TT 110: Superconductivity: Fe-based Superconductors – Theory

Time: Friday 9:30–12:15 Location: H 2053

TT 110.1 Fri 9:30 H 2053

Mass renormalization and unconventional pairing in multi-band Fe-based superconductors- a phenomenological approach — •S.-L. Drechsler[1], S. Johnston[2], D. Efremov[1], V. Grinenko[1], H. Rosner[3], and K. Kikoin[4] — [1]IFW-Dresden — [2]Inst. of Quantum Matter, University of Brit. Coulumbia, Vancouver, Canada — [3]MPI-cPfS, Dresden, — [4]Tel Aviv University, Israel

Combining DFT calculations of the density of states and plasma frequencies with experimental thermodynamic, optical, ARPES, and dHvA data taken from the literature, we estimate both the high-energy (Coulomb, Hund's rule coupling) and the low-energy (el-boson coupling) electronic mass renormalization [H(L)EMR] for typical Fe-pnictides with T_c<40 K, focusing on (K,Rb,Cs)Fe_2As_2, (Ca,Na)122, (Ba,K)122, LiFeAs, and $LaFeO_{1-x}F_xAs$ with and without As-vacancies. Using Eliashberg theory we show that these systems can NOT be described by a very strong el-boson coupling constant $\lambda \gtrsim 2$, being in conflict with the HEMR as seen by DMFT, ARPES and optics. Instead, an intermediate $s_\pm$ coupling regime is realized, mainly based on interband spin fluctuations from one predominant pair of bands. For (Ca,Na)122, there is also a non-negligible intraband el-phonon/orbital fluctuation intraband contribution. The coexistence of magnetic As-vacancies and high-T_c =28 K for $LaFeO_{1-x}F_xAs_{1-\delta}$ excludes an orbital fluctuation dominated s_{++} scenario at least for that system. In contrast, the line nodal $BaFe_2(As,P)_2$ near the quantum critical point is found as a superstrongly coupled system. The role of a pseudo-gap is briefly discussed for some of these systems.

TT 110.2 Fri 9:45 H 2053

Magnetic and orbital ordering in the iron-based superconductors: role of spin-orbit coupling — •Felix Ahn[1], Johannes Knolle[2], Rafael Fernandes[3], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [3]School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, USA

We analyze the magnetic ordering in the iron-based superconductors in presence of spin-orbit coupling. Based on several tight-binding parametrizations of the 3d electron states we show how the spin-orbit coupling introduces the anisotropy of the magnetization of the striped antiferromagnetic state by lifting the degeneracy of all three components of the magnetization m_x, m_y and m_z. The orientation of the magnetic moment is determined by the contribution of the xy, xz, and yz orbitals to the electronic states near the Fermi level of the electron and hole bands and is determined by the electron filling. We find that within an itinerant approach the magnetic ordering is most favorable along the wavevector of the striped AF state. This appears to be a natural consequence of the spin-orbit coupling in the striped AF state where the ferro-orbital order of the xz and yz orbitals is only a consequence of the striped AF order. We further analyze the role of spin-orbit coupling for the C_4 magnetic structure where SDW order parameters with both wavevectors, $Q_x = (\pi, 0)$ and $Q_y = (0, \pi)$, coexist.

TT 110.3 Fri 10:00 H 2053

Superconductivity and Magnetism from First Principles — •Andreas Linscheid, Antonio Sanna, Frank Essenberger, and Eberhard K.U. Gross — Max-Planck-Institut für Mikrostrukturphysik

Magnetism has intriguing effects in superconductors. On the one hand static magnetic fields are known to suppress the superconducting state while dynamic spin-fluctuations are the probable candidate to explain the pairing in the Fe-based Superconductors.

Achieving an ab-initio description is important. First, because this allows to compute the critical field and whether a local coexistence of magnetic and superconducting phases exist. Second, the critical temperature of a material is among the predicted properties which allows to search yet unknown superconductors on a computer.

The Density Functional Theory for Superconductors (SCDFT) has been very successful in predicting T_c of phonon mediated superconductors. We include the magnetic density into SCDFT so that the electronic Kohn-Sham system now reproduces the electronic density $n(\mathbf{r})$, the order parameter of superconductivity $\chi(\mathbf{r}, \mathbf{r}')$ and the magnetic density $\mathbf{m}(\mathbf{r})$. We derive the xc-potential and discuss some first results.

