TT 70: Superconductivity: Fe-based Superconductors - Theory

Time: Thursday 15:00–18:15 Location: HSZ 103

Invited Talk TT 70.1 Thu 15:00 HSZ 103

New Developments in the Theory of STM on Unconventional Superconductors — •Andreas Kreisel — Institut für Theoretische Physik, Uni Leipzig, Germany — Niels Bohr Institute, Copenhagen, Denmark

Scanning Tunneling Microscopy (STM) has become a widely used experimental technique to study superconductivity, yet new approaches are unraveling so far unknown properties. A number theories have been used to explain the qualitative origin of superconducting pairing in Fe-based superconductors (FeSC), but quantitative, material-specific comparisons to experimental results have been made in few cases only. Here, a novel approach to theoretical simulation of STM is outlined which combines first-principles calculations to obtain material-specific Wannier functions and lattice Green functions from BdG or T-matrix calculations. The method takes into account crystal symmetries such that it improves the traditional lattice calculations from two perspectives: Effects of the tunneling layers are contained qualitatively and the spatial resolution is not limited to the lattice spacing, thus comparable to the resolution of experimentally available data. By calculating the local density of states relevant for the tunneling process, it is possible to simulate images of impurities on the surface of superconductors. As examples, we study disorder in a cuprate superconductor and a FeSC and discuss conclusions that can be drawn about the order parameter when comparing to experimental observations.

TT 70.2 Thu 15:30 HSZ 103

Tilting the balance towards d-wave in iron-based superconductors — Mario Fink and •Ronny Thomale — Institut für Theoretische Physik, Universität Würzburg, 97074 Würzburg, Germany

The interplay of interactions and Fermi surface topology in iron-based superconductors can promote s-wave and d-wave superconductivity as competitive canditates. From the theoretical limit of zero temperature, we develop a phenomenological thermodynamic argument how a weak perturbation such as small but finite temperature or an applied Zeeman field H_z can favor a nodal d-wave state over a nodeless s-wave state. This preference occurs as the quasiparticles in the nodal regime gain energy by polarization with respect to the applied field, or generate entropy at small finite temperature. We speculate that $K_xBa_{1-x}Fe_2As_2$ for large hole doping could be a viable scenario for such a magnetically or entropically induced transition from s-wave to d-wave superconductivity.

TT 70.3 Thu 15:45 HSZ 103

Competition of SDW and iCDW and the role of spin-orbit coupling — •Felix Ahn[1], Fabian Lambert[1], Maria N. Gastiasoro[2], Daniel D. Scherer[2], Brian M. Anderson[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark

The magnetic stripe phase is a mutual feature of most the iron-based superconductors and can be described in the basis of the iron $3d$-orbitals or, alternatively, it can be described within the band basis where magnetism occurs as a Fermi surface instability. In this work, we show how spin-orbit coupling causes an intrinsic spin-space anisotropy that is necessarily relevant for the different magnetic phases and that it lifts the Dirac cones of the nodal spin density-wave (SDW) order parameter, in particular. Most importantly, we show that spin-orbit coupling adds an inevitable companion to the SDW phase, namely a charge-current density-wave that is often dubbed imaginary charge density-wave (iCDW).

TT 70.4 Thu 16:00 HSZ 103

s+is Superconductivity with incipient bands: doping dependence and STM signatures — •Jakob Böker, Pavel Volkov, and Ilya Eremin — Institut fur Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Motivated by the recent observations of small Fermi energies and comparatively large superconducting gaps, present on bands located below the Fermi energy(incipient bands) in iron-based superconductors, we analyse the doping evolution of superconductivity in a four-band model in the BCS-BEC crossover regime for the iron pnictides. Similar to the BCS case we find that with hole doping the phase difference between superconducting order parameters of the hole bands changes from 0 to π through an intermediate $s+is$ state breaking time-reversal symmetry. However, in the BCS-BEC crossover phase this transition occurs in the region where electron bands are already above the Fermi level and that the chemical potential renormalization leads to significant broadening of the $s+is$ region. This makes the observation of this phase easier in experiment. We further present the qualitative features of the $s+is$ state that can be observed in scanning tunnelling microscopy (STM) experiments.

