TT 35: Superconductivity: Fe-based Superconductors - 122 and Theory

Time: Tuesday 9:30–13:00 Location: A 053

TT 35.1 Tue 9:30 A 053

Soft phonons reveal finite nematic correlation length in $Ba(Fe_{0.94}Co_{0.06})_2As_2$ — •Frank Weber[1], Michael Merz[1], Thomas Wolf[1], Rafael Fernandes[2], Jörg Schmalian[1], and Dmitry Reznik[3] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota, 55455, USA — [3]Department of Physics, University of Colorado at Boulder, Boulder, Colorado, 80309, USA

Nematicity is ubiquitous in electronic phases of high-T_c superconductors, particularly in the Fe-based systems. While several experiments have probed nematic fluctuations, they have either been restricted to uniform, i.e. $\mathbf{q} = 0$ fluctuations, or measure momentum-averaged effects. Here, we investigate the behavior of finite-momentum nematic fluctuations near $\mathbf{q} \approx 0$ by utilizing the anomalous softening of transverse acoustic phonon modes in optimally doped $Ba(Fe_{0.94}Co_{0.06})_2As_2$. We determine the nematic correlation length and find that it sharply changes its T-dependence at T_c, revealing a strong connection between nematicity and superconductivity.

TT 35.2 Tue 9:45 A 053

Superconductivity induced changes of the phonon lifetime in $Ba(Fe_{0.94}Co_{0.06})_2As_2$ — •Maximilian Kauth[1], Frank Weber[1], John-Paul Castellan[1], Thomas Wolf[1], Thomas Keller[2], and Dmitry Reznik[3] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Max-Planck-Institute for Sodid State Research, Stuttgart, Germany — [3]Department of Physics, University of Colorado atBoulder, Boulder, Colorado, 80309, USA

We have investigated the life time of the transversal acoustic (TA) phonon mode in the Fe-based high-temperature superconductor $Ba(Fe_{0.94}Co_{0.06})_2As_2$ along the [100] direction. We used the thermal neutron triple axis spectrometer (TAS) 1T at LLB at CEA Saclay and the neutron resonant spin echo (NRSE) technique at the TRISP spectrometer at the MLZ in Garching [1]. This phonon mode is the soft mode of the structural phase transition present in lower doped samples. Recent measurements showed evidence that it is sensitive to nematic fluctuations in this compound [2]. We observe a clear maximum of the TA phonon linewidth at the superconducting transition temperature $T_C \approx 24$ K with both measurement techniques (regular TAS and NRSE). This is the first experimental evidence of changes of the phonon lifetime in Fe-based superconductors.

[1] MPI for Solid State Research et al., Journal of large-scale research facilities, 1, A37 (2015).
[2] F. Weber et al., arXiv:1610.00099 (2016).

TT 35.3 Tue 10:00 A 053

Uniaxial strain control of spin-polarization in multicomponent nematic order of $BaFe_2As_2$ — T. Kissikov[1], •R. Sarkar[2], S. L. Bud'ko[3], P. C. Canfield[3], R. M. Fernandes[4], and N. J. Curro[2] — [1]Department of Physics, UC Davis, CA 95616, USA — [2]Institute of Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany — [3]Ames Laboratory Department of Physics and Astronomy,ISU Ames, Iowa 50011, USA — [4]School of Physics and Astronomy, UMN Minneapolis, Minnesota 55455, USA

The iron-based high temperature superconductors exhibit a rich phase diagram reflecting a complex interplay between spin, lattice, and orbital degrees of freedom. The nematic state observed in many of these compounds illustrates this complexity, by entangling a real-space anisotropy in the spin fluctuation spectrum with ferro-orbital order and an orthorhombic lattice distortion. A more subtle and much less explored fact of the interplay between these degrees of freedom arises from the sizable spin-orbit coupling present in these systems, which translates anisotropies in real space into anisotropies in spin space. Here, we present a new technique enabling nuclear magnetic resonance under precise tunable strain control, which reveals that upon application of a tetragonal symmetry-breaking strain field, the magnetic fluctuation spectrum in the paramagnetic phase of $BaFe_2As_2$ also acquires an anisotropic response in spin-space.

