TT 68: Superconductivity: Fe-based Superconductors - Theory I

Time: Wednesday 15:00–18:00 Location: HSZ 201

Invited Talk TT 68.1 Wed 15:00 HSZ 201

Novel Effects of Disorder in Multiband Unconventional Superconductors — •Peter J Hirschfeld — Phys. Dept.. U. Florida, Gainesville FL 32611, USA — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main

Impurities been studied in superconductors for many years because, depending on the type of impurity and on the symmetry of the superconducting state, they may break Cooper pairs. They thus play an important diagnostic role in deducing the type of superconductivity one has in a newly discovered material. I focus here on the Fe-based superconductors, which are multiband in character and probably exhibit unconventional pairing states, including so-called "s+/-" states which change sign of the order parameter between bands. Impurity scattering in such states depends sensitively on the ratio of intra- to interband scattering, giving rise to novel effects of disorder, including possible transitions to conventional "s++" states and lifting of gap nodes. I propose that one can uniquely identify an s+/- state by a sequence of transitions with controlled disorder, observable in bulk quasiparticle transport or NMR. I next focus on STM experiments, and the inability of current lattice-based theories to capture not only the fine structure of STM conductance maps, but also certain local symmetries. I propose to remedy this by using a Wannier-function based extension of the BdG equations of inhomogenous superconductivity. Finally, I discuss the role of correlations in creating C4 symmetry-broken emergent defect states, which may have important consequences for the ubiquitous electronic nematicity observed in these materials.

TT 68.2 Wed 15:30 HSZ 201

Suppression of T_c due to impurity scattering with a phase — •Mareike Hoyer[1], Sergey Syzranov[1,2], and Jörg Schmalian[1,3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Department of Physics, University of Colorado, Boulder, Colorado, USA — [3]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany

We consider weak disorder in a two-band superconductor and investigate the effect of a finite phase of the off-diagonal matrix element of the impurity potential in band representation. In particular, we analyze the impact on the superconducting transition temperature T_c. We concentrate on s^{++} and s^{+-} symmetries of the superconducting order parameter which are widely discussed as possible candidates in iron pnictides.

We argue that the effect of impurity scattering on the transition temperature in complex materials such as iron pnictides cannot be reduced to the consideration of single-particle scattering rates. Depending on the phase ϕ, we find that nonmagnetic impurities can act as pair-breakers for the s^{++} state while such impurities can leave T_c for the s^{+-} state unchanged.

TT 68.3 Wed 15:45 HSZ 201

Electronic and Magnetic Properties of $Ba(Fe_{1-x}Co_x)_2As_2$ — •Gerald Derondeau, Sergiy Mankovsky, Hubert Ebert, and Ján Minár — Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany

Characteristic for most iron arsenides is an antiferromagnetic ordering in form of a commensurate spin-density wave (SDW) at low temperatures, often coupled with a structural phase transition. Superconductivity emerges when these transitions are suppressed, e.g. by chemical doping. As many DFT calculations have still problems to accurately describe the magnetic state [1] further investigations on this issue are needed.

We investigated the low-temperature orthorhombic phase of $Ba(Fe_{1-x}Co_x)_2As_2$ using the Korringa-Kohn-Rostoker-Green function (KKR-GF) [2] approach which allows inclusion of chemical disorder via the coherent potential approximation (CPA). To examine the magnetic structure with different spin states we used a full magnetic unit cell with 8 Fe atoms and antiferromagnetic ordering. In addition spin-spiral calculations for the $\boldsymbol{q}$-dependent induced magnetization were performed to account for the SDW state. Furthermore, the doping dependent evolution of the strong in-plane anisotropy of the electronic structure as observed in ARPES measurements [3] was investigated and connected to the magnetic behavior.

[1] I. I. Mazin, M. D. Johannes, Nature Phys. *5*, 141 (2009)
[2] H. Ebert, D. Ködderitzsch, J. Minár, Rep. Prog. Phys. *74*, 96501 (2011)
[3] M. Yi, D. Lu, J.-H. Chu, *et al.*, PNAS *108*, 6878 (2011)

TT 68.4 Wed 16:00 HSZ 201

Electronic structure modification and ultrafast SDW generation due to coherent oscillation of the A_{1g} phonon mode in $BaFe_2As_2$ — •Bhaskar Kamble and Ilya Eremin — Institut für Theoretische Physik III, Ruhr Universität Bochum, 44801 Bochum, Germany

Time-resolved ARPES experiments on $BaFe_2As_2$ demonstrate an in-phase oscillation of the ARPES spectral function at the Γ and M points [1], while time-resolved (tr) optical conductivity measurements on normal $BaFe_2As_2$ detect a periodic Spin Density Wave (SDW) at ultrafast time scales [2]. The period of oscillation in both cases equals the A_{1g} phonon frequency in which the As atoms oscillate perpendicular to the Fe-planes. With a 5-orbital tight-binding (TB) model with the TB parameters dependent on the As-Fe-Fe angle α, and assuming that the electrons react adiabatically to the α oscillation in the A_{1g} phonon, our calculations for changes in the electronic spectral function match well with tr-ARPES results if (i) α oscillates around a value slightly greater than its equilibrium value, and (ii) the electronic spectral function in the photoexcited state is calculated at a temperature higher than in the absence of the laser pulse. The mean-field magnetic order parameter for the (π,0) SDW state shows that the magnetization increases with α. This, coupled with the enhanced mean-α value in the photo-induced A_{1g} phonon, offers a simple explanation for the ultrafast SDW-generation observed in normal $BaFe_2As_2$.

