TT 32: SC: Fe-based Superconductors - Theory

Time: Wednesday 10:30–13:00 Location: HSZ 304

TT 32.1 Wed 10:30 HSZ 304

Optical spectra and bandstructure in the SDW phase of the iron pnictides using density functional theory — •Johannes Ferber, Yu-Zhong Zhang, Kateryna Foyevtsova, Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe- Universität Frankfurt

Understanding the antiferromagnetic (SDW) phase of the iron pnictides is important as superconductivity in these systems arises from either doping or pressurizing the antiferromagnetic parent compounds. However, density functional calculations in these systems are known to largely overestimate the magnetic moments. In our calculations, we suppress the moments to reasonable values and analyse the optical conductivity and bandstructure, finding that a number of features observed in experiments can be reproduced in this way. In addition, we consider the effect of spin excitations on the optical conductivity. Whereas the static antiferromagnetic order is commonly taken into account in DFT calculations, spin flip terms which lead to spin excitations (magnons) are not considered. Using a high-quality tight-binding model, we include the coupling of the electrons to the magnons into the calculation of the optical conductivity.

TT 32.2 Wed 10:45 HSZ 304

Effect of Impurities and Effect of Ellipticity on the Spin Resonance in Iron-Based Superconductors — •Johannes Knolle[1], Saurabh Maiti[2], Ilya Eremin[3], Andrey Chubukov[2], and Mike Norman[4] — [1]Max-Planck-Institut fur Physik komplexer Systeme, D-01187 Dresden, Germany — [2]Department of Physics, University of Wisconsin-Madison, Madison,Wisconsin 53706, USA — [3]Institut fur Theoretische Physik III, Ruhr-Universitat Bochum, D-44801 Bochum, Germany — [4]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439-4845, USA

Iron-based superconductors are believed to have an unconventional order parameter with $s\pm$ symmetry. Due to the sign change of the superconducting gap a spin resonance develops below the superconducting transition temperature. Based on an effective four-band model we analyze the doping dependence of this spin resonance and its sensitivity to non-magnetic, as well as, magnetic impurities. For zero ellipticity of the electron pockets the resonance becomes incommensurate at a critical doping δ_c, and, overall, the dispersion forms a so-called X-shape. For finite ellipticity, ϵ, the resonance splits into two incommensurate peaks and δ_c increases with increasing ϵ.

Both non-magnetic and magnetic impurities broaden the resonance. Its position depends on the interplay between the two impurity kinds and their intra- and inter-band scattering components. We find that the ratio between ω_{res}/T_c increases with the strength of the interband impurity scattering which is consistent with available experimental data.

TT 32.3 Wed 11:00 HSZ 304

Self-consistent spin wave theory in the collinear phase and its application to iron pnictides — •Daniel Stanek[1], Michael Holt[2], Oleg P. Sushkov[2], and Götz S. Uhrig[1] — [1]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]School of Physics, University of New South Wales, Kensington 2052, Sydney NSW, Australia

A possibility to describe magnetism in the iron pnictide parent compounds in terms of the two dimensional frustrated Heisenberg J_1-J_2 model has been actively discussed recently. However, neutron scattering studies have revealed the three dimensional character of the magnetism in the iron pnictides and an anisotropy between the exchange perpendicular and parallel to the spin stripes. Based on these observations, we study the J_1-J_2-J_c model as the three dimensional generalization of the J_1-J_2 model for $S = 1$ and $S = 1/2$. Using self-consistent spin wave theory, we present a detailed description of the staggered magnetization and magnetic excitations in the collinear state. Interestingly, two qualitatively distinct ways are found how the collinear, magnetically long-range ordered phase becomes unstable. Either the magnetization or one of the spin wave velocities vanishes. In addition, we discuss the relevance of a biquadratic exchange, which explains a part of the anisotropy between the effective in-plane exchange constants on the level of self-consistent spin wave theory.

In the application for the 122 iron pnictides, the experimentally measured spin wave dispersion is compared to the one derived within our model.

TT 32.4 Wed 11:15 HSZ 304

Doping dependence of antiferromagnetism in the pnictides — •Jacob Schmiedt[1], P.M.R. Brydon[1], Maria Daghofer[2], and Carsten Timm[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

Various models have been proposed to describe the antiferromagnetic phase in iron pnictides. Models that take into account five d-orbitals are expected to contain all necessary information that is needed for the explanation of this phase. Based on RPA and mean-field calculations we investigate the doping dependence of the AFM phase in several different five-orbital models. In each of them a strong enhancement of the critical temperature is found for hole doping. We seek to understand this behavior by examining the corresponding change of the Fermi surface and its nesting properties.

TT 32.5 Wed 11:30 HSZ 304

Superconductivity and Magnetism in Iron-Based Superconductors: Insights from Quasiparticle Interference — •Alireza Akbari[1], Johannes Knolle[2], Ilya Eremin[1], and Roderich Moessner[2] — [1]Theoretische Physik III, Ruhr-Universität Bochum, D-44780, Bochum, Germany — [2]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany

The phase diagram of iron-based superconductors exhibits an anti ferromagnetic phase at low doping and an unconventional superconducting phase at larger carrier concentration. Some compounds are even believed to have a microscopic coexistence regime of both orders. We systematically calculate quasiparticle interference (QPI) signatures for the whole phase diagram of iron-based superconductors. Impurities inherent in the sample together with ordered phases lead to distinct features in the QPI images that are believed to be measured in spectroscopic imaging-scanning tunneling microscopy (SI-STM).