TT 70.5 Thu 16:15 HSZ 103

Inelastic STM in LiFeAs — •Patrik Hlobil, Jörg Schmalian, Wulf Wulfhekel, and Jasmin Jandke — KIT

Scanning tunneling microscopy (STM) has been shown to be a powerfulexperimental probe to detect electronic excitations and further allows to deduce fingerprints of bosonic collective modes in superconductors. Here, we demonstrate that the inclusion of inelastic tunnel events is crucial for the interpretation of tunneling spectra of unconventional superconductors and allows to directly probe electronic and bosonic excitations via STM. We apply the formalism to the iron based superconductor LiFeAs. With the inclusion of inelastic contributions, we find strong evidence for a non-conventional pairing mechanism, likely via magnetic excitations.

15 min. break.

TT 70.6 Thu 16:45 HSZ 103

Superconducting fluctuations with small Fermi energies: the case of FeSe — •Pavel A. Volkov, Ilya Eremin, and Konstantin B. Efetov — Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Recent experiments imply the presence of strong superconducting fluctuations above T_c in FeSe. It has been suggested that the observed effects could be due to the presence of a band with an anomalously small Fermi energy $\varepsilon_F \sim \Delta$. We report theoretical analysis of superconducting fluctuations in a two-band model with one of the bands having small ε_F. While close to T_c the system is described by a conventional Ginzburg-Landau theory (unless an accidental degeneracy between superconducting channels is present), the microscopic expressions for the coefficients differ from the ones obtained in the usual BCS ($\varepsilon_F \gg \Delta$) theory. We also present analytical expressions for fluctuation effects valid at elevated temperatures. On the basis of our results, we discuss the possible relevance of the BCS-BEC crossover to the phenomena observed in FeSe.

TT 70.7 Thu 17:00 HSZ 103

Interfacial electron-phonon coupling strength and high-T_c superconductivity in monolayer FeSe/$SrTiO_3$ — •Alex Aperis and Peter M. Oppeneer — Uppsala University, Sweden

Superconductivity in monolayer FeSe on $SrTiO_3$ reaches mysteriously high transition temperatures of typically 50-70 K and up to 100 K, much higher than the T_c=8 K of bulk FeSe. At the FeSe/$SrTiO_3$ interface, a coupling between $SrTiO_3$ phonons and FeSe electrons that manifests as electron replica bands, is commonly believed to enhance T_c moderately but not enough to fully explain it. Here, we employ fully anisotropic, full bandwidth multiband Eliashberg calculations to examine the impact of these phonons on the superconducting state of FeSe/$SrTiO_3$. We find that the interfacial electron-phonon interaction which is hidden behind the seemingly weak coupling constant, λ_m=0.4, fully accounts for the high-T_c while also solving puzzling experimental facts like the s-wave symmetry and replica bands. Our calculations indicate that replica band formation has a T_c-decreasing effect which is nevertheless overcompensated by T_c-enhancing Cooper pairing at bands away from the Fermi level. We predict this mechanism to produce a strong coupling dip-hump signature in the tunnelling spectra.

TT 70.8 Thu 17:15 HSZ 103

Orbitally resolved superconductivity within FLEX: doping evolution of the FeSe monolayer — •Andreas Linscheid[1], Yan Wang[2], Saurabh Maiti[1], Steven Johnston[2], and Peter Hirschfeld[1] — [1]Department of Physics, University of Florida,

Gainesville — [2]Department of Physics and Astronomy, University of Tennessee

FeSe-derived materials have been studied by several recent experiments concerning a number of phenomena that still lack a concise explanation. First, the nature of the pairing in materials with only electron pockets at the Fermi level is still under debate, with proposed explanations by both electronic s++ and s+- and/or phononic pairing. Second, the effective quasi particle mass at the Fermi level is very orbital dependent which likely affects the pairing and may require to solve the superconducting (SC) pairing in the space of orbitals. The effective mass is bound to have consequences for the spin- and charge fluctuations and the problem should therefore be solved self-consistently. In this work, we extend our previous study [PRL 117, 077003] and describe the electron doped FeSe in an orbitally resolved microscopic model. Starting from the normal state DFT band structure, we apply orbitally resolved FLEX to study the system in the SC state, as well as in the magnetic phase. By retaining full momentum resolution, we can also include strong forward scattering by phonons in the FeSe/STO system and discuss the self-consistent influence of the orbitally-resolved quasi particle mass on SC as a function of doping.

