TT 95: Fe-based Superconductors

Time: Friday 9:30–11:45 Location: HSZ/0103

TT 95.1 Fri 9:30 HSZ/0103

Saddle-point-nesting driven formation of charge order and superconducting vortex splitting on heavily hole-doped iron-arsenide superconductors — •Chi Ming Yim — Tsung-Dao Lee Institute & School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai, China

The study of iron-arsenide superconductor $Ba_{1-x}K_xFe_2As_2$ (BKFA) has re-sparked considerable interest following the recent discoveries in this material of superconductivity with broken time-reversal symmetry [1], superconducting vortices with fractional flux quantum [2], and quartic states [3]. Most studies focus on its bulk properties, with much less attention paid to its surface(s). This talk reports on our recent STM/S findings on the surfaces of BKFA in its heavily-hole doped regime: On the As- surface of BKFA (x=0.77), we observe of a density wave order with a 2x2 spatial periodicity, with clear-cut evidence(s) confirming its charge origin. Our calculation results indicate that its formation is saddle-point nesting driven. [4]. On the K- surface of multiband superconductor KFe_2As_2 studied under an external magnetic field, we observe splitting of vortices with integer flux quantum into those with appreciably reduced conductance, demonstrating the possibility of vortex core fractionalization in a multiband superconductor [5].

[1] Grinenko et al., Nat. Phys. 17, 1254 (2021)
[2] Iguchi et al., Science 380, 1244 (2023)
[3] Shipulin et al., Nat. Commun. 14, 6734 (2023)
[4] Hu et al., Nat. Commun. 18, 253 (2025)
[5] Zheng et al., Arxiv 2407.18610 (2024)

TT 95.2 Fri 9:45 HSZ/0103

Measuring Nematic Fluctuations in FeSe under Hydrostatic and Chemical Pressure — •Adrian Merritt[1], Amir Haghighirad[2], Dmitry Reznik[3], Ayman Said[4], Ahmet Alatas[4], Alexei Bosak[5], Michaela Souliou[2,5], and Frank Weber[2] — [1]Karlsruher Institut für Technologie - PHI, 76049 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie - IQMT, 76344 Eggenstein-Leopoldshafen, Germany — [3]University of Colorado, 80309, Boulder, Colorado, USA — [4]Advanced Photon Source, Argonne National Laboratory, 60439, Illinois, USA — [5]European Synchrotron Radiation Facility (ESRF), 38043 Grenoble, France

Nematic correlations in iron-based superconductors have been widely studied through phonon softening measured by INS and IXS. Softening of the transverse acoustic phonons near the tetragonal-orthorhombic transition reflects growing nematic fluctuations, which also appear near the superconducting transition, highlighting the competition between nematicity and superconductivity. Our earlier IXS work on FeSe and Co-doped Ba122 showed similar behavior with and without magnetism and across the superconducting transition, suggesting that nematicity may hinder superconductivity.

Our most recent FeSe studies examine the effects of pressure, using both hydrostatic pressure and isoelectronic chemical pressure via S substitution. Both methods introduce magnetic phases and modify the structural transition order, opening a rich, otherwise inaccessible phase diagram. We present these results and compare how nematic fluctuations evolve across the different pressure-induced phases of FeSe.

TT 95.3 Fri 10:00 HSZ/0103

Magnetic-field-induced Sarma state in atomically thin superconducting FeSe films — •Wantong Huang[1,2], Yuguo Yin[1], Haicheng Lin[1], Wei Chen[1], Yaowu Liu[1], Lichen Ji[1], Zichun Zhang[1], Xinyu Zhou[1], Xusheng Wang[1], Yong Xu[1], Lianyi He[1], Xi Chen[1], Qi-Kun Xue[1], and Shuai-Hua Ji[1] — [1]State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China — [2]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Many-body ground states of imbalanced Fermi gas have long been studied both theoretically and experimentally due to their fundamental significance in condensed matter physics, cold atom physics and nuclear physics. Among the predicted exotic phases, the Sarma state, a gapless spin-polarized superfluid, has remained experimentally elusive. Here, we report direct evidence for the Sarma state in atomically thin FeSe films using a dilution-refrigerator scanning tunneling microscope under high magnetic fields. In the bilayer and trilayer FeSe films, we observe the hallmark signature of the Sarma state: the inner Zeeman splitting coherence peaks cross the Fermi level under high in-plane magnetic fields. The angle dependent critical field exhibits a two-fold symmetry arisng from the anisotropic in-plane g-factor. Moreover, our two-band model shows that the magnetic field induced Sarma phase emerges via a first-order transition at zero temperature, which evolves into a smooth crossover at finite temperature. These findings pave the way to explore the unusual physical properties and potential applications of the spin-polarized Sarma superfluid state.

TT 95.4 Fri 10:15 HSZ/0103

Coupling of Vortex Bound States as a Probe of Majorana Physics in Iron-Based Superconductors — •Raigo Nagashima[1], Iksu Jang[1], and Jörg Schmalian[1,2] — [1]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Motivated by the widespread observation of zero or near-zero vortex bound states on the surfaces of $FeSe_{1-x}Te_x$ and related iron-based superconductors, we investigate how these states evolve and interact as the magnetic-field-induced vortex density increases. Such coupling effects provide a powerful diagnostic of the underlying nature of the bound states. We compare the behavior expected for conventional Caroli-de Gennes-Matricon (CdGM) vortex states with that arising from Majorana zero modes in two-dimensional topological superconductors. To this end, we analyze the multi-vortex problem in the Fu-Kane model and compute the resulting hybridized bound-state wave functions. Our results reveal striking and qualitative differences between the coupling patterns of CdGM states and those of Majorana modes, demonstrating that the field-induced evolution of vortex bound states offers a clear and experimentally accessible fingerprint for identifying Majorana physics in iron-based superconductors.