Furthermore, we discuss an effective electron interaction mediated by spin-flip processes based on the exact spin-susceptibility. We drive a xc-functional for SCDFT that includes this effective interaction and present some results.

TT 110.4 Fri 10:15 H 2053

Coherence-incoherence crossover and non-Fermi-liquid self-energy in Hund's metals - Insights into the normal state of iron pnictide superconductors from a Numerical Renormalization Group study — •Katharina M. Stadler[1], Andreas Weichselbaum[1], Jan von Delft[1], and Gabriel Kotliar[2] — [1]Faculty of Physics, Ludwig-Maximilians-Universität München — [2]Department of Physics and Astronomy, Rutgers University, NJ, USA

In 2008, the iron pnictides were discovered as a new class of strongly correlated high-temperature superconductors [1]. The normal state of these itinerant multi-band materials shows characteristic anomalous properties, which are assigned to a coherence-incoherence crossover at very low temperatures, mediated by Hund's rule coupling.

We study a N-channel Anderson impurity model with Hund's coupling and a filling of N-1, together with the corresponding Kondo model, for the cases N=2 and 3, using the full density-matrix Numerical Renormalization Group (fdmNRG) with non-abelian symmetries [2]. Our high-quality real-frequency NRG results confirm the existence of a Fermi-liquid regime at low temperatures and a non-Fermi-liquid power-law for the self-energy in the incoherent normal state. Further, we analyse the interplay of spin and orbital degrees of freedom to gain insights into the relevant energy scales of the coherence-incoherence crossover and the corresponding renormalization group flow. In addition the lattice model is investigated within DMFT employing fdmNRG as impurity solver.

[1] Takahashi et al., Nature 453 (2008).
[2] A. Weichselbaum, Ann.Phys. 327 (2012).

TT 110.5 Fri 10:30 H 2053

Pair-breaking due to orbital magnetism in iron-based superconductors — •Mareike Hoyer[1,2], Mathias S. Scheurer[1], Sergey V. Syzranov[3,1], and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]Department of Physics, University of Boulder, Boulder, Colorado, USA

We consider superconductivity in the presence of impurities in a two-band model suited for the description of iron-based superconductors. We analyze the effect of interband scattering processes on superconductivity, allowing for orbital, i. e., non-spin-magnetic time-reversal-symmetry-breaking impurities. Pair-breaking in such systems is described by a nontrivial phase in an interband-scattering matrix element. We find that the transition temperature of conventional superconductors can be suppressed due to interband scattering, whereas unconventional superconductors may be unaffected. As an example, we consider impurities associated with orbital density waves that are of interest for iron-based superconductors.

15 min. break.

TT 110.6 Fri 11:00 H 2053

Investigation of substitution effects in the 122-family of the iron superconductors via orbital based CPA — •Alexander Herbig, Rolf Heid, and Robert Eder — Institute for Solid State Physics, Karlsruhe Institute of Technology

The iron-based superconductors are a prominent example how doping can be used as a tuning parameter for the electronic properties of a complex material. A lot of theoretical and experimental effort has been put into the investigation of this class of materials over the last half decade. But until now first principle calculations on the impact of substitution on the electronic structure using supercells and more advanced methods still are rare. Also the role of doping is not fully understood. We recently developed an implementation of Blackman, Esterling and Berk's extension of the coherent potential approximation (BEB-CPA) within a pseudopotential approach using a linear combina-

tion of atomic orbitals (LCAO) basis. We present electronic structure calculations for the 122-family using this method with various species substitutions at different sites and arbitrary impurity concentrations. In particular we investigate orbitally selective effects of substitutional disorder on electronic bands near the Fermi level and the impact of substitution on the electronic density.

