Poster session II:
Fe-based superconductivity and heavy-fermion physics

II.1 It could be either FeSCs or URu_2Si_2 heavy fermions
Girsh Blumberg (Rutgers University)

II.2 Pairing correlation and Kondo-destruction in quantum critical heavy fermions
Ang Cai (Rice University), Jed Pixley, Qimiao Si

Abstract:
How quantum criticality affects superconductivity is a central issue in strongly correlated systems. The problem is particularly pressing when the quantum criticality is beyond the Landau framework of order-parameter fluctuations, such as appearing in heavy fermion systems in the form of Kondo destruction [1]. In addition, T_c in the heavy fermion systems is high as measured by their Fermi temperature. With these motivations, we address the pairing instabilities near a Kondo destruction quantum critical point (QCP). We study the cluster Bose-Fermi Anderson model and, using the Cluster Extended-DMFT approach, the Anderson lattice model. We have identified a Kondo destruction QCP between a heavy fermi liquid and an antiferromagnetic metal phase, and demonstrated enhanced pairing correlations in its vicinity [2]. Finally, we will discuss our initial studies on the role of multipolar degrees of freedom, showing a sequential destruction of a spin-orbital-coupled SU(4) Kondo entanglement and its realization in a cubic heavy fermion system $Ce_3Pd_{20}Si_6$ [3].
[1] Q. Si and F. Steglich, Science 329, 1161 (2010).
[2] A. Cai et al., to be published.
[3] V. Martelli et al., arXiv:1709.09376.

II.3 Memory matrix theory of a disordered antiferromagnetic metal with an effective composite operator
Hermann Freire (Federal University of Goias, Brazil)

Abstract:
We compute the dc resistivity, the Hall angle and the magnetoresistance of the spin-fermion model, which is a phenomenological theory to describe the physics of the cuprates and iron-based superconductors. We investigate both the role of the spin-fermion interaction that couples the large-momentum antiferromagnetic fluctuations to the so-called ‚hot-spots' at the Fermi surface and also of an effective higher-order composite operator in the theory. The latter operator provides a scattering mechanism such that the momentum transfer for the fermions close to the Fermi surface can be small. We also include weak disorder that couples to both the bosonic order-parameter field and the fermionic degrees of freedom. Since the quasiparticle excitations were shown in recent works to be destroyed at the ‚hot-spots' in the low-energy limit of the model, we employ the Mori-Zwanzig memory matrix approach that permits the evaluation of all transport coefficients without assuming well-defined Landau quasiparticles in the system. We then apply this transport theory to discuss universal metallic-state properties as a function of temperature and magnetic field of the cuprates from the perspective of their fermiology, which turn out to be in qualitative agreement with key experiments in those materials.

II.4 Pairing fingerprints in iron-based superconductors

Rudolf Hackl (Bavarian Academy of Sciences), T. Boehm, F. Kretschmar, A.Baum, M. Rehm, D. Jost, R. Hosseinian Ahangharnejhad, R. Thomale, C. Platt, T.A. Maier, W. Hanke, B. Moritz, S. Maiti, P.J. Hirschfeld

Abstract:
Resolving the microscopic pairing mechanism and its experimental identification in unconventional superconductors is among the most vexing problems of contemporary condensed matter physics. We show that Raman spectroscopy provides an avenue for this quest by probing the structure of the pairing interaction at play in an unconventional superconductor. As we study the spectra of the prototypical Fe-based superconductor $Ba_{1-x}K_xFe_2As_2$ for $0.22\le x \le 0.70$ in all symmetry channels, Raman spectroscopy allows us to distill the leading s-wave state. In addition, the spectra collected in the B_{1g} symmetry channel reveal the existence of two collective modes which are indicative of the presence of two competing, yet sub-dominant, pairing tendencies of $d_{x^2-y^2}$ symmetry type. A comprehensive functional Renormalization Group (fRG) and random-phase approximation (RPA) study on this compound confirms the presence of the two sub-leading channels, and consistently matches the experimental doping dependence of the related modes. The synopsis of experimental evidence and theoretical modelling supports a spin-fluctuation mediated superconducting pairing mechanism.

