TT 30: Superconductivity: Fe-based Superconductors - Theory

Time: Tuesday 11:00–13:00 Location: H19

Invited Talk TT 30.1 Tue 11:00 H19

Selective correlations and heavy-fermionic behaviour in Iron-based superconductors — •Luca de' Medici — European Synchrotron Radiation Facility, 71 Av. des Martyrs, 38000 Grenoble, France — Ecole Supérieure de Physique et Chimie industrielles de la Ville de Paris, 10 rue Vauquelin, 75005 Paris - France

The matching between recent experimental evidences from various probes and realistic theoretical calculations highlights the coexistence, in the normal phase of Fe-based superconductors, of strongly correlated and weakly correlated electrons. This peculiar situation can be backtracked to the influence of Hund's coupling exchange interaction between the conduction electrons in these materials, and can be controlled to some degree. In some of these compounds this differentiation can get quite extreme and gives rise to heavy-fermionic behaviour. We will speculate that these and similar d-electron materials could constitute a new ballpark for the exploration of heavy-fermionic physics, and of its applications. A new possible application of the strong thermomagnetic properties that can in principle be found in heavy-fermions is proposed: self-cooling of high-current cables.

[1] L. de' Medici, G. Giovannetti and M. Capone, PRL **112**, 177001 (2014)
[2] L. de' Medici in *Iron-based Superconductivity*, Springer Series in Materials Science **211**, 2015, pp 409-441
[3] L. de' Medici, ArXiv:1506.01674

TT 30.2 Tue 11:30 H19

Hundness versus Mottness in a Three-Band Hund Model with Relevance for Iron-Pnictides — •Katharina M. Stadler[1], Zhiping Yin[2], Jan von Delft[1], Gabriel Kotliar[2], and Andreas Weichselbaum[1] — [1]Ludwig Maximilians University, Munich, Germany — [2]Rutgers University, New Jersey, USA

The recently discovered iron pnictide superconductors (as well as chalcogenides, ruthenates, and other 4d transition metal oxides) show puzzling anomalous properties, like a coherence-incoherence crossover, also in the normal state. While there is consensus about strong correlation effects playing a key role in these materials, their precise origin (Coulomb repulsion or Hund's rule coupling between electrons of different orbitals) has been under debate as one of the major open questions in the field many years. In a recent detailed study of the Hund metal problem [1] the coherence-incoherence crossover was shown to be connected to spin-orbital separation and to be clearly driven by Hund's rule coupling.

In order to better understand the differences between Mott insulators and Hund metals we explore the phase diagram for a three-band model with Coulomb repulsion and Hund's rule coupling on a Bethe lattice at 1/3 filling using the numerical renormalization group to obtain a numerically exact dynamical mean-field theory solution.

[1] K. M. Stadler et al., PRL **115**, 136401 (2015)

TT 30.3 Tue 11:45 H19

Current induced magnetic flux response in frustrated three-band superconductors as a bulk probe of broken time reversal symmetry (BTRS) ground states — Yuriy Yerin[1], Alexander Omelyanchouk[1], •Stefan-Ludwig Drechsler[2], Jeroen van den Brink[2], and Dmitri Efremov[2] — [1]Verkin Inst. for Low Temperature Physics and Engineering. 61103 Kharkiv, Ukraine — [2]Inst. for Theor. Solid State Physics at the Leibniz Inst. for Solid State an Materials Research, IFW-Dresden, D-01171 Dresden, Germany

Within the Ginzburg-Landau formalism we provide a classification of all possible ground states (GS) of a three-band superconductor (3BSC) where either frustrated states with BTRS or a single non-BTRS GS with unconventional/conventional s-wave symmetry, respectively, exist. The necessary condition for a BTRS GS in general cannot be reduced to a "-"sign of the product of all interband couplings (IBC) valid in the case of 3 equivalent bands with repulsive equal IBC, only. It corresponds to a maximal IBC frustration. We show that with increasing diversity of the parameter space this frustration is reduced and the regions of possible BTRS GS start to shrink. We track possible evolutions of a BTRS GS of a 3BSC based doubly-connected system in an external magnetic field. Depending on its parameters, a magnetic flux can induce various current density leaps, connected with adiabatic or non-adiabatic transitions from BTRS to non-BTRS states and vice versa. The current induced magnetic flux response of samples with a doubly-connected geometry e.g. as a thin tube provides a suitable experimental tool for the detection of BTRS GS.