TT 110.7 Fri 11:15 H 2053

Inelastic Scanning Tunneling Microscopy in conventional and unconventional superconductors — •Patrik Hlobil, Jörg Schmalian, Wulf Wulfhekel, and Jasmin Jandke — Karlsruhe Institute of Technologie, Germany

Electron tunneling spectroscopy has been used extremely successful in order to verify the microscopic phonon pairing mechanism in conventional BCS superconductors using the Eliashberg theory. Nevertheless, earlier theories and experiments focused mainly on elastic tunneling processes. We present, motivated by recent experiments, a theoretical description of inelastic tunneling in STM in which an electrons tunnels from the tip into a BCS superconductor and coherently excites a phonon during the tunneling process. This additional channel enhances the measured conductivity and we show that if the superconductor is in the normal state, within some limitations, the derivative $\mathrm{d}\sigma/\mathrm{dV}$ will be proportional to the Eliashberg function α2F. Additionally, the influence of the inelastic contributions on the tunneling spectrum in the superconducting state will be discussed. Finally, we generalize the theory to other bosonic excitations and focus on the question if inelastic tunneling could be used to unveil the electronic pairing mechanism in the iron pnictides.

TT 110.8 Fri 11:30 H 2053

Unexpected impact of magnetic disorder on multiband superconductivity — •Dmitri Efremov[1], Maxim Korshunov[2], Alexander Golubov[3], and Oleg Dolgov[4] — [1]IFW Dresden, Germany — [2]Kirensky Institute of Physics, Krasnoyarsk, Russia — [3]University of Twente, Enschede, The Netherlands — [4]Max-Planck-Institute for Solid State Physics, Stuttgart, Germany

We analyze how the magnetic disorder affects the properties of the two-band s_{++} and s_{+-} models, which are subject of hot discussions regarding iron-based superconductors and other multiband systems like MgB_2 . We show that there are several cases when the transition temperature is not fully suppressed by magnetic impurities in contrast to the Abrikosov-Gor'kov theory, but a saturation of Tc takes place in the regime of strong disorder. These cases are: (1) the purely interband impurity scattering, (2) impurity scattering purely in one of the bands, (3) the unitary scattering limit. We show that the a transition between s_{++} and s_{+-} states may occur with increasing magnetic disorder.

TT 110.9 Fri 11:45 H 2053

Anisotropic transport properties of Ba-122 compounds calculated by the Kubo-formalism — •Gerald Derondeau[1], Sebastian Wimmer[1], Diemo Ködderitzsch[1], Hubert Ebert[1], and Ján Minár[1,2] — [1]Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany — [2]NewTechnologies-Research Center, University of West Bohemia, Pilsen, Czech Republic

We have shown recently that the Korringa-Kohn-Rostoker-Green function (KKR-GF) method, in combination with the coherent potential approximation (CPA), indeed provides a very suitable platform to describe the impact of substitutional disorder on the electronic structure of iron pnictide superconductors. [1]

Based on this we focused on the resistivity anisotropy of Ba-122 compounds, which lately received tremendous interest. [2, 3]

We use the Kubo-formalism to calculate the longitudinal resistivity of doped Ba-122 compounds in their antiferromagnetic state within the framework of the local approximation to density-functional-theory. We are able to reproduce the unusual resistivity anomaly and investigate the transport behavior for different substitution types in $BaFe_2As_2$. The dependence of the transport properties on the type and the concentration of the dopant suggest a crucial influence of impurity scattering for the resistivity anomaly in iron pnictides.

[1] G. Derondeau *et al.*, Phys. Rev. B **90**, 184509 (2014).
[2] J.-H. Chu *et al.*, Science **329**, 824 (2010).
[3] S. Ishida *et al.*, Phys. Rev. Lett. **110**, 207001 (2013).

TT 110.10 Fri 12:00 H 2053

Transport in the spin-density-wave phase of iron pnictides — •Maxim Breitkreiz[1], Jacob Schmiedt[1], Philip M. R. Brydon[2], and Carsten Timm[1] — [1]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, USA 20742

The metallic spin-density-wave phase of iron pnictides shows characteristic and not yet understood features such as the pronounced anisotropy of the resistivity, the enhanced Hall coefficient, and magnetoresistance. We analyze the transport behavior within the linear-response theory and take into account scattering off spin fluctuations and damped magnons. Vertex corrections turn out to be very important because of strong anisotropy in the scattering rates and the reconstructed Fermi surfaces.