II.5 The Charge Transport Phenomenology of the Strange Metal State in Ba-122
Ian Hayes(UC Berkeley), J. G. Analytis, N. Maksimovic, Z. Hao, M. K. Chan, B. J. Ramshaw, R. D. McDonald, P.J.W. Moll

Abstract:
After more than thirty years of research on the high-Tc cuprates, several parts of their phase diagrams remain a mystery, including the Strange Metal regime out of which superconductivity develops at the highest temperatures. The urgency of this problem has been heightened in the last few years with the discovery of the iron based superconductor and the recognition that they exhibited a very similar Strange Metal properties in their transport coefficients, including a T-linear resistivity near optimal doping and an anomalous T-dependence in the Hall effect. I will present measurements of transport coefficients at ultra high magnetic fields (up to 92 Tesla) in the iron-based high-Tc BaFe2(As,P)2 that extend this phenomenology considerably by finding important parallels between their field and temperature dependencies. In particular we identify a scaling relationship in the resistivity that connects the T-linear resistivity in zero field to a B-linear resistivity at low temperatures around optimal doping, and an anomalous field dependence in the Hall effect that is peaked around optimal doping. I will discuss the extent to which these observations may be considered evidence of a nearby quantum critical point and review possibilities for the further exploration of high-Tcs with ultra high magnetic fields.

II.6 Optical conductivity of iron-based superconductors
Christopher Homes (Brookhaven National Laboratory), Yaomin Dai, Xianggang Qiu, Genda Gu

Abstract:
The superconducting cuprates are doped-Mott insulators with a single band crossing the Fermi level. In contrast, the iron-based superconductors are multiband materials with hole and electron pockets at the center and corners of the Brillouin zone, respectively. These metallic materials are either

superconducting, or superconductivity may be induced through chemical substitution. Key questions are: (i) what is the nature of the normal state from which superconductivity emerges, and (ii) how do the superconducting energy gaps manifest themselves on the different bands? By examining the complex optical conductivity of these materials, we can disentangle the contributions from the different pockets to determine the nature of the transport in the different bands. In addition, we can also determine the size of the gaps and the bands to which they correspond.

II.7 AC Elastoresistivity

Alexander Hristov(Stanford University), Johanna C. Palmstrom, Joshua A. W. Straquadine, Tyler A. Merz, Harold Y. Hwang, Ian R. Fisher

Abstract:
Measurements of elastoresistivity have been used to identify the electronic nematic susceptibility in the iron based superconductors, providing evidence for an electronically driven nematic quantum critical point close to optimal doping in several families of iron superconductors. However, measurements close to this critical point are precluded by the onset of superconductivity and are further complicated by observed deviations of the nematic susceptibility from expected functional forms above the superconducting state.

We extend previous measurements by developing a new technique for applying strain at finite frequency, opening a new possibility for the use of dynamical strain as a probe of quantum materials. This AC elastoresistivity technique is applied to the study of the nematic fluctuations near optimal doping to investigate the role of disorder in the deviations of nematic susceptibility from a Curie-Weiss law.

II.8 Orbital-Selective Pairing and Nematic Order in the Iron-Based Superconductors

Haoyu Hu (Rice University), Emilian M. Nica, Rong Yu, Qimiao Si

Abstract:
The considerations of the orbital-selective Mott phase in the normal state [1,2] motivated the theoretical proposal for orbital-selective pairing [3]. The experimental evidence has come from both the iron pnictides [4] and the iron selenides [5]. Motivated by the recent experiments, we theoretically study the role of nematic order in the orbital-selective pairing within multi-orbital models for superconductivity driven by short-range magnetic exchange interactions. We present systematic results on how the pairing-state competition [6], the orbital dependency of the intra-orbital pairing amplitudes, and the gap anisotropy change with the nematicity.

