TT 69: Superconductivity: Fe-based Superconductors - Theory

Time: Friday 9:30–12:15 Location: H21

TT 69.1 Fri 9:30 H21

Fermi surface topology of LaFePO, LiFeP and LiFeAs — •Harald O. Jeschke, Johannes Ferber, and Roser Valenti — Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany

We performed charge self-consistent LDA+DMFT (density functional theory combined with dynamical mean field theory) calculations to study correlation effects on the Fermi surfaces of the iron pnictide superconductors LaFePO, LiFeP and LiFeAs. We find a distinctive change in the topology of the Fermi surface in LaFePO and LiFeP where a hole pocket with Fe $3d_{z^2}$ orbital character changes its geometry from a closed shape in LDA to an open shape upon inclusion of correlations. In LiFeAs correlations influence mostly the shape of the hole pockets. We discuss our results in the context of angle-resolved photoemission spectroscopy and de Haas van Alphen observations.

TT 69.2 Fri 9:45 H21

Finite temperature and pressure molecular dynamics for $BaFe_2As_2$ — •Steffen Backes and Harald Jeschke — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Germany

We investigate the temperature and pressure dependence of the structural and electronic properties of the iron pnictide superconductor $BaFe_2As_2$. We use density functional theory based Born-Oppenheimer molecular dynamics simulations to study the system at temperatures from $T = 5$ K to 150 K and pressures from $P = 0$ to 30 GPa. When increasing the pressure at low temperature, we find the two transitions from orthorhombic to tetragonal to collapsed tetragonal that are also observed in zero temperature structure relaxations and in experiment. However, the first of these transitions is considerably smeared out at finite temperature. We find a negative slope of the tetragonal to collapsed tetragonal transition in the T-P phase diagram in very good agreement with experiment. We also analyze the electronic structure of $BaFe_2As_2$ at finite temperature and work out differences between the time averaged band structure and Fermi surface at finite temperature compared to the known zero temperature results. Our results should be helpful for understanding some contradictions in experimental reports for $BaFe_2As_2$ under high pressure.

TT 69.3 Fri 10:00 H21

Lattice dynamics of binary FeAs from first principles — •Alexander Herbig[1,2], Rolf Heid[2], and Klaus-Peter Bohnen[2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie

Since the discovery of superconductivity in fluorine-doped LaFeAsO in 2008, the research on the so-called iron pnictides is rapidely developing. One of their building blocks, the FeAs layers, seem to play an important role for the physical properties of the iron pnictides. The rare theoretical work on binary FeAs motivated us to perform ab-initio calculations of electronic structure and lattice dynamics of this compound by means of density functional and linear response theory within the mixed-basis pseudopotential method.

We compared different collinear magnetic states with same crystal structure. Thereby an antiferromagnetic state, which is the best collinear approximation to the experimentally observed spin density wave [1], exhibits the lowest total energy in good agreement with previous calculations [2]. Without spin polarization, we found unstable phonon modes while magnetism stabilizes the phonon spectra.

Until now, no direct measurements of the phonon spectra are available. For the purpose of validating our phonon calculations we calculated the phononic heat-capacity and found good agreement with experiment.

[1] E. E. Rodriguez et al., Phys. Rev. B 83, 134520 (2011)
[2] D. Parker, I. I. Mazin, Phys. Rev. B 83, 180403 (2011)

15 min. break

TT 69.4 Fri 10:30 H21

A1g phonon-induced electron dynamics of Fe pnictides at ultra-fast time scales — •Bhaskar Kamble and Ilya Eremin — Theoretical Physics III, Ruhr Universität Bochum, 44801 Bochum

We employ the five-orbital tight-binding model to study the A1g phonon-induced electron dynamics of the Fe pnictides in the context of recent tr-ARPES experiments on BaFe2As2. By analyzing the experimental data we deduce the amplitude of the tetrahedra angle oscillation due to the A1g phonon and the modified band structure topology. We also find that in order to account for the experimental data in the coherent regime, the oscillations of the electronic structure should occur simultaneously with oscillations of the charge density on the iron site and we evaluate the amplitude of these oscillations from the five orbital model. Finally, we analyze the change in the magnetization as a function of the tetrahedral angle and find it is not symmetric around the mean value. This results in a higher value of the average magnetization within a cycle of the A1g phonon compared to the magnetization at the average value of the tetrahedral angle. This suggests that coherent oscillation of the A1g phonon mode may induce transient generation of the SDW state, and also suggests that the interaction strength in the Fe pnictides lies in the weak to the intermediately coupled regimes.

TT 69.5 Fri 10:45 H21

Shedding light on the pairing mechanism in iron-based superconductors — •Christoph Heil, Markus Aichhorn, Heinrich Sormann, Ewald Schachinger, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, University of Technology Graz, 8010 Graz, Austria

Whether superconductivity in iron-pnictides and -chalcogenides stems from local or itinerant effects is a question still debated on. In order to investigate the influence of Fermi surface nesting on the pairing mechanism, we calculate from first-principles calculations the static and dynamic susceptibility of various iron-based compounds. We show that the susceptibility depends sensitively on doping and pressure application and confront our theoretical results with conclusions drawn from experiments. For instance, our results give evidence that pairing through Fermi-nesting mechanisms alone is not sufficient to explain the evolution of the transition temperature with pressure in FeSe.

