DISCUSSION (Wed 10/08): NATURE OF MAGNETISM IN Fe-BASED SUPERCONDUCTORS

Andreyy Chubukov (AC): Itinerant vs localized magnetism in iron pnictides (blackboard talk).

In the itinerant approaches magnetism is enhanced (in an RPA sense) at large Q simply because of the electronic structure with hole and electron pockets, and because the bare bubble involved in the RPA calculation requires one electron and one hole excitation. Nesting is not really required, but it helps. What is required is one band of electron-excitations and one band of hole-excitations.

Leon Balents (LB): ok but enhanced more like FFLO than like Superconductivity. **AC**: agrees

Consequence: the ordered vector is influenced by the physics at high energies.

AC singles out a few interesting points on this topic.

1) Effect of doping (in the rigid model: opposite change in size of the pockets). Another parameter is ellipticity. The transition temperature (2nd order) goes down and disappears at finite doping.
A detail on how it happens: at high T the system first goes in an analog of FFLO and develops magnetism at finite momentum and then becomes first-order.
W Lv: Is this obtained with how many pockets? A.C.: 4 pockets, but degeneracy can be split a little.

2) Type of magnetic order.
Paramagnetic phase C4 symmetry. Two possible order parameters for magnetism: Delta_1=(Pi,0) and Delta_2=(0,Pi)
Depending on the coefficient in front of the term (Delta_1^2-Delta_2^2)^2 in the Ginzburg-Landau free energy being positive or negative one can have respectively |Delta_1|^2=|Delta_2|^2 or one parameter zero and the other finite, thus breaking or not the C4 symmetry.

Qimiao Si (QS): the form of this functional is symmetry-dictated right? **AC**: yes, you start with the fermionic model and integrate out fermions, which gives all the coefficients, which depend on doping.
A. Nevidomskyy (AN): what about hydrostatic pressure like in Phosphorus doping? **AC** I haven't done the calculations for pressure but I can answer about impurities as in Ruthenium doping, and the phase diagram remains the same.
LB: this approach reminds the studies of excitonic insulators (Rice, Keyldish etc). Not settled there if triplet or singlet insulator and it depends on the original interaction put in the model. Is there any assumption for the interaction here in this respect?
AC: all interactions need to be considered and if any of those is attractive then charge physics come into play. But if they are all repulsive then the fixed points obtained with functional RG and parquet RG are such that magnetism and s-wave superconductivity are the only competitors.

It is surprising that in the itinerant approach one obtains the stripe phase (C_2 symmetry) but also in some region and for some values of the parameters a checkerboard phase of C_4 symmetry.

LB: Is the order parameter a complex vector? **AC**: No, it is real because for this magnetic ordering vector Q=(0,Pi), Q is equivalent to -Q, which is what you do with complex conjugation.

3) Relation of this magnetism and superconductivity
Itinerant magnetism favors s+- superconductivity. Indeed it is not required, because only inter-pocket interactions > intra-pocket interaction are needed, but magnetism enhances large-momentum interactions, so it helps.
An interesting fact comes from f-RG and parquet-RG, when treating SDW and SC as coming from the same interactions and seeing who wins.
As a function of a running coupling constant (increasing with decreasing temperature), one has SDW and SC coupling constant diverging (SC even if it starts repulsive becomes attractive and is enhanced thanks to the developing magnetism) and developing the respective instability.
But the final result depends on the specific model.
With 5 pockets, no matter what you do SDW always wins, which means that at zero doping one has always magnetism.
Piers Coleman (PC): but 5 pockets means a lot of parameters, how can you know that you always get this

result?
AC: People working on this claim having analyzed a lot of different choices. We work with 10 parameters and always find this result.
This gives the conventional phase diagram in doping, because for increasing doping magnetism goes down and the attractive SC channel at some point takes over.
But with 4 pockets SC interaction goes up very rapidly and overshoots SDW. Then you only have SC in this model.

Leni Bascones: what happens if the band is not right at the Fermi level but a little below? **AC:** then the story might change because here a simple quadratic dispersion is assumed.

4) Coexistence of SC and SDW
SDW generates another superconductive channel when coexisting with SC and since SDW breaks time-reversal symmetry this channel mixes singlet and triplet (in orbital space) SC. It has been predicted that within the coexistence region of SDW and SC another region with time-reversal symmetry broken (the two order parameters mixed with a pi/2 phase) SC can arise.