TT 70.9 Thu 17:30 HSZ 103

Enhancement of superconductivity by interfacial phonons in perovskite-clad FeAs monolayers — Seokhwan Choi[1], Won-Jun Jang[1], Hyun-Jung Lee[2], Jong Mok Ok[2], Hyun Woo Choi[1], Alex Taekyung Lee[3], •Alireza Akbari[2,4], Ken Nakatsukasa[5], Yannis K. Semertzidis[6], Yunkyu Bang[7], Steven Johnston[5], Jun Sung Kim[2], and Jhinhwan Lee[1] — [1]Korea Advanced Institute of Science and Technology, Daejeon, Korea — [2]Asia Pacific Center for Theoretical Physics, Pohang, Korea — [3]Columbia University, New York 10027, USA — [4]Pohang University of Science and Technology, Pohang, Korea — [5]University of Tennessee, Knoxville, Tennessee, USA — [6]Institute of Basic Science, Daejeon, Korea — [7]Chonnam National University, Kwangju, Korea

The physics at interfaces between monolayer iron-based superconductors (FeSC) and perovskite substrates has received considerable attention due to the unusually high T_c of 100 K found recently in monolayer FeSe on $SrTiO_3$. We present a quasiparticle interference (QPI) study which provides a strongest-ever proof of enhancement of the Fe-based superconductivity (FeSC) by the forward-scattering interfacial phonons in the system of the perovskite-clad FeSC monolayers. Furthermore, the self-assembled heterostructure studied here shows stronger electron-phonon coupling consistent with the doubled interfaces per FeSC monolayer and has greater applicability due to its massively parallel superconducting layers compared with the monolayer counterpart.

[1] S. Choi et al., arXiv:1608.00886.

TT 70.10 Thu 17:45 HSZ 103

Structural Properties and Magnetic Behavior of the New Iron-based Superconductor $CaKFe_4As_4$ — •Felix Lochner[1,2], Ilya Eremin[2], and Tilmann Hickel[1] — [1]Computergestütztes Materialdesign, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany

The iron-based superconductor $CaKFe_4As_4$ is one of the most famous representative of the new 1144 family of the iron pnictides. Because of the combination of alcali and alcaline-earth metals $CaKFe_4As_4$ is hole-doped itself and reaches a transition temperature of $T_c = 35$ K [1]. We calculate *ab initio* the electronic structure and internal parameters by using density functional theory for several magnetic configurations. In contrast to other iron-based superconductors we find that the d_{xy}-orbital contributes not much to the Fermi-surface, whereas the $d_{x^2-y^2}$- and d_{z^2}-orbitals are showing a strong contribution. This behavior is related to the shift of the FeAs-layer away from its high-symmetry position [2]. Hereby we focus on the orbital-resolved electronic bandstructure to estimate the strength of the electronic interactions.

[1] W. R. Meier *et. al.*, PRB **94**, 064501 (2016)
[2] D. Mou *et. al.*, arXiv:1606.05643

TT 70.11 Thu 18:00 HSZ 103

Chromium analogues of iron-based supercondictors — •Martin Edelmann[1], Giorgio Sangiovanni[1], Massimo Capone[2], and Luca de' Medici[3] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136 Trieste, Italy — [3]European Synchrotron Radiation Facility, 71 Av. des Martyrs, Grenoble, France

The present talk encompasses the results of our studies of $BaCr_2As_2$, the Cr equivalent of the 122 iron-based superconductor (FeSC) $BaFe_2As_2$. In the respective compound, Cr nominally hosts 4 electrons in its d orbitals, whereas Fe hosts six, placing Cr on the other side of half-filling. Therefore, one expects behaviour of the Cr compound that is specular to $BaFe_2As_2$. We conducted DFT+DMFT studies on the PM and G-type AFM phase as well as slave-spin mean field (SSMF) calculations on the PM phase [1]. We show that dynamical correlations are necessary to narrow the discrepancy between the Sommerfeld coefficient as accessed by theoretical studies and the experimental value. Through SSMF one finds that the $BaCr_2As_2$ mirrors the $BaFe_2As_2$ compressibility, where the $BaCr_2As_2$ compound phase diagram displays a crossover from a weakly to a strongly correlated metal. We infer that, similar to $BaFe_2As_2$, $BaCr_2As_2$ can be pushed into the SC regime with the proper amount of electron doping and/or negative pressure, introducing a new, interesting family of SCs.

[1] M. Edelmann, G. Sangiovanni, M. Capone, L. de' Medici, arXiv:1610.10054