TT 35.4 Tue 10:15 A 053

Superconductivity with broken time reversal symmetry in $Ba_{1-x}K_xFe_2As_2$ single crystals — •Vadim Grinenko[1,2], Philipp Materne[1], Rajib Sarkar[1], Sirko Kamusella[1], Kunihiro Kihou[3], Chul-Ho Lee[3], Shavkat Akhmadaliev[4], Dmitriy Efremov[2], Stefan-Ludwig Drechsler[2], Hubertus Luetkens[5], and Hans-Henning Klauss[1] — [1]Institute for Solid State and Material Physics, TU Dresden, 01069 Dresden, Germany — [2]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [3]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8560 Japan — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [5]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute (PSI), CH-5232 Villigen, Switzerland

Over the last years a lot of theoretical and experimental efforts have been made to find states with broken time reversal symmetry (BTRS) in multi-band superconductors below the superconducting transition temperature (T_c). In particular, it was theoretically proposed that in the $Ba_{1-x}K_xFe_2As_2$ system either an $s + is$ or an $s + id$ BTRS state may exist at high doping levels in a narrow region of the phase diagram. Here we report the observation of an enhanced zero field muon spin relaxation rate at $T^* \lesssim T_c$ for a high quality crystalline samples in the doping range $0.8 \gtrsim x \gtrsim 0.7$. We found that T^* is strongly doping dependent. Our results are consistent with the multi-band $s + is$ superconducting state in $Ba_{1-x}K_xFe_2As_2$ in this doping range.

TT 35.5 Tue 10:30 A 053

Mass enhancements and band shifts in hole overdoped Fe-based pnictide superconductors: KFe_2As_2 and $CsFe_2As_2$ — •S.-L. Drechsler[1], H. Rosner[2], V. Grinenko[3], S. Aswartham[1], I. Morozov[4], L. Ming[4], A. Boltalin[4], K. Kihou[5], C. H. Lee[5], T. K. Kim[6], D. Evtushinsky[7], J.M. Tomczak[8], S. Johnston[9], and S. Borisenko[1] — [1]IFW-Dresden, Germany — [2]MPI-CPfS Dresden, Germany — [3]TU Dresden, Germany — [4]Moscow University, Russia — [5]AIST, Tsuk. Japan — [6]Diamond Light Source, U.K. — [7]Ec. de Fed., Lausanne, Switzerland — [8]Vienna-University of Technology, Austria — [9]Tennesee University, Knoxville, USA

The interplay of high- and low energy (LE) mass renormalizations with band shifts as seen in the positions of van Hove singularities (VHS) in the normal state of the strongly correlated and most hole-overdoped AFe_2As_2 (A122), A = K,Rb,Cs Fe pnictides is discussed phenomenologically from ARPES data and band structure (GGA) with full spin-orbit coupling and microscopically applying the GW-self-energy. The increase of the Sommerfeld coefficient γ from K122 to Cs122 is ascribed to an enhanced coupling to LE bosons in the vicinity of a quantum critical point to an yet unknown incommensurate phase different from the tetragonal Mott phase. We find no sizable increase of correlation for Cs122 in contrast to scenarios proposed in the literature. The ARPES positions of VHS as compared with GGA and GW results point to slightly weaker correlations in accord with the low-T susceptibility data and the reduced Wilson ratio $\chi(0)/\gamma$. Other quasi-2D systems with generic VHS and their el-el interactions are briefly discussed.

TT 35.6 Tue 10:45 A 053

Synthesis and Characterization of $YbFe_2As_2$ Single Crystals — •Nilotpal Ghosh[1], Santhosh Raj[2], and R Navamathavan[2] — [1]Science and Engineering Research Board, Department of Science and Technology, Vasant Kunj, New Delhi, India — [2]School of Advanced Sciences ,VIT University, Chennai, Tamilnadu, India

We report synthesization of a new compound $YbFe_2As_2$ crystals using melt growth technique. The crystals have been characterized by Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Analysis (EDX). Rietveld refinement of crushed single crystals has shown that the $YbFe_2As_2$ has monoclinic unit cell structure. Transport measurement has shown metallic behavior with a down turn in resistivity around 17K for $YbFe_2As_2$ which is similar to superconducting transition. The detailed magnetic studies by SQUID on these crystals have revealed the co-existence of strong antiferromagnetic and weak ferromagnetic characteristics. Influence of anti-ferromagnetic spin fluctuation in the normal state transport property has been found. Effect of oxygen adsorption on $YbFe_2As_2$ have been studied in detail.