[1] R. Yu and Q. Si, PRL 110, 146402 (2013); PRB 84, 235115 (2011).
[2] M. Yi et al., PRL 110, 067003 (2013).
[3] R. Yu, J.-X. Zhu and Q. Si, PRB 89, 024509 (2014).
[4] C. Zhang et al., Phys. Rev. Lett. 111, 207002 (2013).
[5] P. O. Sprau et al., Science 357, 75 (2017).
[6] E. M. Nica, R. Yu and Q. Si, Npj Quantum Materials 2, 24 (2017).

II.9 Frustrated magnetism and quantum transitions of nematic phases in FeSe

Wenjun Hu (Rice University), Hsin-Hua Lai, Shou-Shu Gong, Rong Yu, Andriy H. Nevidomskyy, and Qimiao Si

Abstract:
The iron-based superconductivity has been known to develop near an antiferromagnetic order, but this paradigm apparently fails in FeSe. This system displays a nematic order while being non-magnetic, raising the puzzle about the origin of its nematic order. Here we show that the phase diagram of FeSe can be fully described by a quantum spin model with highly frustrated interactions. We perform density matrix renormalization group calculations on a frustrated spin-1 bilinear-biquadratic model on the square lattice, and find three stable phases breaking C4 rotational symmetry, including the antiferromagnetic states with wave vectors (0,pi) and (pi/2,pi), and a (pi,0) antiferroquadrupolar state. Tuning the ratio of competing interactions, we show quantum transitions from the (pi,0) antiferroquadrupolar order to the (pi,0) antiferromagnetic state, either directly or through the (pi/2,pi) antiferromagnetic order. Our findings explain the dramatic experimental observations of an orthorhombic antiferromagnetic order in the pressurized FeSe, and suggest that superconductivity in a wide range of iron-based materials has a common origin in the antiferromagnetic correlations of strongly correlated electrons.

II.10 Renormalization group study on the coupled nematic-magnetic quantum phase transitions in the presence of quenched disorder
Jian Kang (NHMFL/Florida State University), Rafael Fernandes and Laimei Nie

Abstract:
Recent elasto-resistance measurements in iron-based superconductors revealed a puzzling interplay between disorder and nematic quantum criticality. Theoretically, in the case in which nematic order is promoted by magnetic fluctuations in an itinerant system, renormalization group calculations of the appropriate low-energy model predict a simultaneous first-order nematic-magnetic quantum phase transition, and, consequently, the absence of a nematic quantum critical point. Here, we investigate how these results are affected by the presence of isotropic quenched disorder, which is manifested as a random-mass term in the low-energy model. By combining the replica trick and the renormalization group approach, we investigate the existence of nematic fixed points, and discuss whether disorder can promote a second-order nematic quantum phase transition that is split from the magnetic quantum phase transition.

II.11 Orbital physics in iron based superconductors
Elio Koenig (Rutgers University), Piers Coleman, Alexei M. Tsvelik

Abstract:
We investigate the role of orbital degrees of freedom in the context of quasi 1D and quasi 2D iron based superconductors. Motivated by the recent experimental discovery of superconductivity in the ladder material BaFe2S3 we present an RG study of an effective 2-leg ladder with spin and orbital degrees of freedom which captures the essential physics of iron based quasi 1D materials. The RG analysis shows a rich phase diagram, including Mott phases and an s_{+--} superconductor which is stabilized by Hund\'s interaction. The quasi 1D material also motivates a Fermi surface geometry independent explanation of the robustness of Tc with respect to Coulomb repulsion. We thoroughly study the question and conclude that the flexibility of moving gap nodes and orbital degrees of freedom is unlikely capable to explain the robustness, it is too expensive in Tc. We therefore discuss alternative pairing mechanisms.

