quality of our wave functions can be improved systematically towards the exact solution. We show that the considered ansatz provides accurate correlation functions and momentum distributions that compare well with those from other theoretical approaches. Our formalism provides an intuitive physical picture that describes well the quantum fluctuations in the considered systems.

Fuxiang Li, Texas A&M University

6. “Braid group phase transition in Full counting statistics and spin noise spectroscopy”

When the interaction of a quantum system with a detector is changing from weak to strong coupling limits, the system experiences a transition from the regime with quantum mechanical coherent oscillations to the regime with a frozen dynamics. In addition to this quantum Zeno transition, we show that the full counting statistics of detector signal events also experiences a topological phase transition at the boundary between two phases at intermediate coupling of a quantum system to the detector. We demonstrate that this transition belongs to the class of topological phase transitions that can be classified by elements of the braid group. We predict that this transition can be explored experimentally by means of the optical spin noise spectroscopy.
7. “Global phase diagram of heavy fermion metals: Insights from an Ising-anisotropic Kondo lattice model tuned by a transverse magnetic field”


Johnpierre Paglione, University of Maryland

8. “Quantum-critical quasiparticle scattering in the superconducting state of CeCoIn5”

Low-temperature thermal conductivity measurements in the normal and superconducting states of the heavy-fermion metal CeCoIn5 for magnetic fields parallel to the [100] direction reveal an unprecedented increase in the electronic thermal conductivity with decreasing temperature at fields lower than the upper critical field Hc2. We will present an analysis of the temperature dependence of this contribution that indicates divergent electron-electron scattering upon approach to Hc2 from both above and below, proving the existence of a continuous field-tuned quantum critical point and an extension of quantum-critical scattering into the superconducting state. Suppression of the relative strength of inelastic magnetic scattering upon superconducting condensation provides strong evidence for a direct link between superconducting pairing and magnetic fluctuations.
Jedediah Pixley, Rice University

9. “Unconventional Superconductivity near a Kondo Destroyed Quantum Critical Point”

Experiments on quantum critical heavy fermion metals have clearly established the existence of magnetic quantum phase transitions concomitant with the suppression of Kondo entanglement. The destruction of the Kondo effect gives rise to inherently quantum modes, and leads to unusual scaling properties that go beyond conventional Landau theory. There is now strong experimental evidence, e.g. from the heavy-fermion material CeRhIn5, that such a quantum critical point (QCP) underlies a completely new and unconventional form of superconductivity. With this in mind, we study the superconducting pairing correlations in the Kondo lattice model, within a cluster extended dynamical mean field theory. We find that the Kondo energy scale is continuously suppressed at the magnetic QCP. In addition, we find the pairing susceptibility to be strongly enhanced when the QCP is approached, both from the paramagnetic Kondo screened side and from the Kondo-destroyed magnetically ordered side. Our results point to a new form of unconventional superconductivity associated with both magnetic fluctuations and a proximity to electronic localization.

Binod Rai, Rice University

10. “Intermediate valence in Yb3Rh4Ge13 single crystals”

The hybridization of the localized f-electrons with conduction electrons gives rise to unusual behavior, such as intermediate valence states, Kondo insulator, pseudogap, superconductivity, heavy fermion and non-Fermi liquid behavior, quantum criticality etc. The cubic crystal structure R3T4M13 (R = rare earth, T = transition metal, M = Si, Ge or Sn) is a family of compounds which have shown such wide variety of properties. In this presentation, I will discuss the physical properties of the new intermediate valence compound Yb3Rh4Ge13. The magnetic susceptibility is consistent with the interconfigurational fluctuations (ICF) model, while resistivity reveals poor metal behavior. The findings will be discussed in the context of search new Yb based strongly correlated systems.
Eteri Svanidze, Rice University

11. “Novel Itinerant Antiferromagnet With Nonmagnetic Constituents”

While many systems exhibit both local and itinerant magnetism, only two are known to display magnetism while being composed of non-magnetic elements - Sc$_3$In and ZrZn$_2$. Drastic differences in dimensionality, critical scaling and susceptibility to perturbations suggest that more systems like this would be useful in identifying the origin of their magnetic properties. In this talk, the properties of a new itinerant antiferromagnet with no magnetic constituents, are presented. Specific heat, resistivity and magnetization data indicate magnetic ordering below $T_N \approx 36$ K. Above this temperature, the susceptibility displays Curie-Weiss-like behavior, with an unexpectedly large paramagnetic moment $\mu_{PM} \approx 0.8 \, \mu_B \, F.U.^{-1}$. The magnetism is confirmed by band structure calculations, which suggest a spin-density wave ground state with a modulation wavevector $Q = (0, 2\pi/3b, 0)$. In collaboration with J. K. Wang, T. Besara, M. Gamza, T. Siegrist, M. C. Aronson, A. Nevidomskyy and E. Morosan.