[1] S. S. Raj, N. Ghosh, R. Navamathavan, J. Supercond. Novel Magnetism 30 (2017) 287;
[2] S. S. Raj, N. Ghosh, R. Navamathavan, Mater. Res. Express 4 (2017) 086101;

TT 35.7 Tue 11:00 A 053

Interplay of magnetism and superconductivity in the triclinic $Ca_{10}Pt_3As_8(Fe_{1-x}Pt_xAs)_{10}$ system — •Felix Brückner[1], Vadim Grinenko[1], Rajib Sarkar[1], Maksym Surmach[1], Hubertus Luetkens[2], Dmytro Inosov[1], and Hans-Henning Klauss[1] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, Villigen, Switzerland

Among iron-based superconductors, $Ca_{10}Pt_3As_8(Fe_{1-x}Pt_xAs)_{10}$ is the first system with a triclinic crystal structure. The usually tetragonal symmetry of the characteristic FeAs layers is slightly distorted by insertion of a skutterudite-like interlayer.

We report comprehensive studies of magnetic probe experiments including ^{75}As and ^{195}Pt nuclear magnetic resonance (NMR), muon spin rotation and inelastic neutron scattering (INS). Broadening of NMR spectra below $T^* \sim 45$ K provides evidence for static magnetic correlations far above the superconducting $T_c = 13$ K. At T^*, a sudden drop of the spin-lattice relaxation rate, that is insensitive to external magnetic field up to 30 T, is observed. INS spectra exhibit a resonant mode at higher energies just below T^*. This was previously interpreted as a manifestation of preformed cooper pairs, which can be ruled out by ^{195}Pt Knight-shift experiments. Furthermore an additional magnetic transition at 3 K and strong but slow magnetic fluctuations peaking at ~ 120 K are detected by NMR. In addition to the magnetic probe investigations, we compare our results with transport measurements and specific heat studies.

15 min. break.

TT 35.8 Tue 11:30 A 053

Consequences of Orbital Selectivity for Magnetism and Superconductivity in Fe-based Superconductors — •Andreas Kreisel[1], Brian Andersen[2], and Peter Hirschfeld[3] — [1]Universität Leipzig, Germany — [2]Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark — [3]University of Florida, Gainesville, FL, United States

Recently, it has been observed that electronic correlations in iron pnictides and chalcogenides affect electrons in different d-orbitals quite differently. The resulting reduced coherence of the quasiparticle states has consequences for the normal state properties and affects the superconducting state. The renormalization of the d_{xy} orbital is known to be largest, thus its quasiparticle weight smallest. In the Fe based systems, this leads to a reduction of Néel type (π, π) magnetic fluctuations and makes stripe fluctuations relatively stronger. Within a modified spin fluctuation pairing theory, this makes the sign-changing s-wave state more competitive. In this work, we investigate these effects of orbital selectivity with a focus on the FeSe system, which allows us to study the effect of nematicity due to the breaking of tetragonal symmetry without magnetic order at low temperatures. Consequences include different renormalization of the d_{yz} and d_{xz} orbital states, leading to an anisotropic superconducting order parameter and enhancements of the $(\pi, 0)$ magnetic fluctuations, an effect seen in neutron scattering experiments. The strongest effects of the reduced coherence are observed in the KFe_2As_2, system where we discuss implications for the superconducting order parameter.

TT 35.9 Tue 11:45 A 053

Orbital loop currents in iron-based superconductors — •Markus Klug[1], Jian Kang[2], Rafael M. Fernandes[2], and Jörg Schmalian[1,3] — [1]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA — [3]Institute of Solid State Physics, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany

We show that the stripe spin-density wave state commonly observed in the phase diagrams of the iron-based superconductors necessarily triggers loop currents characterized by charge transfer between different Fe 3d orbitals. This effect is rooted on the glide-plane symmetry of these materials and on the existence of an atomic spin-orbit coupling that couples states at the X and Y points of the 1-Fe Brillouin zone. We show that the two main manifestations of the orbital loop currents are the emergence of magnetic moments in the pnictide/chalcogen site and an orbital-selective band splitting in the magnetically ordered state, both of which could be detected experimentally. Our results highlight the unique intertwining between orbital and spin degrees of freedom in the iron-based superconductors, and reveal the emergence of an unusual correlated phase that may impact the normal state and superconducting properties of these materials.

