Discussion session on various topics as covered below:

Steve Kivelson on Cs3C60

Steve gave a blackboard presentation where he first reviewed some of the material and experimental properties of Cs3C60, where Cs donates 3 electrons to C60. The T versus 1/a (a=lattice spacing) phase diagram has a Mott insulating (MI) phase at small 1/a with Neel order and a first order transition to a superconducting phase at larger 1/a.

Cs3C60 forms either an FCC lattice or BCC/A15 structure, where the FCC is disordered (C60 anions oriented randomly; "merihedral") but BCC is ordered and samples are of high quality. [Other A3C60 compounds are FCC.] Neel transition seen (by NMR) in BCC and much lower T_N seen (about order of magnitude lower) in FCC. [Greg Stewart points out the BCC structure is not really BCC but this is how the literature refers to it.] The highest SC Tc is about 38K (in FCC; the BCC has a slightly lower Tc.)

Greg Stewart asks if Cs is really a vegetable and Steve replies that the only difference between the FCC and BCC samples is the difference in Neel temperatures, all other electronic properties are very similar so that suggests Cs is not doing anything but donating 3 electrons.

The mean free path is very short (0.25 angstrom) and the resistivity is linear. A spectacular example of a bad metal. Chubukov: does it remain linear at low T? Kivelson: no it flattens out before Tc.
NMR sees s-wave (full) gap. The ratio 2Delta/Tc is BSC at low density but rises as 1/a decreases, so becomes more strong coupling-like near MI. See Hebel-Schlichter peak in one material, not other.

Steve then moves on to the theory: in MI phase can look at one molecule at time. 3 electrons go into l=1 state, so can have (s,l)=(3/2,0), (½,2) or (½,1). Note all are magnetic. Experiments find the ordered moment & fluctuating moment consistent with ½. MI transition is 1st order, so unlikely to be so tuned that fluctuations suppress from 3/2 to ½.] So how to get an l=0 MI state?

One idea is a dynamic Jahn-Teller effect. J-T would cause structural transition that isn't seen. Dynamic means no structural distortion. Distort molecular, such that one has an l=2 phonon mode and combine with (½,2) electron state to make el-ph (½,0) state. It's a composite object (entanglement, not order). This may explain the MI phase.

Another point Steve makes is the size of mu*. Phonon freq ~ band width ~ 0.1 eV. So mu* is of the order of 1, not small as el-phonon calculations for A3C60 assume. Chubukov: how do you overcome this to form SC? Kivelson: Numerical calculations of the Hubbard model on simpler 12 site truncated tetrahedron gave attractive

interactions (attractive pair energy) provided U is not too large. Q Si – is it obvious you get s-wave? Elihu Abrahams: NMR shows it's nodeless.

Greg Stewart: Some cautions about specific heat jumps and extracting numbers

Data is shown for Ba(Fe1-xCox)2As2. Gamma of the normal state, γ_n, is not well determined and ranges from 14.6 to 22.1. Also should the jump be renormalized by the fraction of the sample that is SC or not?

Data is shown for Ba1-xKxFe2As2. Some groups try to idealize their broadened data and then determine ΔC, others take it from raw data which depends on exactly which points are used. In the raw data, the jump is tiny on high Tc materials, 1% or so, the peak is not sharp, and Cv above Tc has T dependence. Shows plot of the ratio, $R=\Delta C/\gamma Tc$ for several different materials, LiFeAs, FeSe, etc. R varies from less than ½ to ~3.3. Notes that the low Tc Fe SC have small R, may be because they are d-wave.

The data above was using normalized jumps. If you use unnormalized, then R ranges from 0.4 to 2.5. Chubukov: Is the message that higher Tc have higher ratio Stewart. Yes, that is one message. Another message is the error bars on gamma and on the ratio R. At low T, phonons are less important, subtraction less important. In general, can get factor of 2 variation depending whether you take max,min, fit to an idealized curve, normalize, etc.

