TT 17: SC: Iron-Based Superconductors - Theoretical Approaches

Time: Tuesday 14:00–16:15 Location: H20

TT 17.1 Tue 14:00 H20

Relation of structure, magnetism, doping and pressure in $AFe_{2-x}T_xAs_2$ (T=Co,Rh,Ru) — •Helge Rosner, Walter Schnelle, Deepa Kasinathan, Miriam Schmitt, Ulrich Schwarz, Michael Nicklas, Christoph Geibel, and Andreas Leithe-Jasper — MPI-CPfS Dresden, Germany

We present an overview of our recent investigations on the $SrFe_{2-x}T_xAs_2$ (T = Co, Ru, Rh) compounds. In our joint experimental and theoretical study, we report the influence of hydrostatic pressure and substitution at the Fe site on the magneto-structural and superconducting transitions. The magnetism is weakened upon the application of pressure as indicated by resistivity, X-ray data and density functional band structure calculations. Similar to substitution on the Sr site, substitutions on the Fe-site quench the magnetic transition and induce bulk superconductivity with T_c up to 20 K for ambient pressure and up to 27 K for underdoped $SrFe_{2-x}Co_xAs_2$ for pressures of 2.6GPa. In our analysis, we attempt to disentangle the interplay of charge doping and structural changes induced by the substitution and by external pressure.

TT 17.2 Tue 14:15 H20

Magnetism and pairing symmetries in a three-orbital model for pnictides — •Maria Daghofer[1], Andrew Nicholson[2,3], Adriana Moreo[2,3], and Elbio Dagotto[2,3] — [1]IFW Dresden, Dresden, Germany — [2]University of Tennessee, Knoxville, USA — [3]Oak Ridge National Laboratory, USA

While the shape of the Fermi surface (FS) obtained with the local density approximation (LDA) can be reproduced by a two-orbital model, three orbitals are needed to produce the degeneracy of the hole pockets. We discuss a three-orbital model including the xz, yz, and xy orbitals of the iron ions, which qualitatively reproduces the FS shape and orbital composition obtained by LDA calculations for undoped pnictides [1,2]. Since this model is not at half filling, orbital order becomes a possibility in addition to various magnetic phases. Using numerical techniques, we find an antiferromagnetic metal at realistic Coulomb interaction, while orbital order is only induced at at interaction strengths that are probably too strong to be realistic for pnictides. We also investigate possible pairing operators allowed by the lattice symmetry. We find that almost all of them lead to intra- as well as inter-band pairing, i.e., Cooper pairs that are formed by two electrons coming either from the same or from different bands. We also discuss consequences of inter-band pairing.

[1] A. Moreo, M. Daghofer, A. Nicholson, E. Dagotto, PRB **80**, 104507 (2009)

[2] M. Daghofer, A. Nicholson, A. Moreo, and E. Dagotto arXiv:0910.1573

TT 17.3 Tue 14:30 H20

Spin Density Waves in the Iron Pnictides - Itinerant Magnetic Excitations — •Johannes Knolle[1], Ilya Eremin[1,2], and Andrey Chubukov[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany — [2]Institut für Mathematische und Theoretische Physik, TU Braunschweig, D-38106 Braunschweig, Germany — [3]Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

We study the spin wave excitations of the parent iron-based superconductors employing the three band model which consists of one hole pocket centered around the Γ-point, and two elliptic electron pockets centered around $(\pi, 0)$ and $(0, \pi)$ points of the Brillouin zone (BZ), respectively. Without taking ellipticity into account, the spin wave excitations are degenerate at $(\pi, 0)$ and $(0, \pi)$ points representing the degeneracy of the underlying spin state. The ellipticity removes the degeneracy and selects the required $(\pi, 0)$ or $(0, \pi)$ state. Simultaneously, it also leaves only one gapless Goldstone mode. We analyze the dispersion of the spin waves along the symmetry points of the first BZ for various strengths of the ellipticity parameter and compare the results with available experimental data. We find that neutron scattering data on the damping of the spin waves and their dispersion can be well described within the itinerant description.