TT 35.10 Tue 12:00 A 053

Mixed magnetic order in iron pnictides — •Chris Koschenz and Carsten Timm — Institute of Theoretical Physics, Technische Universität Dresden, Germany

Multiband and multiorbital physics are crucial for understanding superconductivity and magnetism in iron pnictides. We present recent results for multiorbital Hubbard models representative of iron pnictide compounds using restricted and unrestricted generalized Hartree-Fock methods. The generalized Hartree-Fock method introduced by [1] allows to study phases with mixed magnetic order. In this talk, we revisite the magnetic phases in the vicinity of superconductivity for compounds for which a reentrance of tetragonal magnetic order was found [2,3]. We employ a realistic multiorbital model for $Ba_{1-x}Na_xFe_2As_2$ and $Ba_{1-x}K_xFe_2As_2$ and elucidate the role played by orbital effects. Furthermore, we study the coexistence and competition of tetragonal or mixed magnetic order with superconductivity as well as the possibility of phase separation (mixed phases).

[1] E. Langmann and M. Wallin, J. Stat. Phys. **127** (2007) 825
[2] S. Avci *et al.*, Nature Comm. **5** (2014) 3845
[3] M. Gastiasoro, B. Anderson, Phys. Rev. B **92** (2015) 140506(R)

TT 35.11 Tue 12:15 A 053

Collective modes and short-time dynamics of time-reversal symmetry broken superconductors — •Marvin A. Müller[1], Pengtao Shen[2], Maxim Dzero[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, German — [2]Department of Physics, Kent State University, Kent, OH 44242 USA

Motivated by the recent observation of the time-reversal symmetry broken state in K-doped $BaFe_2As_2$ systems, we theoretically study the collective modes and the short time dynamics of this state using density-matrix theory on an effective four-band model with two hole and two electron pockets. Hole doping moves the electron bands away from the Fermi surface and leads to frustration between superconducting channels. This results either into $s+is$ or $s+id$ superconductivity, which are both time-reversal symmetry breaking (TRSB) states. Consequently, the Higgs and Leggett modes are coupled and the superconducting ground state accommodates a variety of collective modes. In extremely overdoped systems with incipient electron bands, we find the Higgs mode at $\omega = 2\Delta_h$ with an absent Leggett mode similar to a two band model. At dopings before the TRSB occurs and within the TRSB state, we uncover a new coupled collective mode both in the amplitude and in the relative phase of the superconducting gaps. This mode becomes gapless at the boundaries of the TRSB state.

TT 35.12 Tue 12:30 A 053

Superconductivity in presence of spin-orbit coupling in strongly electron-doped iron-based superconductors — •Jakob Böker[1], Felix Ahn[1], Peter Hirschfeld[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Department of Physics, University of Florida, Gainesville, FL 32611, USA

Motivated by recent experimental reports on sizeable spin-orbit coupling (SOC) in the iron pnictides, we study the SOC induced mixing of the spin singlet and the spin triplet pairing for the leading s- and d-wave superconducting instabilities. We focus on highly electron doped systems where only electron $d_{yz}/d_{xz}/d_{xy}$ pockets are present at the M-point of the two-iron unit cell. Using a orbitally projected effective low energy model for the iron pnictides with pairing driven by atomic onsite interactions, we present the gap structure close to Fermi level and discuss consequences of the induced triplet pairing to experiment.

TT 35.13 Tue 12:45 A 053

Enhanced Nernst effect by nematic fluctuations in an iron based superconductor — •Steffen Sykora[1], Christoph Wuttke[1], Federico Caglieris[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

Nematic fluctuations are expected to enhance superconductivity in iron based superconductors which undergo a transition to nematic order.

Motivated by recent Nernst effect measurements we investigate theoretically transport properties within a minimal electronic model consisting of two orbitals, with interactions that enhance nematic fluctuations. We apply a many-particle renormalization method to calculate current-current correlation functions and show that the correlation between currents in perpendicular directions are particularly enhanced by interactions between different orbitals. This property gives rise to a direct coupling of the Nernst effect to nematic fluctuations. We discuss our results in the context of recent Nernst effect experiments in $BaFe_2As_2$.