II.12 Model for Ferromagnetic Quantum Critical Point in a 1D Kondo Lattice
Yashar Komijani (Rutgers University), Piers Coleman

Abstract:
Motivated by recent experiments, we study a quasi-one dimensional model of a Kondo lattice with Ferromagnetic coupling between the spins. Using bosonization and dynamical large-N techniques we establish the presence of a Fermi liquid and a magnetic phase separated by a local quantum critical point, governed by the Kondo breakdown picture. Thermodynamic properties are studied and a gapless charged mode at the quantum critical point is highlighted.

II.13 Spin excitation anisotropy and nematic fluctuations in the iron pnictides
Chia-Chuan Liu (Rice University), Elihu Abrahams, Qimiao Si

Abstract:
To elucidate the electronic nematic correlations in the iron pnictides, we study the spin excitation anisotropy defined by the difference between the dynamical spin susceptibilities at (pi,0) and (0,pi) [1]. We consider an effective theory for the spin and Ising-nematic degrees of freedom [2] in the presence of a small external C4-symmetry-breaking potential. Our analysis is carried out both perturbatively and in a large N limit [3]. We connect the spin excitation anisotropy to the dynamical spin susceptibility and the nematic susceptibility. This relationship provides the understanding of the singular energy dependences observed in the optimally Ni-doped $BaFe_2As_2$ under a uniaxial strain.
[1] Y. Song, X. Lu, D. L. Abernathy, D. W. Tam, J. L. Niedziela, W. Tian, H. Luo, Q. Si, and P. Dai, Phys. Rev. B 92, 180504 (2015).
[2] J. Dai, Q. Si, J. X. Zhu, and E. Abrahams, PNAS 106, 4118, (2009).
[3] J. Wu, Q. Si and E. Abrahams, Phys. Rev. B 93, 104515 (2016).

II.14 Fe-vacancy and superconductivity in FeSe superconductor
Tung-Sheng Lo (Institute of Physics, Academia Sinica), C.H. Wang, K.C. Huang, T.S. Lo, K.Y. Yeh, P.M. Wu, M.J. Wang, and Maw-Kuen Wu

Abstract:
It was found that with a careful control of material synthesizing processes, numerous rich phases have been observed in the FeSe-based system. Detailed studies show that the Fe-vacancy ordered phases, which are non-superconducting Mott insulators, are the parent compounds of the superconductors. Superconductivity emerges from the parent phases by disordering the Fe vacancy, often by a simple annealing treatment. Recent high temperature X-ray diffraction experiments show that the degree of structural distortion associated with the disorder of Fe-vacancy is closely related to volume fraction of the superconductivity observed. These results suggest the strong lattice to spin coupling are important for the occurrence of superconductivity in FeSe based superconductors.

II.15 Quantum Monte Carlo study of pairing in systems with incipient bands
Thomas Maier(Oak Ridge National Laboratory), Vivek Mishra, and Douglas Scalapino

Abstract:
The nature and mechanism of superconductivity in the extremely electron-doped iron-chalcogenides continues to be a matter of wide debate. In these systems, the hole-like band has dropped below the Fermi energy, challenging the leading spin-fluctuation based theory of pairing that relies on the presence and nesting

properties of both electron- and hole-Fermi surface pockets. Here, we use dynamic cluster quantum Monte Carlo calculations of a bilayer Hubbard model to gain insight into this problem. These calculations show that s+- pairing remains robust and dominant over d-wave pairing, even when the hole band does not cross the Fermi energy. The gap on the submerged band has the opposite sign and larger magnitude than the gap on the electron band. Consistent with previous phenomenological calculations, this demonstrates that an incipient band can have a decisive effect on the pairing symmetry of the Fermi surface states.