TT 95.5 Fri 10:30 HSZ/0103

Intertwined superconductivity and orbital selectivity in a three-orbital Hubbard model for the iron pnictides — Vito Marino[1,2], Alberto Scazzola[2], Federico Becca[3], Massimo Capone[1], and •Luca F. Tocchio[2] — [1]International School for Advanced Studies (SISSA), Trieste, Italy — [2]Politecnico di Torino, Italy — [3]University of Trieste, Italy

We study a three-orbital Hubbard-Kanamori model relevant for iron-based superconductors, using variational wave functions which explicitly include spatial correlations and electron pairing. We span the nonmagnetic sector from filling $n = 4$, which is representative of undoped iron-based superconductors, to $n = 3$, where a Mott insulating state with each orbital at half filling is found. In the strong-coupling regime, we observe spontaneous differentiation in the occupation of the d_{xz} and d_{yz} orbitals, leading to an orbital-selective state with nematic character that becomes stronger with increasing density. One of these orbitals remains half-filled for all densities, while the other hosts (together with the d_{xy} orbital) the excess electron density. Most importantly, in this regime, long-range pairing correlations appear in the orbital with the largest occupation. Our results highlight a strong link between orbital-selective correlations, nematicity, and superconductivity, which requires the presence of a significant Hund's coupling. The interplay with magnetism is also discussed.

[1] V. Marino, A. Scazzola, F. Becca, M. Capone, and L.F. Tocchio, PRL 134, 196502 (2025).

15 min. break

TT 95.6 Fri 11:00 HSZ/0103

Predicting isostructural collapses in the $ThCr_2Si_2$ structure type - fast and efficient — •Adrian Valadkhani[1], Paul Canfield[2], and Roser Valentí[1] — [1]Goethe Universität ITP, Frankfurt am Main, Germany — [2]Ames National Laboratory, Ames, USA

Isostructural collapse transitions in tetragonal $ThCr_2Si_2$(122) compounds strongly affect magnetism, topology, and superconductivity, yet most studies treat materials on a case-by-case basis, making the overall approach computationally inefficient. Here, we present a general, efficient framework to predict isostructural collapses across the

122 family - readily extensible to other structure types. We classify collapsibility from the ambient-pressure unit cell using a linear, supervised classifier. In addition, an ambient-pressure calibration of the density-functional-theory-based calculations anchored to the experimental structure determines both the form of collapse and the critical pressure, if it exists. We validate the method against literature data and recent work on $SrCo2P_2$, and we show how the same calibration subsequently enables efficient exploration of the pressure-dependent electronic structure. Because the procedure requires minimal experimental input and fast, efficient and standard computations, it is directly transferable to other structure families where isostructural transitions or distortions occur. This establishes a practical route for screening and designing materials with collapse-tunable functionalities.

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TT 95.7 Fri 11:15 HSZ/0103

Inelastic neutron scattering study of magnetic fluctuations in iron germanides YFe_2Ge_2 and $LuFe_2Ge_2$ — •Ran Tao[1], Jiasheng Chen[1], Stephen Hodgson[1], Philipp Niklowitz[2], Malte Grosche[1], Travis Williams[3], David Voneshen[3], Devashibhai Adroja[3], Paul Steffens[4], Alexandre Ivanov[4], and Andrea Piovano[4] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Department of Physics, Royal Holloway, University of London, UK — [3]ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, UK — [4]Insitut Laue-Langevin, Grenoble, France

The iron-based superconductor YFe_2Ge_2 ($T_c \simeq 1.8$ K) exhibits strong electronic correlations [1,2], and a prior neutron scattering study has demonstrated enhanced magnetic fluctuations [3]. The isoelectronic and isostructural sister compound $LuFe_2Ge_2$ orders antiferromagnetically with $Q_F = (0, 0, 1)$ below $T_N \simeq 6.5$ K, and in clean crystals shows a resistive superconducting transition below 1 K.

Our inelastic neutron scattering experiments in YFe_2Ge_2 indicate that the dynamic response near Q_F deviates from the commonly assumed overdamped oscillator form and could instead best be fitted with an underdamped form. A similar response is also seen in the sister compound $LuFe_2Ge_2$ in the paramagnetic phase. The similarities between the two materials suggest that resonant spin fluctuations may be a more general feature in iron germanides.

[1] J. Chen et al., Phys. Rev. Lett. **125,** 237002 (2020).
[2] J. Baglo et al., Phys. Rev. Lett. **129,** 046402 (2022).
[3] H. Wo et al., Phys. Rev. Lett. **122,** 217003 (2019).

TT 95.8 Fri 11:30 HSZ/0103

Local-moment magnetism in Mn-based pnictides — •Matteo Crispino[1], Niklas Witt[1], Tommaso Gorni[2], Giorgio Sangiovanni[1], and Luca de' Medici[2] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]LPEM, ESPCI Paris, PSL Research University, CNRS, Sorbonne Université, 75005 Paris, France

We report a comprehensive study of electronic-correlation effects in Manganese-based antiferromagnetic pnictides $BaMn_2Pn_2$ (Pn=P,As,Sb,Bi). Our density functional theory plus slave-spin mean-field simulations indicate that all the compounds lie on the strong-coupling side of an itinerant-to-localized moment crossover, corresponding to the critical interaction strength for the Mott transition in the high-temperature paramagnetic phase. We also show that the experimental Néel temperature of each compound scales with the distance from this crossover.