TT 3: Superconductivity: Properties and Electronic Structure

Time: Monday 9:30–13:00 Location: H23

TT 3.1 Mon 9:30 H23

Is lead really a prototypical type I superconductor? New results on the phase diagram at ultra-low temperatures — Thomas Gozlinski, Qili Li, Rolf Heid, Jörg Schmalian, and •Wulf Wulfhekel — Karlsruhe Institute of Technology

Superconductors are classified by their behavior in a magnetic field into type I, which transitions from a superconducting Meissner to a normal state at the critical field and type II, which have an additional Shubnikov phase consisting of magnetic vortices with one magnetic flux quantum, each. For type I superconductors of finite lateral dimensions, the transition to the normal state is, however, known to occur locally in form of domains in the so-called intermediate Landau state. Basis for this classification are thermodynamic considerations near the critical temperature and a single band description of superconductivity. Although bulk lead (Pb) is classified as a prototypical type I superconductor, we surprisingly observe single and multi-flux quanta vortices in the intermediate state at temperatures far below the critical temperature using a 25 mK scanning tunneling microscope hand in hand with a complex superconducting behaviour of the two distinct Fermi surfaces of Pb. By probing the quasiparticle local density of states (LDOS) inside the vortices and comparison with quasi-classical simulations based on DFT band-structure calculations, we identify the Caroli-de-Gennes-Matricon states of the two superconducting bands of Pb and are consequently able to determine their winding number.

TT 3.2 Mon 9:45 H23

High-precision impedance measurements near the Berezinski-Kosterlitz-Thouless transition in strongly disordered superconductors — •Lea Pfaffinger[1], Alexander Weitzel[1], Thomas Huber[1], Klaus Kronfeldner[1], Lorenz Fuchs[1], Sven Linzen[2], Evgeni Il'ichev[2], Nicola Paradiso[1], and Christoph Strunk[1] — [1]University of Regensburg, Germany — [2]Leibniz Institute of Photonic Technology, Jena, Germany

We investigate the Berezinskii-Kosterlitz-Thouless (BKT) transition - a vortex induced topological phase transition - in 3 nm thin atomically layer deposited NbN films. The samples are placed inside a RLC-resonator, whose design enables us to perform AC measurements of the superfluid stiffness J_s and four-probe current-voltage (IV) characteristics in the same cooling cycle. In contrast to earlier experiments, we observe a sharp discontinuous jump of J_s at the BKT transition temperature T_{BKT}. Comparison of the J_s and the DC resistance measurements reveal quantitative agreement of both T_{BKT} and T_{c0}. Powerlaw exponents extracted of IV characteristics agree quantitatively with J_s and calculations based on renormalization group. Surprisingly, if a DC current is added to the rf-drive, $J_s(I)$ reaches a pronounced maximum before dropping sharply to zero at a current much smaller than the pair breaking critical current. This behaviour may be tentatively explained as a cut-off of the BKT renormalisation flow by the current.

TT 3.3 Mon 10:00 H23

Prediction of ambient-pressure superconductivity in ternary hydride $PdCuH_x$ — •Riccardo Vocaturo[1], Cesare Tresca[2], Giacomo Ghiringhelli[3], and Gianni Profeta[2,4] — [1]IFW-ITF, Dresden, Germany — [2]Università degli studi dell'Aquila, L'Aquila, Italy — [3]Politecnico di Milano, Milano, Italy — [4]CNR-SPIN, L'Aquila, Italy

We present an ab initio study of the ternary hydride $PdCuH_x$, a parent compound of the superconducting PdH, at different hydrogen content (x=1,2). We investigate its structural, electronic, dynamical, and superconducting properties, demonstrating that, at low hydrogen content, the system is not a superconductor above 1K; however, the highly hydrogenated structure is a strongly coupled superconductor. We give a solid rationale for the unusual increase of the superconducting critical temperature in hydrogenated palladium when alloyed with noble metals (Cu, Ag, and Au), as observed in Stritzker's experiments in 1972 but never investigated with modern experimental and theoretical techniques. We highlight the important role played by H-derived phonon modes at intermediate frequencies, dynamically stabilized by anharmonic effects, as they strongly couple with states at the Fermi level. We hope that the present results will stimulate additional experimental investigations of structural, electronic, and superconducting properties of hydrogenated palladium-noble metal alloys. Indeed, if confirmed, these compounds could be considered a novel class of superconducting hydrides, showing different coupling mechanisms, which can be exploited to engineer new ambient-pressure superconductors.