Ilya Vekhter: what about parity? AC: Parity it is not broken by SDW.

5) Magnetism and nematicity
The two transitions (normal to nematic, and nematic to magnetic) are seen both coincident and separate in different materials.
Calculations (in quasi-2D) show that as a function of electronic doping 3 possibilities are found. Simultaneous 1st order (small doping), split 2nd order (large doping), slightly split and nematic 2nd order while magnetic 1st order (intermediate doping). This last region is called meta-nematic and seems to be observed experimentally (see slides).

Qimiao Si: Refer to the slides: "Discussion - Nature of magnetism in Iron Pnictides and Chalcogenides"

I want to reverse the historical perspective and imagine if the first discovered were the chalcogenides. One would have known first the most strongly correlated ones.

Extreme case: the 245 is found insulating for some compositions. Ordered moment by neutrons very large (3.3 mu_B/Fe).
La_2O_3Fe_2Se_2 is also found insulating and with large moments (2.8 mu_B/Fe). LDA predicts metallic phases, so the insulating behavior has to come from interactions. Kinetic energy is reduced compared to the pnictides by 25%.

In-between case: metallic Iron chalcogenides.
Fe_1-xTe, two unusual things compared to pnictides: the magnetic moment is large (2.3 mu_B/Fe), and the ordering is (Pi/2,Pi/2) which is strange from the perspective of the nesting of the Fermi surface (which is very practically identical to the pnictides case).
By substituting with Se AF order goes away and SC emerges. The two are separated by a phase with no bulk superconductivity but where magnetic fluctuations survive. The are seen (neutron resonance) to survive until the part of the phase diagram where SC develops.
AC: Don't they see the peak in the susceptibility at (0,Pi) however? **QS**: In the SC phase, not in the metallic phase above where the larger signal is still (pi/2, pi/2). But there are no normal-state magnetic-fluctuation spectrum measurements for further substitution, i.e. for the case of FeSe, however, and it would be very important to know what happens there.

For Fe(Te,Se) and single-layer FeSe, two things argue for sizable interactions: some mass enhancements are measured 10-20 contrary to 3 for pnictides, and Orbital-selective Mott phase is observed. Another thing to notice is that for KFeSe and the single layer the Fermi pockets are only electron-like but the Tc is comparable to pnictides. This points to sizable short-range interactions.

Iron Pnictides. Optics: Drude reduction is of order 2-3. Room T resistivity is already at the Mott-Ioffe-Regel limit.

The total spin spectral weight (ordered + fluctuating) measured by neutrons corresponds for 122 pnictides to a fully developed spin 1/2 moment. XES spectroscopy gives numbers compatible with this. Much larger number than implied by the areas of Fermi pockets.
Luca de' Medici (LdM): these numbers could be even higher actually because neutrons have resolution problems at high energies (thus the integrated spin spectral weight could be even larger) and XES cannot do absolute measurements so they adapt their scale on neutron measurements. Thus these moments could be even larger.
QS: I agree, but to me the important feature from these measurements is that they see relatively sharp features at the zone boundary.

Thus I argue that these families from a continuum.
PC: What instead, would you need to you to say the opposite (experimentally)? **QS**: If they were to have very different Tc's for example.
AC: FeTe is very different from pnictides, the magnetic order is different for example. **QS**: I think that the FeSeTe phase diagram pushes us to consider it all together. [some confuse discussion…] **QS**: I am just saying that there is superconductivity in these materials and trying to find a common starting point to access the physics of this phase. The question is can I do that or do I have to use very different starting points…I think that this question has consequences especially in cases where you have only electron Fermi pockets.
AC: Ok but where would you put the pnictides on this diagram? I think at x=0.5 because there the fluctuations are at (Pi,0) like in pnictides. Then at higher temperature the (pi/2,pi/2) takes over, it is an interesting physics but not connected to pnictides.
QS: I only want to say that wherever there is high-Tc there are magnetic fluctuations in the normal state. **AC**: yes but magnetic fluctuations of FeTe are very different from FeTeSe at x=0.5. FeTe is definitely a local moment system.

If I consider these materials part of a continuum, and I would obviously use the localized moment picture for the insulating one, I want to show that one understands also the spin dinamics in the more itinerant ones, assuming that most of the electron spectral weight is in the incoherent part.