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II.16 Experimental Evidence for non-quasiparticle dynamics in quantum critical metals
Ross Mcdonald (Los Alamos National Lab), Arkady Shekhter, Laurel Winter, Mun Chan, Jon Betts, Kim Modic, Brad Ramshaw, James Analytis

II.17 Competing electronic phases in Na-doped SrFe2As2
Christoph Meingast (Karlsruhe Institute of Technology), L. Wang, M. He, F. Hardy, M. Merz, P. Schweiss, Th. Wolf, P. Adelmann

Abstract:
Hole-doped ReFe2As2 (Re = Ba, Sr, Ca) exhibit much richer phase diagrams than the corresponding electron-doped systems. In particular, the phase diagram of Na-doped BaFe2As2 K-doped BaFe2As2 exhibits a small pocket of a double-Q reentrant C4 magnetic phase [1], as well as another yet unidentified magnetic phase [2]. In strong analogy with the charge order observed in underdoped cuprates [3], these additional phases strongly compete with the emerging superconducting order [2,4].

Here we present a detailed phase diagram of the Na-doped SrFe2As2 system using thermodynamic probes (heat capacity, thermal expansion and magnetization). The double-Q C4 reentrant phase is much more stable in this system, and our data demonstrates that the phase diagram of Na-doped SrFe2As2 exhibits even more complexity than the K- and Na-doped BaFe2As2 counterparts. We discuss our results in terms of spin and possible charge-ordering phenomena.
[1] J. M. Allred et al., Nature Physics 12, 493,Äì498 (2016).
[2] L. Wang et al., Phys. Rev. B93, 014514 (2016).
[3] B. Keimer et al. Nature 518, 179 (2015).
[4] A. E. Boehmer et al., Nat. Commun. 6, 7911 (2015).

II.18 Intertwined orders in superconducting CeCoIn5
Roman Movshovich (Los Alamos National Lab), Duk Y. KIM, Franziska WEICKERT, Michel KENZELMANN, Eric D. BAUER, Filip RONNING, J. D. THOMPSON

Abstract:
We will present measurements of the thermal conductivity of heavy-fermion superconductor CeCoIn5 in rotating magnetic field, that provide a clear evidence for intertwined orders in its high field superconducting (HFSC) phase [1]. Experiments were performed in a dilution refrigerator coupled with a superconducting magnet, allowing investigations down to 20mK and fields up to 14T. The sample, polished with a long axis in the [110] direction of tetragonal

CeCoIn5, nodal for its dx2-y2 order parameter, was mounted with c-axis parallel to the horizontal axis of rotation of a piezo-electric rotator. Recent neutron scattering measurements [2] indicated that the SDW order in the HFSC phase is single-domain. The ordering wave-vector Q switches abruptly when magnetic field is rotated through the anti-nodal [100] direction, with Q choosing the direction (node) more perpendicular to the magnetic field. Q in our experiment, therefore, switched from being parallel to perpendicular to the direction of the heat current. The observed anisotropy of the heat current calls for a presence of a third order intertwined with the d-wave and SDW. A p-wave pair-density-wave, suggested theoretically to exist in a d-wave superconductor with an SDW order, can explain our results.

II.19 Critical Properties of Bulk Doped BaFe2As2 Pnictides for Magnet Design
Martin Nikolo (Saint Louis University), Jeremy D. Weiss, John Singleton, Jianyi Jiang, and Eric E. Hellstrom

Abstract:
A comprehensive study of upper critical (Hc2) and irreversibility magnetic fields (Hirr) in (Ba0.6K0.4)Fe2As2 (critical temperature Tc = 38.3 K), Ba(Fe0.95Ni0.05)2As2 (Tc = 19.2 K), Ba(Fe0.94Ni0.06)2As2 (Tc = 18.5¬†K), Ba(Fe0.92Co0.08)2As2 (Tc = 23.2¬†K), and Ba(Fe0.91Co0.09)2As2 (Tc = 25.3¬†K) polycrystalline bulk pnictide superconductors with different average grain sizes was made in pulsed fields at the Los Alamos National Laboratory. The magnetic field-temperature (Hc2-T) phase diagrams with Hc2 as high as 65¬†T at 28¬†K for the K-doped samples and critical current density (Jc) measurements as high as 105¬†A/cm‚Äì2 for the smallest, sub-micrometer grain size samples were obtained. The high Hc2, Hirr, and Jc data shows the suitability of these materials for magnet design as their mechanical strength and random grain alignment show promise in the manufacturing of next generation magnets.