TT 3.4 Mon 10:15 H23

Theory of spin-excitation anisotropy in the nematic phase of FeSe obtained from RIXS measurements — •Andreas Kreisel[1], Peter Hirschfeld[2], and Brian M. Andersen[3] — [1]Institut für Theoretische Physik, Universität Leipzig — [2]Department of Physics, University of Florida, Gainesville — [3]Niels Bohr Institute, University of Copenhagen

Recent resonant inelastic x-ray scattering (RIXS) experiments have detected a significant high-energy spin-excitation anisotropy in the nematic phase of the enigmatic iron-based superconductor FeSe [1], whose origin remains controversial. We apply an itinerant model previously used to describe the spin-excitation anisotropy as measured by neutron scattering measurements [2], with magnetic fluctuations included within the RPA approximation. The calculated RIXS cross section exhibits overall agreement with the RIXS data [3], including the high energy spin-excitation anisotropy such that the picture of a localized Heisenberg model does not need to be evoked in order to explain the experimental data.

[1] X. Lu et al., Nat. Phys. (2022)
[2] T. Chen et al. Nat. Mater. **18**, 709 (2019)
[3] A. Kreisel, P. J. Hirschfeld, B. M. Andersen, Frontiers in Physics **10**, 859424 (2022)

TT 3.5 Mon 10:30 H23

Local measurements of (super-)conducting microstructure in $Rb_xFe_{2-y}Se_2$ — •Donald M Evans[1], Stephan Krohns[1], Dorina Croitori[2], Vladimir Tsurkan[1,2], and István Kézsmárki[1] — [1]Experimental Physics V, University of Augsburg, 86135 Germany — [2]Institute of Applied Physics, MD 2028 Chisinau, Moldova.

There are many reports on the bulk coexistence of competing orders in iron-based superconductors. In some of these systems, such as $RbFe_2Se_2$, this is because even single crystals spontaneously phase separate into a superconducting phase made up of micron scale islands, within an antiferromagnetic host matrix. Such phase coexistence makes any bulk data challenging to interpret and, rather, requires local measurement techniques.

In this work, we use low-temperature conducting atomic force microscopy (cAFM) to map the local current response of the superconducting islands in $RbFe_2Se_2$. Below T_c ($\sim 32K$) these islands show large current values, as expected for a superconductor. Unexpectedly, there is no distinct change in these current values when heating through Tc: rather, the high currents persist within the islands until they becoming as insulating as the bulk matrix at $\sim 150K$. This enhanced conductivity vanishes in response to external magnetic fields. This implies that the reported bulk Tc is the temperature at which the superconductivity is strong enough to connect the islands, i.e. the percolation limit, while the superconductivity within individual islands persists to higher temperatures. This work shows the strength of cAFM to understand the local properties of inhomogeneous superconductors.

TT 3.6 Mon 10:45 H23

Cascade of collapsed phases in $SrNi_2P_2$ and $CaKFe_2As_2$ under various strain conditions — •Adrian Valadkhani[1], Shuyang Xiao[2], Igor Mazin[3], Seok-Woo Lee[2], Paul Canfield[4], and Roser Valenti[1] — [1]Goethe University, Frankfurt am Main, Germany — [2]University of Connecticut, Connecticut, United States — [3]George Mason University, Fairfax, USA — [4]Iowa State University, Ames, United States

Most of crystalline solids have a maximum recoverable strain of less than 1%. Further strain will cause plastic deformation or fractures. In the current work we present $SrNi_2P_2$, whose maximum recoverable compressive strain is $\sim 14\%$ and tensile is $\sim 6\%$. These widespread values of strain are realizable due to a double lattice collapse-expansion mechanism. The ab initio density functional theory calculations are in very good agreement with the experiment[1,2]. Instead of the usual uncollapsed to collapsed tetragonal transition for the generic tetragonal 122s, a second transition to an orthorhombic superstructure is observed. By a detailed investigation of the electronic and geometric structures for various strains, and substitutions of the Sr, Ni, (and /) or P from first principles, we are able to give a deeper insight in the theory description of this doubly lattice collapse-expansion mechanism. Within this framework we will also discuss structural phases in $CaKFe_2As_2$ under varios strain conditions.

This work is support by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) for funding through TRR 288.