J1-J2 model with biquadratic J1-J2 terms.

Natalia Perkins (NP): it seems to me that in chalcogenides these biquadratic terms are important but not in pnictides.
QS: they are not important for the order itself, but to understand the high-energy part of the spectrum.
AC: In the calchogenides, to explein the pi/2, pi/2 order they are crucial. QS: Yes.
NP: but why in chalcogenides J1 is small. QS: there are arguments, but it is next level of sophistication. The question of principle is if I can successfully use these models with local interactions to understand spin dynamics.

Here one starts from the outset with a lot of incoherent spectral weight but can also control itinerancy and e.g. understand the role of (phosphorus in 122) doping

------ back to superconductivity
Details of fermi surfaces are much less important for the pairing. This is important in view of materials having no nesting but comparable Tc with pnictides.

Sri Raghu: but can you get both SC and magnetism right (I.e. (pi,0) vs (pi/2,pi/2))?
QS: Yes but different materials may have different J1,J2,J3. Then the right measure for SC is the energy of the zone-boundary magnetic excitations and for all materials the numbers are comparable, 200-300 meV. With that you understand that the pairing amplitudes are comparable very naturally.

AC shows a slide (available) with data of the spin susceptibility of BaFe2As2. He points out that at 150meV the data are completely incoherent and do not see any clear peak.
AC: There is clearly Mott physics around, e.g. as Luca de' Medici showed, no question about it. The question is how many steps away from it are the optimally doped materials.
In cuprates we get d-wave with the two approaches, and maybe we can get also here everything both ways, but what approach gives better details? We don't need to take one approach and apply it to everything.

Leni Bascones (refer to the slides)

Shows magnetic results of 5-orbital model with U and J, within Hartree-Fock for (Pi,0) ordering.
There is a region, between the fully localized and fully itinerant limit, in which the system is partially localized and partially itinerant. Compares with 3 regions found in slave-spin calculations, of which the intermediate is the Hund's metal. Correlations seen in experiments are consistent with the Fe-based materials being in this intermediate region.
It is remarkable that the U for the onset of magnetic order is quite symmetric around the filling of 6 electrons but that for the onset of the intermediate region monotonically increases with the filling instead.
Origin of magnetism: a mixture of both localized and itinerant.
Assuming (pi,0 order) one can calculate the exchange couplings between the orbitals. Itinerant electrons want to be ferromagnetic along y direction, the localized electrons want to be antiferromagnetic.

AC: how you can be sure, quantitatively?
Leni: the shape of the phase diagrams is very similar with Slave-spins, and the order of orbitals with Slave-spin and DMFT. H-F overestimates interactions, Slave-spins underestimate them. They are both approximations.
QS: Yes and the reported diagram done with Slave-spin was for a simplified model.
LdM: The shape of that phase diagram and the values are found very analogous in all realistic and model calculations, but these method are semi-quantitative anyway.

Another result (slide 2) concerns the estimate of the magnetic couplings (J1, J2,..) in the localized picture. We have estimated them in the simplest way, 2nd order perturbation theory in the hoppings. They depend on U and on Hund's coupling. We considered two high-spin atomic configurations with 6 electrons as starting points that are close in energy, and the couplings are different in the two cases because of the different hoppings involved. We have then calculated the Hartree-Fock phase diagram, and we find that the (pi,pi) ordered state wins at low J/U, whereas the (Pi,0) wins at large J/U. At large U and J a double-stripe order is found, like in FeTe. These results could be inferred by the atomic limit estimates, and their dependence on some crystal-field splittings too.

One can also study the 5 electron case and we find that the (pi,pi) order always wins, which is experimentally observed in Manganese and Cr-doped arsenides. Also the dependence of the magnetic couplings on the Fe-As angle has been evaluated, and it shows that the order can vary with this parameter.

QS: In KFe2As2, with 5.5 electrons/Fe the exchange couplings are all found very small, of the order of 40meV, instead of 300meV, I wonder if this trend can teach us something.

AC: Is there a (pi/2,pi/2) state when going from the (pi,0) state you find at n=6 and the (pi,pi) you find at n=5?
Leni: We find the double stripe phase more easily when doping with electrons than with holes.

NP: The double stripe can be stabilized at n=6 only when additional terms are added to the standard tight-binding, like non-Heisenberg terms. Once you go towards n=7 the double stripe becomes stable, like it is seen here.