In the spin-density wave phase the rotational symmetry of the electronic structure is broken, signatures of which are also seen in the coexistence regime with both superconducting and magnetic order.

In the superconducting regime we show how the different scattering behavior for magnetic and non-magnetic impurities allows to verify the $s\pm$ symmetry of the order parameter. The effect of possible gap minima or nodes is discussed.

[1] A. Akbari, J. Knolle, I. Eremin, and R. Moessner, Phys. Rev. B, 82, (2010) (in press).
[2] J. Knolle, I. Eremin, A. Akbari, and R. Moessner, Phys. Rev. Lett. 104, 257001 (2010).

15 min. break

TT 32.6 Wed 12:00 HSZ 304

Cleavage behavior and surface states in Ferropnictides — •Klaus Koepernik[1], Alexander Lankau[1], Helmut Eschrig[1], Jeroen van den Brink[1], Sergey Borisenko[1], Erik van Heumen[2], and Mark S. Golden[2] — [1]IFW Dresden, Germany — [2]Zeeman Institute, University of Amsterdam, Netherlands

We present a density functional study of the surface electronic structure and the cleavage behavior of LiFeAs and Co-doped $BaFe_2As_2$. The results are discussed together with angle resolved photo emission (ARPES) and low energy electron diffraction (LEED) data. The two systems behave rather differently and we conclude that LiFeAs will be the ideal system for surface sensitive probes among the iron pnictide family.

TT 32.7 Wed 12:15 HSZ 304

Dichotomy between Large Local and Small Ordered Magnetic Moments in Iron-Based Superconductors — •Alessandro Toschi[1], Philipp Hansmann[1], Ryotaro Arita[2], Shiro Sakai[1], Giorgio Sangiovanni[1], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, Austria — [2]Department of Applied Physics, University of Tokyo, Japan

We study a four-band model for iron-based superconductors within the local density approximation combined with dynamical mean-field theory (LDA + DMFT). This successfully reproduces the results of models which take As p degrees of freedom explicitly into account and has several physical advantages over the standard five d-band model. Our findings[1] reveal that the new superconductors are more strongly correlated than their single-particle properties suggest. Two-particle correlation functions unveil the dichotomy between local and ordered magnetic moments in these systems, calling for further experiments to better resolve the short time scale spin dynamics.

[1] P. Hansmann, R. Arita, AT, S. Sakai, G. Sangiovanni, K. Held, Phys. Rev. Lett. **104**, 197002 (2010)

TT 32.8 Wed 12:30 HSZ 304

Order-Parameter Anisotropies in the Pnictides - An Optimization Principle for Multi-Band Superconductivity — •Christian Platt[1], Ronny Thomale[2], and Werner Hanke[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg — [2]Department of Physics, Princeton University

Using general arguments of an optimization taking place between the pair wave function and the repulsive part of the electron-electron interaction, we analyze the superconducting gap in materials with multiple Fermi-surface (FS) pockets, with application to two proto-type (P-based and As-based) ferropnictides. The main point of our work is to show that the SC state, its gap and, in particular, its anisotropy in momentum space is determined by an optimization, which balances the interplay between the attractive interaction in the sign-reversing $s_{\pm}$-channel and the Coulomb repulsion. This Coulomb repulsion, as discussed below, is unavoidable in a multi-band SC situation: it appears because of a kind of frustration in the $s_{\pm}$-channel, when more than two FS-pockets are involved in setting up the pairing interaction. On the basis of functional Renormalization Group (fRG) calculations for a wide parameter span of the bare interactions and for the different FS topologies applying to these two characteristic Fe-based superconductors, we show that the symmetry of the gap and the nodal versus nodeless behavior is driven by this optimization requirement.

TT 32.9 Wed 12:45 HSZ 304

Antiferromagnetic order in multi-band Hubbard models for iron-pnictides — •Tobias Schickling[1], Florian Gebhard[1], and Jörg Bünemann[2] — [1]Fachbereich Physik, Philipps Universität, Renthof 6, 35032 Marburg — [2]Institut für Physik, BTU Cottbus, Postfach 101344, 03013 Cottbus

In our presentation, we discuss the physics of multi-band Hubbard models for LaOFeAs which we have investigated by means of the Gutzwiller variational theory [1]. An analysis of the paramagnetic ground state shows that neither Hartree–Fock mean-field theories nor effective spin models describe these systems adequately. In contrast to Hartree–Fock-type approaches, the Gutzwiller theory predicts that antiferromagnetic order requires substantial values of the local Hund's-rule exchange interaction. For a three-band model, the antiferromagnetic moment fits experimental data for a broad range of interaction parameters. However, for the more appropriate five-band model, the iron e_g electrons polarize the t_{2g} electrons and they substantially contribute to the ordered moment. Therefore, we argue that an inclusion of the arsenic $4p$ bands is essential for a proper description of the magnetic order in LaOFeAs.

[1] T. Schickling, F. Gebhard, and J. Bünemann, arXiv:1011.6219