TT 69.6 Fri 11:00 H21

The effect of weak disorder on the phase competition in unconventional superconductors — •Mareike Hoyer and Jörg Schmalian — Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie

We investigate the phase competition between magnetism and superconductivity for iron pnictides in the presence of weak disorder. The competition of these two ordered states has been studied in detail by Fernandes and Schmalian [1] who came to the conclusion that in the case of unconventional s^{+-} pairing, the superconducting and antiferromagnetic phase may coexist microscopically but are near to a parameter regime of mutual exclusion. Correspondingly, the multicritical point in the phase diagram is close to the transition from from a tetracritical to a bicritical point.

Close to the multicritical point, the free energy of the system can be expanded simultaneously in terms of magnetic and superconducting order parameters and the coefficients can be determined microscopically. We include the effect of impurity scattering in the model and investigate its influence on the phase diagram of iron pnictides.

[1] Rev. B **82**, 014521 (2010)

TT 69.7 Fri 11:15 H21

Manifestations of impurity induced $s_{\pm} \rightarrow s_{++}$ transition: multiband model for dynamical response functions — •Dmitri Efremov[1], Oleg Dolgov[2], and Alexander Golubov[3] — [1]IFW, Dresden — [2]FKF, Stuttgart — [3]University of Twente

We investigate effects of disorder on the density of states, the single particle response function and optical conductivity in multiband superconductors with $s_{\pm}$ symmetry of the order parameter, where $s_{+-} \rightarrow s_{++}$ transition may take place. In the vicinity of the transition the superconductive gapless regime is realized. It manifests itself in anomalies in the above mentioned properties. As a result, intrinsically phase-insensitive experimental methods like ARPES, tunneling and terahertz spectroscopy may be used for revealing of information about the underlying order parameter symmetry.

TT 69.8 Fri 11:30 H21

Breaking of fourfold lattice symmetry in a model for pnictide superconductors — Maria Daghofer and •Andre Fischer — IFW Dresden, Dresden, Germany

We investigate the interplay of onsite Coulomb repulsion and various mechanisms breaking the fourfold lattice symmetry in a three-band model for the iron planes of iron-based superconductors using cluster perturbation theory[1]. Previously investigated anisotropic magnetic couplings are compared to an orbital ordering field and anisotropic hoppings. We find that all three mechanisms lead to similar signatures once the onsite interactions are strong enough to bring the system close to a spin-density wave state.

[1] M. Daghofer and A. Fischer, Supercond. Sci. Technol. 25, 084003 (2012)

TT 69.9 Fri 11:45 H21

Emergence of superconductivity in the presence of a metallic spin density wave — •Jacob Schmiedt, Philip M. R. Brydon, and Carsten Timm — Institut für Theoretische Physik, TU Dresden, Germany

The coexistence of spin density wave (SDW) and superconducting (SC) order has gained significant attention in the field of iron pnictides since there is strong experimental evidence for microscopic coexistence in a number of compounds. Both types of order gap out the Fermi surface - at least partially. We study how the existence of a SDW gap influences the formation of the SC state and determines the preferred gap symmetry. In contrast to previous studies that use phenomenological pairing potentials, we take a more realistic approach of calculating the effective pairing interaction in the SDW background from the bare interactions using the random phase approximation. This scheme can also be applied to models with orbital degrees of freedom, which can lead to a deeper understanding of the coexistence and the interplay between SDW and SC order in multi-orbital systems such as the pnictides.

TT 69.10 Fri 12:00 H21

Theoretical study of magneto-crystalline anisotropy in Fe pnictides — •Alexander Yaresko — MPI FKF, Stuttgart, Germany

If spin-orbit coupling is taken into account, LSDA band structure calculations for parent Fe pnictides successfully reproduce the correct magnetic ground state with stripe antiferromagnetic (AFM) order and Fe moments aligned along a, i.e., along AFM Fe chains. They also predict that the out-of-plane (ac) magneto-crystalline anisotropy (MCA) in LaFeAsO and $BaFe_2As_2$ is stronger than the in-plane (ab) one. However, recent polarized inelastic neutron scattering experiment showed the opposite: the gap at zone center is larger for in-plane spin excitations than for out-of-plane ones, which means that it is easier to deviate Fe spins in the ac plane. In this work it is shown that MCA in LaFeAsO, $BaFe_2As_2$, and NaFeAs is a non-monotonous function of the exchange splitting of Fe d states. For large values of the splitting the out-of-plane MCA is stronger. However, for sufficiently small exchange splittings, which correspond to reduced Fe moments, the order of the MCA energies is reverted: in agreement with the experiment the in-plane ab anisotropy becomes stronger. The microscopic origin of MCA in pnictides is also discussed.