Theory summary-- Peter Hirschfeld
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- **When is a localized/itinerant description appropriate for magnetic properties? (Bernevig, Boeri, van den Brink, Eremin, Ku, Si, Tesanovic,Valenti)**

1. *distinguish between 3 cases:*
a) itinerant magnetism at weak coupling, comes from fermions very near FS
b) itinerant magnetism, fermions are still propagating, but magnetism comes from fermions at energies generally comparable to a bandwidth
c) fermions are localized, and magnetism == magnetism of localized fermions

Nobody argues a) for pnictides, the real distinction should be between b) and c). However, from theory point of view, b) is just a moderate coupling version of a), i.e., the existence of magnetism at weak coupling for nested electron and hole FSs is good theoretical justification to discuss moderate coupling and get magnetism within RPA.

2. *type of magnetic order*.
a) (0,π) order is selected both in localized spin and itinerant description [but for different reasons] In itinerant description, it appears already in weak coupling
b) double stripe phase is not easily obtained in the itinerant scenario at weak coupling, but was claimed to be reproduced in the RPA for moderate coupling/particular form of the FSs. In the localized spin approach, it can be reproduced if you assume that J_a is very different from J_b (see Dai). Si claims that it can be obtained in J1-J2-J3 model with isotropic J. Kuroki gets (π/2,π/2) from RPA. Can anyone show that correct phase (1 of 4 different possible OPs) is produced & understand why?

NB: DFT reproduces magnetic order and bonding correctly (Boeri,Ku,Valenti), but requires large moment, still controversial why. Ku: telling us that bonding character, As p-polarization important. Challenge: explain origin of INS anisotropy J1a>>J1b.

3. *Spin-wave spectrum:*
a) in ORDERED phase, it doesn't matter what description one uses -- there are undamped spin waves at low energies, with anisotropic dispersion (because order is either (0,π) or (π,0), it breaks tetragonal symmetry.
b) in the itinerant scenario, there is continuum above some energy (2 Δ_SDW), and magnetic excitations rapidly decay into a continuum. In localized scenario, they remain essentially propagating. Localized approaches must add Landau damping-- makes approach similar to itinerant one. The issue then is what is larger at frequencies around 200 meV: damping term $\Gamma \sim \omega$ or ω^2 (are spin excitations overdamped or propagating).

4. *pairing*:

Here we deal with fermions near the FS, up to some energy E. E_F is already ~ 100 meV. There is a generic agreement that magnetic response at energies < 100 meV is described within itinerant scenario. Then, the issue is whether some contribution to SC comes from higher energies.

There exist two qualitatively different "spin-fluctuation" scenarios for the nodes: two dimensional, with "vertical" nodes on electron FSs, and 3D scenario (Graser), with nodes on hole FSs.

- **Normal state transport & nematic order (Ku, Korshunov)**

What drives the nematic order above magnetic transition?

Can it extend beyond structural transition?

2 expts. (Fisher, Matsuda-Shibauchi) show nematic tendencies.
Scenario 1: nematic susceptibility above Ts.
Scenario 2: nematic order above Ts, below some T_nem near critical pt.

Challenges for theory:

1) does orbital order, magnetism or Pomeranchuk drive nematicity?
2) if nematic LRO extends above Ts, how to understand jump in orthorhombicity there?
3) importance of critical fluctuations?

Normal state transport even outside SDW range is anomalous—dominance of one sign of carriers—importance of d_{xy} states.

- **Pairing mechanism (Bernevig, Honerkamp, Kuroki, Thomale, Hanke, Scalapino, Maier, Kontani, Ikeda, Arita, Ku)**

Is pairing in pnictides driven primarily by one physical effect (spin/orbital fluctuations, phonons) or are more than one important, at least in some materials?

Well known (at this pt.):
π,0 spin fluctuations $\Rightarrow$ s+/- pairing
π, π spin fluctuations $\Rightarrow$ d-wave pairing

But: role of orbital fluctuations: driven by *U'*, enhanced by electron-phonon interaction $\Rightarrow$ s++? Effective negative *U* center (Little, Allender-Bray-Bardeen, Scalapino-Hirsch)?

$$\Gamma(k,k') \sim const. + U^s \chi_s U^s - U^c \chi_c U^c$$

$$\Gamma_c \sim \frac{1}{1+(U-2U')\chi_0(q)}$$

$U' \Rightarrow U' + U_{eph} \Rightarrow$ orbital susceptibility diverges 1st, gives s++ (Kontani).

Connection between lattice structure ⇒ band structure ⇒ pairing (Kuroki: As height). Need more insights of this type to give theory predictive power.

Theoretical description of transitions d → d+is → s+- → s++?

d-wave at end of doping sequences (only hole or only electron pockets, KFe2As2 or KFe2Se2)?

Methods: FLEX vs. RPA vs. fRG
FLEX smears out anisotropy; double counting problem
RPA exaggerates nodes relative to fRG

- **Superconducting properties (Vorontsov,Vavilov, Graser, Kontani)**

Why is behavior of pnictides/chalcogenides in SC state so diverse? What causes extreme sensitivity to small changes in electronic structure?

New tests for sign changing order parameter?

Importance of 3D nature of FS pockets—nodes on hole surfaces (Graser,Kuroki)?

To s++ nonbelievers: explain apparent slow Tc suppression, Lee plots (Kontani)

What can we do to make disorder studies relevant to phenomenology of Fe-based materials? Too many parameters to separate pairbreaking, “chemical pressure” effects. Is Tc suppression really slow? Depends on order parameter, different DOS on different sheets, inter/intraband scattering, magnetic/nonmagnetic, Born/unitary. Goal: theory where impurity parameters determined ab initio for given impurity, host (Arita, Ikeda).