[1] Nano Lett. 2021, 21, 19, 7913
[2] Phys. Rev. B 56, 13796 (1997)

TT 3.7 Mon 11:00 H23

3DSC - A new dataset of superconductors including crystal structures — •Timo Sommer, Roland Willa, Jörg Schmalian, and Pascal Friederich — Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

More than 100 years after the discovery of superconductivity in mercury, the search for new superconducting materials still remains challenging. In contrast to most other phenomena, making theoretical predictions about the superconductivity of a certain material is extremely difficult, due to the need to model the comparably tiny energy gain of the superconducting phase, compared to the other energy scales of the problem. Data-driven methods, in particular machine learning, are well-known for finding complex patterns in existing datasets. In the case of superconductors, the use of data science tools is to date slowed down by a lack of accessible data. Here we present a new and publicly available superconductivity dataset ("3DSC"), featuring the critical temperature T_c of superconducting materials additionally to tested non-superconductors. In contrast to existing databases such as the SuperCon database, the 3DSC contains not only the chemical composition, but also the approximate three-dimensional crystal structure of each material. We perform machine learning experiments which show that access to this structural information improves the prediction of the critical temperature T_c. Additionally, we provide ideas for further research to improve the 3DSC in multiple ways. We argue that expanding and developing the 3DSC is a promising direction towards the reliable prediction of new superconductors using machine learning.

15 min. break

TT 3.8 Mon 11:30 H23

Control of the critical temperature of a superconductor/chiral magnet heterostructure — •Julius Grefe[1], Jannis Willwater[1], Rodrigo de Vasconcellos Lourenço[2], Markus Etzkorn[2,3], Stefan Süllow[1], and Dirk Menzel[1,3] — [1]IPKM, TU Braunschweig, Germany — [2]IAP, TU Braunschweig, Germany — [3]LENA, TU Braunschweig, Germany

Recently, theory has predicted that spin valves consisting of a superconducting film and a magnetic substrate exhibiting a non-collinear spin structure can be controlled via the proximity effect by changing the spin orientation of the magnet. The critical temperature T_c of a thin superconducting Nb film on top of a magnetic MnSi substrate is supposed to be altered when the spin helix vector switches from the inplane to the out-of-plane direction [1]. We have prepared substrates for molecular beam epitaxy from MnSi single crystals. After preparation the surface roughness has been investigated by AFM and TEM and is in the order of 1 nm. Afterwards, a 20 nm superconducting Nb thin film has been deposited on top of the MnSi substrate. In dependence of the orientation of the external magnetic field and, thus, the direction of the spin helix vector in the MnSi substrate, we observe a change of T_c in the Nb film. To distinguish between the influence of the helix on T_c and pure geometry effects, we compare the result with observations on a Nb film deposited on an isostructural but non-magnetic CoSi substrate.

[1] N. G. Pugach et al., Appl. Phys. Lett. **111**, 162601 (2017)

TT 3.9 Mon 11:45 H23

Gate controlled switching in A15 and non-centrosymmetric superconducting devices — •Jennifer Koch, Leon Ruf, Simon Haus, Roman Hartmann, Elke Scheer, and Angelo Di Bernardo — Universität Konstanz, Konstanz, Germany

Gate-controlled superconducting devices have become of great interest for the development of energy-efficient hybrid superconductor/semiconductor computing architectures. The idea behind this technology stems from the recent discovery that superconducting devices can be controlled electrically with the application of a gate voltage [1-3]. We investigate gate-controlled switching devices made of A15 and non-centrosymmetric superconductors like Nb_3Ge (A15) and $Nb_{0.18}Re_{0.82}$ (non-centrosymmetric). These materials promise a low switching voltage due to their disordered structure and high spin-orbit coupling and should therefore be more suitable for the realization of devices working at voltages comparable to those used for the control of CMOS transistors.

[1] G. de Simoni et al., Nat. Nanotechnol. 13, 802 (2018)
[2] F. Paolucci et al. , Nano Lett. 18, 4195 (2018)
[3] F. Paolucci et al., Phys. Rev. Applied 11, 024061 (2019)

TT 3.10 Mon 12:00 H23

Fano interference of the Higgs response and CDW fluctuations in cuprate high-T_c superconductors — •Liwen Feng[1,2,3], Hao Chu[1,2,4], Sergey Kovalev[5], Lukas Schwarz[1], Tao Dong[6], Min-Jae Kim[1,2,3], Gideok Kim[1], Gennady Logvenov[1], Bernhard Keimer[1], Dirk Manske[1], Nanlin Wang[6], Jan-Christoph Deinert[5], and Stefan Kaiser[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]4th Physics Institute, University of Stuttgart, Stuttgart, Germany — [3]Institute of Solid State and Materials Physics, Technical University Dresden, Dresden, Germany — [4]Quantum Matter Institute, University of British Columbia, Vancouver, Canada — [5]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [6]International Center for Quantum Materials, Peking University, Beijing, China

Cuprate high-T_c superconductors exhibit a rich phase diagram due to the presence of multiple orders. The interplay of these orders is difficult to access directly by experimental probes. Here, we introduce phase-resolved Higgs spectroscopy, i.e. THz driven amplitude oscillations of the superconducting order parameter. We find a Fano interference of the driven Higgs mode with charge density fluctuations in superconducting $La_{2-x}Sr_xCuO_2$ ($0.05 \leq x \leq 0.25$). The interference manifests itself as a distinct jump in the phase of the driven Higgs oscillation, which we characterize in an extensive doping- and magnetic field-dependent study. As such, Higgs spectroscopy provides a novel and direct view on the intriguing interplay of charge density fluctuations and superconductivity in high-T_c cuprates.