Ilya Vekhter, Louisiana State University

12. “Heavy antiferromagnetic phases in Kondo lattices”

We propose a microscopic physical mechanism that stabilizes coexistence of the Kondo effect and antiferromagnetism in heavy-fermion systems. We consider a two-dimensional quantum Kondo-Heisenberg lattice model and show that long-range electron hopping leads to a robust antiferromagnetic Kondo state. By using a modified slave-boson mean-field approach we analyze the stability of the heavy antiferromagnetic phase across a range or parameters, and discuss transitions between different phases.
Jianda Wu, Rice University


Quantum critical point (QCP) occurs at a continuous phase transition at zero temperature. It follows from hyperscaling argument that, near a QCP, the Grneisen ratio (ratio of thermal expansion coefficient to specific heat) diverges and entropy accumulates [1]. The enhanced entropy has been observed near the field-induced metamagnetic QCP in Sr3Ru2O7[2]. Here we present a detailed theoretical study of entropy across itinerant-magnetic QCPs, with a focus on the ferromagnetic cases. We propose a regularization scheme for the effect of a dangerously irrelevant quartic coupling on the free energy [3], and calculate the entropy using this scheme. While the entropy accumulation near the QCP basically follows the hyperscaling arguments, the correction to scaling is sizable especially for the 2D case. We compare the theoretical results with the experimental data for Sr3Ru2O7 [2], providing an entropic characterization of the degree to which the metamagnetic QCP in this system is described by the itinerant-magnetic quantum criticality. [1] L. Zhu et al., PRL 91, 066404 (2003). [2] A.W. Rost et al., Science 325, 1360 (2009). [3] J. Wu, L. Zhu, and Q. Si, J. Phys.: Conf. Series. 273 012001.

Jianda Wu¹ and Marton Kormos²
¹ Rice University and ² University of Pisa

14. “Finite-temperature spin dynamics near the quantum critical point of transverse field Ising chain with a small longitudinal field”

When the transverse-field Ising chain at its quantum critical point is subjected to a small longitudinal field, the perturbed conformal field theory led to a field theory with an exotic E8 symmetry [1]. Recent neutron scattering experiments have provided evidence for the lightest two particles in this E8 model in the quasi-1D Ising ferromagnet CoNb2O6 [2]. While the zero temperature dynamic of the model is well known, its finite-temperature counterpart has not yet been systematically studied. We study the low-frequency dynamical spin structure factor at finite temperatures using the form-factor method. We show that the dominant contribution to the spin dynamics comes from the channel between two lightest particles, and demonstrate how the spin dynamics differ from a diffusion form. Using these results, we determine the temperature dependence of the NMR relaxation rate. We suggest that, for CoNb2O6, measurements of the NMR relaxation rate provide a means to further test the applicability of the E8 model. In collaboration with Qimiao Si and Marton Kormos [1] A. B. Zamolodchikov, Int. J. Mod. Phys. A4, 4235(1989).
Grain boundaries (GBs) are structural imperfections that typically degrade the performance of materials. Here we show that dislocations and GBs in two-dimensional (2D) metal dichalcogenides MX2 (M = Mo, W; X = S, Se) can actually improve the material by giving it a qualitatively new physical property: magnetism. The dislocations studied all have a substantial magnetic moment of 1 Bohr magneton. In contrast, dislocations in other well-studied 2D materials are typically non-magnetic. GBs composed of pentagon-heptagon pairs interact ferromagnetically and transition from semiconductor to half-metal or metal as a function of tilt angle and/or doping level. When the tilt angle exceeds 47 the structural energetics favor square-octagon pairs and the GB becomes an antiferromagnetic semiconductor. These exceptional magnetic properties arise from an interplay of dislocation-induced localized states, doping, and locally unbalanced stoichiometry. Purposeful engineering of topological GBs may be able to convert MX2 into a promising 2D magnetic semiconductor.
List of Participants

Elihu Abrahams  
UCLA

Meigan Aronson  
Stony Brook University,  
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Ramachandhran Balasubramanian  
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Ireneusz Bulik  
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Brian DeSalvo  
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Gleb Finkelstein  
Duke University

Zachary Fisk  
UC Irvine

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Sayed Ali Akbar Ghorashi  
University of Houston

Sarah Grefe  
Rice University

Will Hardy  
Rice University

Shayan Hemmatiyan  
Texas A&M University

Randy Hulet  
Rice University

Leonid Isaev  
Louisiana State University

Carlos Jimenez-Hoyos  
Rice University

Kevin Kelly  
Rice University

Thomas Killian  
Rice University

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