Iron-based Superconductivity: Towards Optimizing T_c through Orbital Selectivity

1. **Discovery of orbital-selective Cooper pairing in FeSe**
   Authors: P. O. Sprau, A. Kostin, A. Kreisel, A. E. Böhmer, V. Taufour, P. C. Canfield, S. Mukherjee, P. J. Hirschfeld, B. M. Andersen, J. C. Séamus Davis
   Science **357**, 75 (2017)
2. **Formation of Hubbard-like bands as a fingerprint of strong electron-electron interactions in FeSe**
   Authors: M. D. Watson, S. Backes, A. A. Haghighirad, M. Hoesch, T. K. Kim, A. I. Coldea, and R. Valenti
   Phys. Rev. B **95**, 081106(R) (2017)
3. **Direct observation of dispersive lower Hubbard band in iron-based superconductor FeSe**
   Authors: D. V. Evtushinsky, M. Aichhorn, Y. Sassa, Z.-H. Liu, J. Maletz, T. Wolf, A. N. Yaresko, S. Biermann, S. V. Borisenko, and B. Büchner
   arXiv:1612.02313

Recommended with a Commentary by Qimiao Si, Rice University

The iron-based superconductors (FeSCs) involve multiple electronic degrees of freedom (spin, orbital and nematic). As such, there are two questions that are particularly important to the study of their microscopic physics:

- Can we achieve simplicity in the understanding given this level of complexity?
- How to take advantage of the multiple degrees of freedom to realize even higher superconducting transition temperature (T_c)?

One promising setting to explore these issues is the iron chalcogenides, which host the highest T_c among the FeSCs (65 K, as determined by the onset of the Meissner effect [1]). There is an emerging consensus that the electron correlations are strong in these systems. Because of the strong correlations, the low-energy physics may be considered in an orbital-selective way. This notion has been verified by orbital-selective measurements using angle-resolved photoemission spectroscopy (ARPES) [2]. Particularly important are the d_{xz} and d_{yz} orbitals of the 3d-electrons, which are degenerate so long as the C_4 symmetry of the tetragonal crystal is preserved, and the d_{xy} orbital.

The highlighted studies concern the bulk iron selenide FeSe ($\alpha-$FeSe, to be more precise) [3], a member of the iron chalcogenide superconductors. It stands out in having the simplest structure. One can picture it as a simple repetition of an FeSe plane, with two Se-layers sandwiching a square lattice of Fe ions. The system undergoes a transition into an electronic nematic order (the breaking of the C_4 rotational symmetry of the electronic degrees of freedom, accompanied by a tetragonal to orthorhombic structural phase transition; see a Commentary on the July 2016 issue of JCCM) at about 90 K, and superconducts with a T_c of 9 K. The FeSe plane is the structural basis for the iron chalcogenides with the highest T_c.

In article #1, P. O. Sprau and collaborators used STM to study the interference of electronic quasiparticles induced by impurities in FeSe. They performed experiments at a (sub-Kelvin) temperature that is low compared to T_c. The interference pattern in the wavevector space, derived from a Fourier transform of the STM pattern in real space, allows for extracting the gap of the Bogoliubov quasiparticles. A surprisingly strong variation of the gap was found on each Fermi-surface sheet.

Sprau *et al.* found that the gap anisotropy can be understood in terms of strongly orbital-dependent pairing amplitudes, once the interaction-induced strong and orbital-selective quasiparticle renormalization factors are taken into account. Their interpretation seems to be natural: The extracted Fermi surfaces are compatible with the ARPES and quantum oscillation results [4], and the gap amplitude tracks the orbital content of the (normal-state) electronic states on the Fermi surfaces.

The orbital-selective pairing was theoretically advanced [5] from the perspective of superconductivity driven by short-range spin-exchange interactions involving the multiple 3d orbitals. (Inter-orbital pairing was found to be negligibly small.) When the local Coulomb (Hubbard and Hund's) interactions are sufficiently strong, orbitals become a natural basis to consider superconducting pairing. The work of Sprau *et al.* extended this notion by adding an important new ingredient: the pairing amplitude is different not only between the d_{xy} orbital and the d_{xz}/d_{yz} orbitals, but also between the d_{xz} and d_{yz} orbitals. The latter manifests the electronic nematic order, which breaks the degeneracy between the d_{xz} and d_{yz} orbitals due to the reduction of the C_4 symmetry to C_2.

The interpreation of Sprau et al. rests on the Coulomb interactions being strong in FeSe. Is that really so? In article #2, by M. D. Watson and collaborators, and article #3, by D. V. Evtushinsky and collaborators, ARPES studies were reported which provide evidence for Hubbard-like bands in FeSe on the scale of several eVs. These are incoherent single-electron excitations that are sufficiently away from the Fermi energy and are generated by the local Coulomb interactions. As such, they are hallmarks of strong correlations.

The ARPES results in FeSe connect well with the bad-metal behavior of the normal state that has been observed in the FeSCs from the beginning of the field: The DC resistivity at room temperature is so large that it reaches the Mott-Ioffe-Regel limit (the mean free path being the same order as the inverse Fermi wavevector), and the Drude component of the AC conductivity is strongly reduced from its non-interacting counterpart.

Taken together, the new developments have several implications and also raise a number of intriguing possibilities for future exploration:

- First, the strong correlations allow us to build up intuition about how to control the low-energy physics by tuning local degrees of freedom. For instance, an emerging notion is that the multi-orbital nature provides a new handle to engineer the low-energy electronic states and raise T_c. Even when the superconductivity is primarily driven by magnetic correlations, tuning the orbital levels and orbital-dependent couplings may optimize superconductivity. Some recent evidence along this direction has come from the monolayer FeSe system in the work of X. Shi et al. [6], which provided evidence that T_c can be further increased from the current record by the tuning of the electronic states of particular d-orbitals.

- Second, similar line of consideration even suggests some welcoming simplicity out of the complex entwining in the multiple degrees of freedom. For the FeSCs, there are strong indications that superconductivity is primarily driven by magnetic correlations; yet, there is also evidence that it is influenced by nematicity. Perhaps the primary form of this influence is for the nematicity to cause a change to the orbital selectivity, which, in turn, modulates the magnetically driven superconductivity?

References

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