TT 30.4 Tue 12:00 H19

Dynamical coupled modes theory for an $s_{\pm}$-pairing mechanism of superconductivity in doped iron pnictides — Mikhail Kiselev[1], •Dmitry Efremov[2], Stefan-Ludwig Drechsler[2], Konstantin Kikoin[3], and Jeroen van den Brink[2] — [1]International Center for Theoretical Physics, I-34151 Trieste, Italy — [2]Institute for Theoretical Solid State Physics at the Leibniz Institute for Solid State an Materials Research Dresden, IFW-Dresden, D-01171 Dresden, Germany — [3]School of Physics and Astronomy, Tel Aviv University, 69978 Tel Aviv, Israel

We develop a high-temperature approach to the problem of the interplay between magnetic and superconducting phases in multi-band iron pnictides. A dynamical mode-mode coupling theory is derived from the the microscopic theory based on the solution of the coupled Bethe-Salpeter equations. We focus on the vicinity to a spin density wave (SDW) where spin fluctuations enhance the onset of superconducting ordering. Special attention is paid to arsenic deficient materials where As vacancies behaves as effective magnetic defects [1]. The proposed theory allows generalization to multi-mode regimes.

[1] K. Kikoin, S.-L. Drechsler, K. Koepernik, J. Málek, and J. van den Brink, Nature, Scientific Reports **5**, 11280 (2015).

TT 30.5 Tue 12:15 H19

Robust Determination of the Superconducting Gap Sign Structure via Quasiparticle Interference — •Dustin Altenfeld[1], Peter Hirschfeld[2], Ilya Eremin[1,3], and Igor Mazin[4] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Department of Physics, University of Florida, Gainesville, Florida 32611, USA — [3]Kazan Federal University, Kazan 420008, Russian Federation — [4]Code 6393, Naval Research Laboratory, Washington, DC 20375, USA

Using an electronic theory, we present a qualitative description to identify sign changes of the superconducting order parameter via quasiparticle interference (QPI) measurement in Fe-based superconductors (FeSc). In particular, we point out that the temperature dependence of the momentum-integrated QPI data can be used to differentiate between s_{+-} and s_{++} states in a system with typical iron pnictide Fermi surface. We show that the signed symmetrized and antisymmetrized QPI maps are useful to obtain a characteristic signature of a gap sign change or lack thereof, starting from two-band model up to ab initio based band structure calculation. We further suggest this method as a robust way of the determination of the superconducting gap sign structure in experiment and discuss its application to the LiFeAs compounds.

TT 30.6 Tue 12:30 H19

The role of the d-filling in DFT+DMFT calculations of pnictides containing Chromium — •Martin Edelmann[1], Luca de' Medici[2], Massimo Capone[3], Gianluca Giovannetti[3], and Giorgio Sangiovanni[1] — [1]ITPA Universitaet Wuerzburg, Wuerzburg, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy

In the recent years, transition-metal-pnictides gained attention as among them there are new high-T_c superconductors. The physical effects are strongly influenced by the Hund's coupling and the extent of this influence directly depends on the orbital occupation. We calculate quasiparticle properties in Chromium-pnictide materials of different classes via DFT+DMFT. To this aim, we construct various localized bases, consisting of only the transition-metal d orbitals located around the chemical potential or also including ligands' p states. We then analyze the orbital-resolved quasiparticle weight and the scattering rates as well as modifications of the Fermi surfaces due to electronic correlation. These help in understanding why the electronic properties of the various families are compatible with a localized as well as an itinerant picture.

TT 30.7 Tue 12:45 H19

Spin-wave Excitations in Tetragonal and Orthorhombic Spin-Density-Wave Phases of Iron Pnictides — •Daniel David Scherer and Brian Møller Andersen — Niels Bohr Institute, University of Copenhagen, 2100, Copenhagen, Denmark

The most prominent and abundant spin-density-wave (SDW) state found theoretically and experimentally in the Fe-based superconductor materials features stripy orthorhombic magnetic order in the Fe layer with ordering vectors $\mathbf{Q}_1 = (\pi, 0)$ or $\mathbf{Q}_2 = (0, \pi)$. Recently, however, tetragonal magnetic orders have been discovered in these systems [1-4]. A candidate for a commensurate tetragonal SDW state is a spin- and charge-ordered state (SCO) that was previously understood [5,6] as a superposition of two stripy orders with an induced checkerboard charge order. Starting from a DFT-derived 5-orbital model for the electronic degrees of freedom, we here focus on a theoretical investigation of the spin-wave spectra in the orthorhombic stripy SDW and tetragonal SCO states within an itinerant weak-coupling approach, and present a comprehensive comparison of our results to experimental data.

[1] S. Avci et al., Nat. Commun. **5**, 3845 (2014).
[2] A. E. Böhmer et al., Nat. Commun. **6**, 7911 (2015).
[3] J. M. Allred et al., arXiv:1505.06175.
[4] L. Wang et al., arXiv:1510.03685.
[5] X. Wang and R. M. Fernandes, Phys. Rev. B **89**, 144502 (2014).
[6] M. N. Gastiasoro and B. M. Andersen, Phys. Rev. B **92**, 150506(R) (2015).