TT 92: Superconductivity: Fe-based Superconductors - Theory II

Time: Thursday 15:00–16:15 Location: HSZ 201

TT 92.1 Thu 15:00 HSZ 201

Superconducting gap in LiFeAs from three-dimensional spin-fluctuation pairing calculations — •Yan Wang[1], Andreas Kreisel[1], Volodymyr B. Zabolotnyy[2,3], Sergey V. Borisenko[2], Bernd Büchner[2,4], Peter J. Hirschfeld[1], Thomas A. Maier[5], and Douglas J. Scalapino[6] — [1]Department of Physics, University of Florida, USA — [2]Leibniz-Institute for Solid State Research, IFW-Dresden, Germany — [3]Physikalisches Institut, EP IV, Universität Würzburg, Germany — [4]Institut für Festkörperphysik, Technische Universität Dresden, Germany — [5]Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, USA — [6]Department of Physics, University of California, Santa Barbara, USA

The lack of nesting of Fermi-surface sheets in the Fe-based superconductor LiFeAs, with a T_c of 18 K, has led to questions as to whether the origin of superconductivity in this material might be different from other Fe-based superconductors. Here we present calculations of the superconducting gap and pairing in the random-phase approximation using Fermi surfaces derived from ARPES. The gaps obtained are qualitatively different from previous 2D theoretical works and in good agreement with ARPES on the main Fermi-surface pockets. We analyze the contributions to the pairing vertex thus obtained and show that the scattering processes between electron and hole pockets still dominate the pairing as in other Fe-based superconductors despite the lack of nesting, leading to gaps with anisotropic $s_\pm$ structure.

TT 92.2 Thu 15:15 HSZ 201

Superconductivity from repulsion in LiFeAs: novel s-wave symmetry and potential time-reversal symmetry breaking — •Felix Ahn[1], Ilya Eremin[1], Johannes Knolle[2], Volodymyr Zabolotnyy[3], Sergey Borisenko[3], Bernd Büchner[3], and Andrey Chubukov[4] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, D-01171 Dresden,Germany — [4]Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

Using the ten orbital tight-binding model, derived from the ab-initio LDA calculations and fitted to the ARPES experiments, we analyze the structure of the superconducting gap in LiFeAs. We treat superconductivity as quasi-2D and decompose the pairing interaction for various k_z cuts into $s-$ and d-wave components. Analyzing the leading superconducting instabilities we find that in addition to the conventional s^{+-}-wave order parameter where the gap changes sign between electron and hole pockets LiFeAs possesses another instability where the superconducting gap also changes sign between two smaller inner hole pockets. This occurs due to relatively large repulsion between these two small pockets and also relatively weak interaction between outer and inner hole pockets. The sizes of the gaps on the inner hole pockets is larger than the average value of the superconducting gap on the outer hole pockets and electron pockets which agrees with experimental data.

TT 92.3 Thu 15:30 HSZ 201

$BaFe_2P_2$ and $LaFe_2P_2$: What makes the difference? — •Tobias Förster[1], Helge Rosner[2], Andrey Polyakov[1], Marek Bartkowiak[1], Andrea D. Bianchi[3], and Jochen Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Deutschland — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Deutschland — [3]Département de Physique and RQMP, Université de Montréal, Montréal H3C 3J7, Canada

The Fermi-surface topology of iron-pnictide superconductors stimulated many theories on the pairing mechanism in these materials. Especially the degree of nesting between quasi-two-dimensional hole and electron bands is regarded as a key ingredient. However, also more localized pictures and the duality of both itinerant and localized degrees of freedom of the Fe 3d electrons are considered.To challenge the different scenarios, a precise knowledge of the electronic structure is necessary. We, therefore, present a detailed DFT study on $LaFe_2P_2$ and $BaFe_2P_2$. Using the full potential local orbital (FPLO) code we work out the difference between both compounds and show in detail what changes when replacing Ba with La. As a surprise, we find that a rigid-band-like description is inappropriate, since the La 5d states provide sizable contributions to a part of the Fermi surface. Additionally we use our de Haas-van Alphen measurements of $LaFe_2P_2$ and literature data of $BaFe_2P_2$ to refine our calculations and estimate the renormalization strength acting on the electronic structure.

TT 92.4 Thu 15:45 HSZ 201

Is $LiFeO_2Fe_2Se_2$ a typical iron-based superconductor? — •Christoph Heil, Lilia Boeri, Markus Aichhorn, Heinrich Sormann, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, University of Technology Graz, Austria

We study the electronic and magnetic properties of the recently synthesised [Lu et al., arXiv 1309.3833 (2013)] new iron-based superconductor $LiFeO_2Fe_2Se_2$ from first principles using GGA, LDA+U and LDA+DMFT. This material is a very interesting new member of the class of iron superconductors as it features an intercalated $LiFeO_2$ layer with a Fe $3d^5$ configuration. We calculate different magnetic configurations with first-principle methods, and find that the $3d^5$ Fe in the $LiFeO_2$ layer has a very big magnetic moment of $\mu \approx 3.6$, which would block all spin fluctuations in the FeSe layer. Based on our LDA+U and LDA+DMFT results, we will compare $LiFeO_2Fe_2Se_2$ with other typical iron-based superconductors and also more "exotic" ones.

TT 92.5 Thu 16:00 HSZ 201

Spin fluctuations and superconductivity in $K_xFe_{2-y}Se_2$ — •Andreas Kreisel[1], Yan Wang[1], Thomas A. Maier[2], Peter J. Hirschfeld[1], and Douglas J. Scalapino[3] — [1]Department of Physics, University of Florida, USA — [2]Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, USA — [3]Department of Physics, University of California, USA

Superconductivity in alkali-intercalated iron selenide, with T_c's of 30 K and above, may have a different origin than that of the other Fe-based superconductors, since the Fermi surface seems not to have any sheets centered around the Γ point. Here we investigate the symmetry of the superconducting gap in the framework of spin-fluctuation pairing calculations using DFT bands downfolded onto a 3D, ten-orbital tight-binding model, treating the interactions in the random-phase approximation. We find a leading instability towards a state with d-wave symmetry, but show that the details of the gap function depend sensitively on electronic structure. The crystal symmetry requires quasi-nodes to occur, which are either horizontal, looplike or vertical depending on details. We investigate the possibility that spin-orbit coupling effects on the one-electron band structure, which lead to enhanced splitting of the two M-centered electron pockets in the 2-Fe zone, may stabilize the bonding-antibonding $s_\pm$-wave states. Finally, we discuss our results in the context of current phenomenological theories and experiments and address the question of the origin of the spin-resonance that has been observed in inelastic neutron scattering experiments.