TT 17.4 Tue 14:45 H20

Itinerant spin excitations in the spin-density-wave state of the iron pnictides — •Philip Brydon and Carsten Timm — Technische Universität Dresden, Dresden, Germany

The proper understanding of the antiferromagnetism of the iron pnictide parent compounds is expected to provide important insights into the superconductivity of these materials. We consider a model where the spin density wave (SDW) arises from an excitonic instability of nested electron-like and hole-like Fermi pockets [1]. Using the random phase approximation, we obtain the transverse spin susceptibility within the SDW state, which allows us to determine the collective spin-wave dispersions and the single-particle continua [2]. Our results are compared to experimental findings, and the implications for electronic-only models of the SDW order are discussed.

[1] P. M. R. Brydon and C. Timm, Phys. Rev. B 79, 180504(R) (2009).

[2] P. M. R. Brydon and C. Timm, Phys. Rev. B 80, 174401 (2009).

15 min. break

TT 17.5 Tue 15:15 H20

The Curious Iron Pnictides: A Mottness Point of View — •Mukul Laad[1] and Luis Craco[2] — [1]Institut für Theoretische Physik, RWTH Aachen D-52056, Aachen, Germany — [2]MPI-CPfS, Nöthnitzer Strasse 40, 01187 Dresden, Germany

Based on perusal of various experiments, we propose that Fe pnictides are "bad metals" close to a Mott-Hubbard instability, as in the classic V_2O_3. First-principles LDA+DMFT calculations confirm this suspicion, giving excellent quantitative agreement with a host of one- and two-particle responses.

We have studied the instability of this "bad metal" to an unconventional SC, whose gap function has an admixture of extended-s and s_{xy} components. This, to our knowledge, is the first time that such an instability has been studied within LDA+DMFT.

Invited Talk TT 17.6 Tue 15:30 H20

Nature of Pairing in the FeAs Superconductors — •Siegfried Graser[1], Thomas A. Maier[2], Alexander F. Kemper[3], Peter J. Hirschfeld[3], and Douglas J. Scalapino[4] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Oak Ridge National Laboratory, Oak Ridge, USA — [3]University of Florida, Gainesville, USA — [4]University of California, Santa Barbara, USA

A comparison of the new high-T_c superconductors of the iron pnictide and chalcogenide family to the cuprates reveals startling similarities between the two classes: both are layered materials with mainly 2D character, a conductivity that is dominated by d-electrons, and an antiferromagnetic or spin-density wave phase in proximity to the superconducting state. However, the pronounced multiband character of the iron pnictides, that becomes manifest in several disconnected Fermi surface sheets, distinguishes them from the cuprates and requires a multiorbital description of its electronic properties. This multiorbital character of the bands at the Fermi level together with the rich momentum structure of the Fermi surface allows for a wide variety of possible superconducting ground states. We have explored the symmetry of the superconducting state assuming a pairing mechanism based on the exchange of spin fluctuations using a 5-orbital tight-binding Hamiltonian fitted to the LDA band structure of LaOFeAs. We could show that not only the symmetry but also the anisotropy of the pairing state depends sensitively on the intra- and interorbital interaction parameters.

TT 17.7 Tue 16:00 H20

Superconductivity in the Fe-Pnictides - From first principle calculations to effective RG studies — •Christian Platt[1], Ronny Thomale[2], Andrei Bernevig[2], Carsten Honerkamp[3], and Werner Hanke[1] — [1]Universität Würzburg — [2]Princeton University — [3]RWTH Aachen

The functional Renormalization Group (fRG) is used to determine the superconducting (SC) mechansim in the ferropnictides, with the main emphasis on distiguishing universal and material-specific aspects. To this end we use a five-band d-orbital whose interactions, in contrast to earlier fRG studies, are not taken as scalar model parameters, but calculated "a priori" from constrained RPA calculations. We universally find a SC pairing instability, driven by inter-Fermi surface (FS)

scattering and resulting in a sign-changing s+- wave order parameter. However, the gap anisotropy is shown to be dependent on material-specific orbital parameter deviations not only by the "non-interacting" (i.e. LDA) part of the d-orbital Hamiltonian, but also by self-energy corrections.