Andrey Chubukov: Specific heat jump near the onset of co-existence with AF

As we heard from, jump not universal in Fe Sc, but larger for larger Tc and larger than BCS ratio 1.43. Even within MFT, i.e. with no AF get BCS jump, when there is co-existence with AF there is another jump in C because of the condensation of the second order parameter. Within MFT including Gaussian fluctuations, the ratio R has a maxima when you go into the coexistence state, which is larger than BCS (no AF) . Data of C. Meingast et al and theory (Vorontsov et al) shows ratio as function of Tc can be captured MFT. Other data on BaFe2(As1-xPx)2 as function of doping x can be fit by Gaussian fluctuations in the normal state. Main point is specific heat data can be understood within simple theory including Guassian fluctuations.

Peter Hirschfeld: low Tc is more anisotropic, high Tc has more isotropic gaps. This could account for the rise in C jump or R as Tc increases. Chubukov: differences are minor from calculations. Peter thinks it is factor of 2, Andrey disagrees. It is pointed out that phosophorus doped at low Tc is not anisotropic, so won't fit this hypothesis. Andrey agrees this effect, anisotropy, should be included on top of the effect of co-existence.

Leon Balents: 1d quantum Magnetism – frustrated ferromagnets

Leon gives a blackboard talk about a 1d chain with FM NN (J1) and AFM NNN (J2) interactions in B field. At zero temperature, this system is ferromagnetically ordered if J2/J1<1/4. At intermediate fields and J2/[J1+J2]>1/5 there are spin nematic phases, with a cascade of multipolar orders. At higher fields one again is in the FM phase, connecting to the small J2 FM. At J2/[J1+J2]=1/5 there is a QCP between the FM and a vector chiral phase.

Kivelson: What happens at H=0? Balents: Complicated double crossover with zero magnetization. Can't break SU(2) except for FM. This is peculiar to 1d. In 2d, would expect these multipolar states to have a gap. Writes down a non-linear sigma model description.
Chubukov: Does cascade go on to infinity? Balents: solving close to QCP the finite H transition terminates in a 1st order line so the QCP goes into 1st order line. A vector chiral phase with magnons is below all these multipolar orders. Can interpret these multipolar phases emerging from coexistence of FM and vector chiral phase with magnons.

Qimiao Si: exchange interactions in bad metals near Mott transition

Introduces the Hubbard model in slave rotor representation (as first introduced by Florens & Georges), as per work with W. Ding, R Yu and E Abrahams.
Split electron into spinon (spin) and rotor (charge) and require that ang mom of rotor is equal to number of spinons to project back into physical electron Hilbert space.
Hirschfeld: what's the motivation for slave rotor? Si: incoherent part of spectrum is already included in saddle point approx. Incoherent part comes in from L^2. Calcuate spinon and rotor propagators in saddle point approx. Saddle point justified either if spinon is SU(N) or rotor O(N) for large N. Incoherent electron spectral weight comes from rotor part. For large U, spectral weight is gapped above Mott transition. Incoherent peaks smoothly evolve through the Mott transition so are also present in bad metal phase.
Can also calculate the effective exchange interaction in one-loop approximation and gives J_eff=4t^2/U at large U/t, but is enhanced over this as MI transition approached (monotonic increase from large U to MI U_crit). J_eff peaks at the MI and then decreases in bad metal phase. Q: Is this at half-filling? Si: Yes, this is all at half filling of one band Hubbard model on square lattice.
Tarun Grover: MI is continuous? Si: Yes. Grover: Must be spinon FS in MI? Rotors have gap but spinons are gapless, right? Si: Yes, gapless spinons but still get usual 4t^2/U.
Chubukov: can you understand qualitatively why Jeff is maxima at U_crit? Si: The incoherent part of the spectral weight decreases below U_crit because of the transfer of weight to the coherent part.