II.20 Pressure-driven Lifshitz and Other Transitions in 122-Pnictides
Khandker Quader (Kent State University), Michael Widom

Abstract:
Using first principles calculations, we discuss that observed pressure-driven anomalies in the 122 iron-arsenic pnictides family (AFe_2As_2; A = alkali earth element Ca, Sr, Ba) can be understood [1-3] as consequences of Lifshitz transitions arising from changes in Fermi surface topology at T=0. Our results for band dispersions, spectra, lattice parameters, enthalpies, magnetism, and elastic constants over a wide range of hydrostatic pressure provide a coherent understanding of multiple transitions in these compounds: enthalpic, magnetic, and tetragonal (T) collapsed tetragonal (cT) transitions. We also show that the while the enthalpic transition from striped AFM orthorhombic (OR) to nonmagnetic tetragonal (T) state occurs at a pressure, P_H, the OR state remains metastable up to a higher pressure, P_M > P_H. We find anomalies in magnetism and orthorhombicity as P ‚Üí PM and a trend towards elastic instability [4].
[1] K. Quader, M. Widom, Phys. Rev. B 90, 144512 (2014).
[2] M. Widom, K. Quader, Phys. Rev. B 88, 045117 (2013).
[3] K. Quader , M. Widom, Contrib, Plasma Phys. 55, 128 (2015).
[4] M. Widom, K. Quader, Supercond. Nov. Magn. (2015).

II.21 Structure prediction and origin of competing magnetism, nematicity and superconductivity in Fe-based superconductors
Zhiping Yin (Beijing Normal University), Yundi Quan

Abstract:
Understanding the structure-property relation of materials is the central theme of condensed matter physics. Standard density functional theory (DFT) calculations are usually unsatisfactory in predicting the structures and electronic properties of strongly correlated materials. The family of iron-based superconductors (IBS) is one of such examples, where DFT calculations severely underestimate the distance between the iron and pnicogen/chalcogen planes, leaving microscopic understanding of their complex phase diagram impossible when experimental input is limited. Here we use first-principles many-body theory calculations to optimize the crystal structure of a number of IBS by minimizing the free energy. We obtain the pnicogen/chalcogen position within one percent of experimental values for most compounds, in strong contrast to 10 percent error from plain DFT calculations. We further predict the Se position in FeSe under pressure where different experimental measurement gave rather diverse Se positions. With the optimized Se position, we are able to understand the complex phase diagram of FeSe under pressure which consists of competing nematic, magnetic and superconducting orders. Our results point to the key role of spin fluctuations in understanding the phase diagram of IBS. Our ability to accurately predict the structure of IBS has great potential in designing novel correlated materials and studying existing materials (such as monolayer thin films) whose structures are difficult to measure in experiments.

II.22 Polarized Inelastic Neutron Studies of Dynamical Magnetism in Parent and Superconducting Fe(Te,Se)

Igor Zaliznyak (Brookhaven National Lab), J. Tranquada, G. D. Gu, Z. Xu, G. Xu, A. Savici, O. Garlea

Abstract:
We present recent polarized inelastic neutron scattering surveys of the temperature-dependent magnetic response in parent material of the chalcogenide family, Fe(1+y)Te, and the optimally doped superconductor, FeTe0.55Se0.45. We observe that the structure of local dynamical correlations in the superconducting sample in the energy range of spin resonance, at high temperature acquires features similar to those found in the under-doped samples [1], and which are also observed in the optimally doped samples at higher energy. Our results indicate the unusual and energy- and temperature-dependent orbital composition of dynamical magnetism in these unconventional superconductor family materials.

[1] I. Zaliznyak, A. T. Savici, M. Lumsden, A. Tsvelik, R. Hu, C. Petrovic.``Spin-liquid polymorphism in a correlated electron system on the threshold of superconductivity”, Proc Natl Acad Sci USA, (2015).