[1] L. Rettig, Ph.D. thesis (Freie-Universität Berlin) (2012)
[2] K. W. Kim et al., Nature Mat. 11, 497 (2012)

TT 68.5 Wed 16:15 HSZ 201

LDA+DMFT study of the iron-pnictide superconductor KFe_2As_2 — •Steffen Backes, Daniel Guterding, Harald Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität, Frankfurt

We study the electronic structure of the iron pnictide superconductor KFe_2As_2, including electronic correlations within dynamical mean field theory. The recent theoretical studies based on density functional calculations (DFT) turned out to be unable to satisfactorily describe experimental observed properties of the electronic band structure. However, treating electronic correlations beyond the local density approximation within an LDA+DMFT (dynamical mean field theory) approach has shown to be a very effective method to overcome some of these discrepancies. Therefore, we perform a comprehensive LDA+DMFT investigation focused on features of the KFe_2As_2 compound that have not been dealt with in existing studies. We also benchmark our findings with ARPES measurements. Our results indicate that KFe_2As_2 is a moderately correlated metal, where the Fe 3d orbitals show an electron mass enhancement of a factor of about 2. We find that only when including correlations beyond DFT the shape and size of the hole Fermi surface in experiment can satisfactorily be described. Furthermore, due to correlations a topological change in the Fermi surface is induced, where compared to DFT the hole pocket at the Z point vanishes in LDA+DMFT in agreement with experiments. We also observe a strong k_z-dispersion of the middle hole cylinder around Γ along the k_z-axis , which is not seen in DFT.

15 min. break.

TT 68.6 Wed 16:45 HSZ 201

de Haas-van Alphen effect and effective masses in KFe_2As_2 from LDA+DMFT — •Daniel Guterding, Steffen Backes, Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

We investigate changes in de Haas-van Alphen (dHvA) frequencies and effective masses in the iron-based superconductor KFe_2As_2 upon inclusion of correlation effects beyond the local density approximation (LDA). Quantitative comparison of our findings to dHvA measurements shows that a combination of density functional theory with

dynamical mean-field theory (LDA+DMFT) solves the disagreement between previous *ab-initio* calculations and experiment. We also show how to numerically extract de Haas-van Alphen frequencies and effective masses from band structure calculations.

TT 68.7 Wed 17:00 HSZ 201

Wannier orbitals via the projector method for LAPW and effects of correlation in the (collapsed) tetragonal phases of $CaFe_2As_2$ — •Jean Diehl and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

We present a scheme for constructing Wannier orbitals from a (linear) augmented plane wave basis set via projection. This method shows strong sensitivity on the chosen energy window as we discuss. On this projector method we build our code to implement dynamical mean field theory based on density functional theory.

The former introduced method is then used to study the effects of correlation by means of Hubbard U and Hund's rule J in one of the iron pnictides $CaFe_2As_2$. We present results for the band structure, Fermi surface and mass enhancements of the room-temperature ambient-pressure tetragonal and the high-pressure low-temperature collapsed tetragonal phase.

TT 68.8 Wed 17:15 HSZ 201

Using Space Group Representations to Unfold the Band-structures of Iron Pnictides — •Milan Tomic, Roser Valentí, and Harald Jeschke — Institut für Theoretische Physik, Goethe-Universität, Frankfurt am Main, Germany

We present a general method for unfolding bandstructures beyond the limit of translational symmetry, utilizing irreducible representations of space groups. We demonstrate the method on the representative materials of 11 and 122 iron-pnictide family and discuss the result in context of ARPES experiments.

TT 68.9 Wed 17:30 HSZ 201

Topological Surface States in Paramagnetic, Antiferromagnetic, and Superconducting Iron Pnictides — •Alexander Lau — Institute of Theoretical Physics, Technische Universität Dresden, Dresden, Germany

Motivated by the topologically nontrivial electronic structure of iron pnictides, we study surface states in various strip geometries. For the paramagnetic phase, the existence of these states can be understood from a topological argument. If we go to the antiferromagnetic phase, the surface bands split, depending on the geometry of the strip. In the superconducting phase, assuming an $s_{\pm}$-wave gap structure, the topological surface states under certain conditions remain in the gap. Interestingly, they exist side by side with Andreev bound states for small superconducting gaps and even merge with them for increasing gap amplitude. The bulk and surface dispersions are obtained from exact diagonalisation of two- and five-orbital models.

TT 68.10 Wed 17:45 HSZ 201

Negative transport times in Fe-based superconductors — •Maxim Breitkreiz[1], Philip M. R. Brydon[2], and Carsten Timm[1] — [1]Institute of Theoretical Physics, Technische Universität Dresden, Dresden, Germany — [2]Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, USA

Negative transport times lead to unexpected transport behavior such as negative magnetoresistance, strongly enhanced Hall coefficient, and reduced resistivity. Within a semiclassical Boltzmann approach beyond the relaxation-time approximation, we demonstrate that negative transport times can arise in iron pnictides due to scattering of charge carriers at spin fluctuations. To explore this effect, we consider the temperature dependence of transport coefficients for a phenomenological two-band model relevant for iron pnictides.