The Ironics: Strong Coupling or Weak Coupling in the Wonderland

- **Mott-Kondo Insulator Behavior in the Iron Oxychalcogenides**

  B. Freelon, Yu Hao Liu, Jeng-Lung Chen, L. Craco, M. S. Laad, S. Leoni, Jiaqi Chen, Li Tao, Hangdong Wang, R. Flauca, Z. Yamani, Minghu Fang, Chinglin Chang, J.-H. Guo and Z. Hussain,
  arXiv:1410.3435

- **FeSe: a model system for Fe based superconductors**
  B. Büchner, IFW Dresden, at KITP Program: Magnetism, Bad Metals and Superconductivity, Nov 04, 2014,
  http://online.kitp.ucsb.edu

Recommended with a Commentary by Chandra Varma,
University of California.

The discoveries of several Pnictogen and Chalcogen Iron compounds, with contiguous Antiferromagnetism, high temperature Superconductivity, and structural transitions in their phase diagram as a function of dopants, has been followed by intense activity, both theoretical and experimental. The level of activity does not rival the frenzy in the decade following the discovery of superconductivity in the cuprates, but is only an order of magnitude lower.

The compounds have well separated layers of Fe and superconductivity appears below a region of anomalous non-Fermi-liquid transport properties characteristic of quantum-critical fluctuations. In this respect, the problem is less perplexing than the cuprates, where the non-Fermi-liquid properties above superconductivity have, at one boundary in the phase diagram, a much more subtle transition than the easily observed Antiferromagnetism in the ironics (a term used to describe such compounds which I heard Sri Raghu use at the KITP workshop on this problem last fall). But unlike in the Cuprates, there are multiple bands from the closely spaced Fe-orbitals near the Fermi-surface and not too far below and above it because Fe is near the middle of the 3d-transition metal series. The near orbital degeneracy introduces intra-atomic Hund's rule correlations together with inter-atomic interactions and appears much more complicated at the level of the minimal Hamiltonian. But is it so at the level of basic principles?

One outlook has been that the interactions parameters, though numerous are not much larger than the kinetic energy parameters. So, why not address the problem by using the all-purpose calculations of the density functional type, (too numerous to refer to here but referred in the papers highlighted and below) which have rationalized through imaginative use the properties of so many magnetic metals and compounds. The difficulty in Cuprates, which led to rejection of such methods, that they predict the 1/2 filled state to be a metal are absent in the Ironics. And the ground state properties like itinerant Antiferromagnetism can be obtained by the spin-polarized density functional methods. Being variational,

such methods give good account of ground states. Superconductivity may then be calculated by exchanging spin-fluctuations in the bands crossing the Fermi-level using ideas of nesting. These also promote electronic-fluctuation induced superconductivity. Some of the successes follow because such methods incorporate the right symmetries.

The other outlook is that such weak-coupling methods are the wrong way to think on these problems. This outlook is supported by two kinds of calculations, (also too numerous to give references here) those of the dynamical mean-field type, in which dynamics of small clusters embedded in a self-consistent media are well calculated, and those of the phenomenological type in which model Hamiltonians are proposed. Definite answers, on for example the antiferromagnetic states and the fluctuation spectra, can only be approximately calculated. Questions of judgement on choice of model and parameters necessarily accompany such an approach. So the debate rages on between the two outlooks.

Do experiments definitely favor one or the other outlook? The fact pointed out, for example many years ago in Ref.(1) below, that the total number of electrons **plus** holes in the bands crossing the Fermi-surface in the Ironics, is only of $O(10^{-1})$ per unit-cell, while the magnetic order is often of $O(1)\mu_B$ per unit-cell, would argue against the weak-coupling outlook. Such magnetic moments can only come from states well below the chemical potential. Such states are required to be many-body states because to be magnetic, they must result in partially-filled orbitals and yet lie below the chemical potential with their partners lying above the chemical potential. Partially-filled orbitals below the chemical potential imply Mott-like states discoverable in one-hole spectra. Then their partners must be observable in one-electron spectra above the chemical potential. The former should be visible in photoemission experiments and the latter in, for example, X-ray absorption experiments. The two papers above, each using one of these methods appear to succeed in discovering such states. They appear as broad states and have other spectroscopic signatures of being Mott states.

There appears to be an issue which at first appears surprising and thought-provoking. In the calculations in which the correlations are considered explicitly[2], the number of bands crossing the Fermi-surface and the shapes of the Fermi-surfaces are quite similar to those calculated by one-electron methods of the density functional type, (although states away from the chemical potential do not bear such a correspondence). And they agree with the photoemission experiments! In the calculations with explicit correlations, partial occupation of some orbitals creates an effective attractive potential for the occupied states such that some other orbitals have to be pushed down (relative to the one-electron type calculations) so as to maintain charge neutrality. It appears that the effective potential *for the conduction bands* despite all this re-arrangement has the full symmetry of the lattice. Only then can the Fermi-surface shapes in the two kinds of calculations be identical. This seems to require more than the old result that, for example in heavy fermions, the shape of the Fermi-surfaces are similar to those in one-

electron calculations, despite the masses being more than an order of magnitude different, because the self-energy is momentum-independent. One may conjecture a generalized version of a Friedel like theorem that the pseudo-potential for the conduction bands is almost unaffected in a *partial* Mott localization.

It is worth also mentioning a great simplification that the experiments suggest in the form that the theory with correlations might take. Consistent with the small number of electrons and holes in the bands crossing the Fermi-level, the bottoms of such bands with respect to the Fermi-level is typically less than 0.1eV. The measured spin-fluctuation spectra extends at least up to the upper limit, about 0.25 eV, of the measurements using neutron scattering[3]. This together with magnetism arising from orbital below the chemical potential implies that quite different states are responsible for the fluctuations and for conduction and super-conductivity. The problem is akin to electron-phonon problem in that the basis states for fluctuations and that of the Cooper pairing are orthogonal to leading order. This should make the problem simpler. But the fluctuations and the conduction band-width are in the anti-Migdal limit. That suggests that superconductivity may not of the BCS type, but closer to superconductivity due to Bose condensation of preformed pairs, due to the much larger scale of pairing interactions compared to the conduction band. Is this possibly a reason why the uniform magnetic susceptibility in such compounds is observed to decrease fairly strongly as temperature decreases, being often less than 1/2 near T_c of O(30 K) compared to that near room temperature? Or is it due just to a very large region in temperature of Antiferromagnetic fluctuations, or are the two the same thing, said in different words.

(1) G.M. Zhang et al., arXiv:0809.3874v3.
(2) M. Aichhorn et al., Phys. Rev. B 82, 064504 (2010). (3) For example, J. Zhao et al, Nature Physics 5, 555 (2009).