TT 3.11 Mon 12:15 H23

Clarifying the origin of CDW and finding the routes to superconductivity in Ti-Se systems. — •Andrii Kuibarov, Yulia Shemerliuk, Alexander Fedorov, and Sergey Borisenko — IFW Dresden, Deutschland

Two-dimensional chalcogenides have gained renewed attention mainly because of the novel topological properties observed in single crystals and thin films. Although $TiSe_2$ has been intensively researched over the last 20 years, the true nature of its charge density waves (CDW) state remains controversial. Several different theories have been proposed during these years to explain CDW formation: Fermi surface nesting, Jahn-Teller effect and excitonic insulator.

We try to answer this question using high-resolution ARPES measurements and DFT calculations for different Ti-Se systems: $TiSe_2$, Cu_xTiSe_2, TiSeS. We show that the CDW state does disappear at various Cu-doping in Cu_xTiSe_2 as it was thought before.

TT 3.12 Mon 12:30 H23

Superconductivity in the type-I Weyl semimetal trigonal-$PtBi_2$ — •Arthur Veyrat[1], Valentin Labracherie[1], Federico Caglieris[1,2], Jorge I. Facio[1], Grigory Shipunov[1], Jeroen van der Brink[1,3], Bernd Büchner[1,3], Saicharan Aswartham[1], and Joseph Dufouleur[1,4] — [1]Leibniz Institute for Solid State and Materials Research (IFW Dresden), Dresden, Germany — [2]CNR-SPIN, Genova, Italy — [3]Department of Physics, TU Dresden, Dresden, Germany — [4]Center for Transport and Devices, TU Dresden, Dresden, Germany

Symmetry breaking in topological matter became a key concept in condensed matter physics to unveil novel electronic states. In particular, the interplay between topology and superconductivity in topologically non-trivial materials is of great interest for the study of unconventional superconducting states. In this talk, I present DFT calculations showing a type-I Weyl semimetal band structure in trigonal $PtBi_2$. We also evidenced, via transport measurements, that single crystals of trigonal $PtBi_2$ are superconducting ($T_c \sim 600mK$), which represents the first unambiguous report of bulk superconductivity in a type-I Weyl semimetal. We further characterized the superconductivity in exfoliated thin flakes of trigonal $PtBi_2$ to be 2-dimensional, up to 126 nm, and we evidence a Berezinskii-Kosterlitz-Thouless transition in flakes up to 60nm thick, with $T_{BKT} \sim 310mK$. This discovery makes trigonal $PtBi_2$ a very interesting platform to study the interplay between low dimensional superconductivity and topology, into relatively thick and easily fabricated samples.

TT 3.13 Mon 12:45 H23

Vortex inductance as a directional probe of Lifshitz invariants in synthetic Rashba-superconductors — Lorenz Fuchs[1], Denis Kochan[1], Christian Baumgartner[1], Simon Reinhardt[1], Sergei Gronin[2], Geoffrey C. Gardner[2], Tyler Lindemann[2], Michael J. Manfra[2], Christoph Strunk[1], and •Nicola Paradiso[1] — [1]University of Regensburg — [2]Purdue University

In type II superconductors, the magnetic field penetrates the sample in quantized units of flux, which correspond to vortices in the superfluid. To save condensation energy, vortices tend to be pinned to defects. If these are sharp, the pinning potential $U(\vec{r})$ is harmonic near the vortex core, where it mirrors the superfluid density $|\Psi(\vec{r})|^2$. In this work, we show that in 2D Rashba superconductors the combination of spin orbit interaction and in-plane magnetic field leads to an anisotropic squeezing of the vortex core. This, in turn, produces a strong enhancement of the pinning strength, which can be measured by vortex inductance measurements. To this end, we developed a technique to measure small inductances which is compatible with the application of both DC bias and strong magnetic fields. Vortex inductance is sensitive to the curvature of the pinning potential along the direction perpendicular to the supercurrent. Thus, our method enables a full tomography of the vortex core, obtained by measuring inductance as a function of the angle between current and field. Our results can be interpreted as the effect of the spin orbit-induced Lifshitz invariant term in the Ginzburg-Landau free energy.