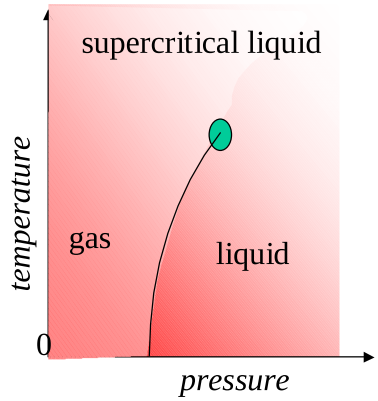
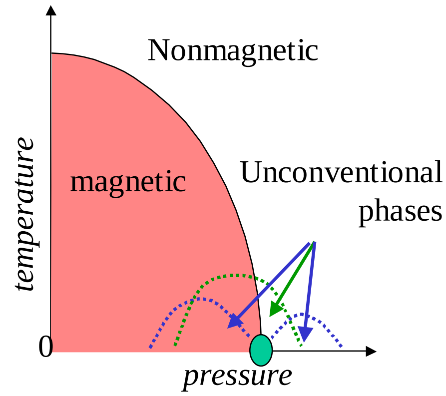
What is quantum criticality?



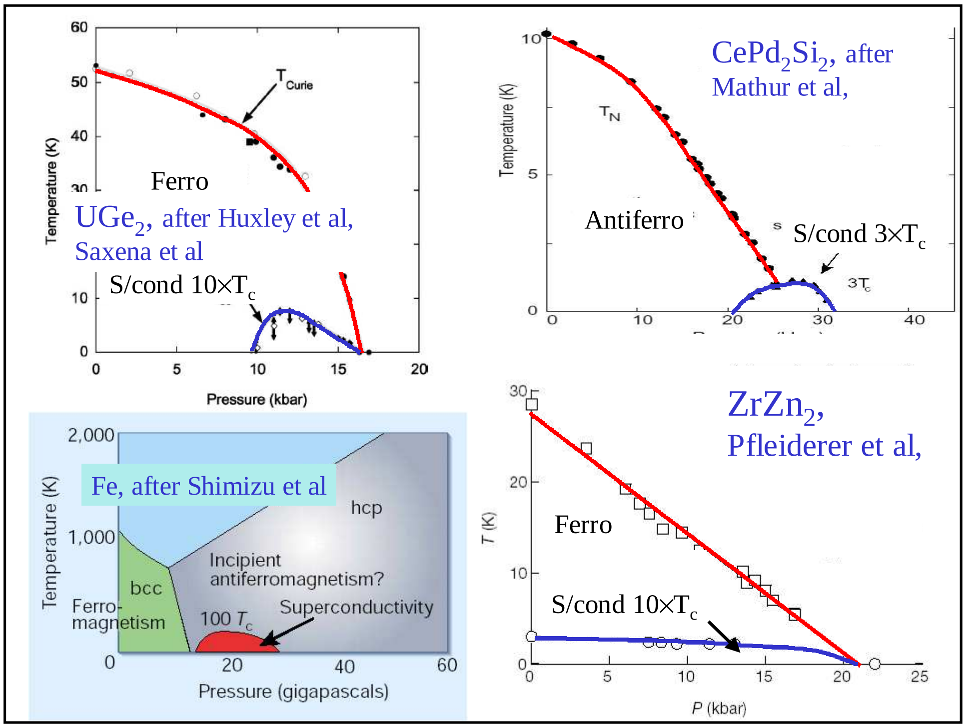
Classical criticality: Thermal density fluctuations grow indefinitely close to the Critical Point (CP).

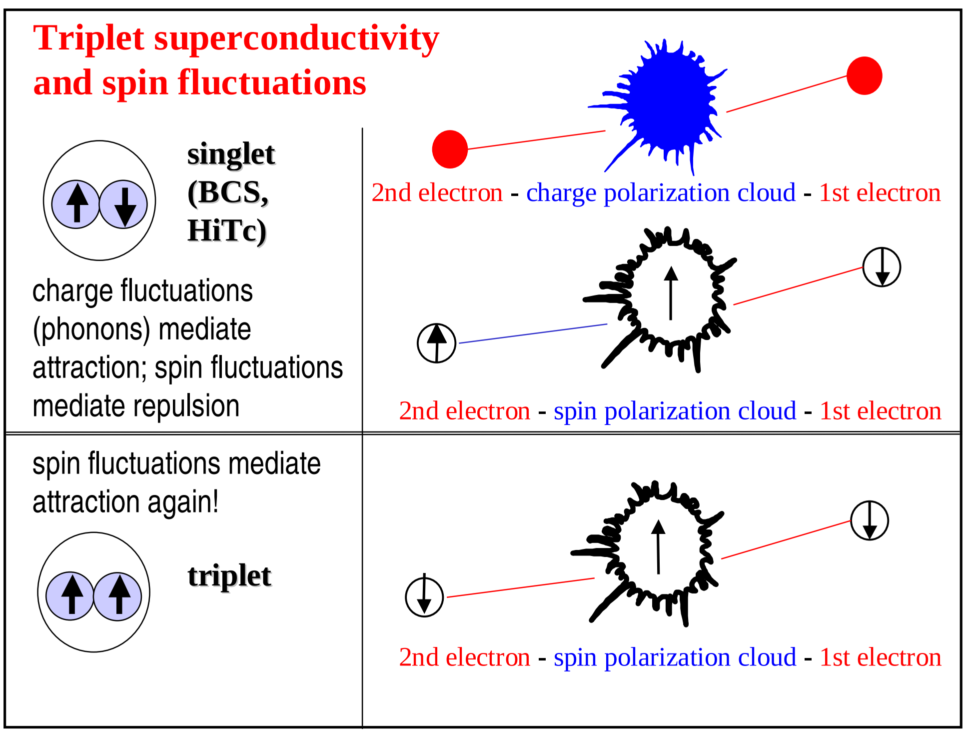


Quantum criticality: Quantum density fluctuations grow indefinitely close to the Quantum Critical Point (QCP).

Statistics games with ISI

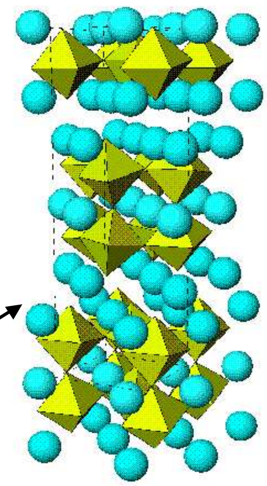
- of every **6** paper mentioning *quantum criticality*, one is in PRL/Nature/Science
- *superconductivity*: one of every **20** papers (*triplet superconductivity:* one of every **7.5**)
- *DMFT*: one of every **9.7**
- *quantum computing*: one of every **8**


UGe2, after Huxley et al, Saxena et al
Temperature (K)
Pressure (kbar)
T Curie
Ferro
S/cond 10×Tc
CePd2Si2, after Mathur et al,
Temperature (K)
TN
Antiferro
S/cond 3×Tc
3Tc
Fe, after Shimizu et al
Temperature (K)
Pressure (gigapascals)
hcp
bcc
Incipient antiferromagnetism?
Ferro-magnetism
100 Tc
Superconductivity
ZrZn2, Pfleiderer et al,
T (K)
P (kbar)
Ferro
S/cond 10×Tc


Triplet superconductivity and spin fluctuations
singlet (BCS, HiTc)
charge fluctuations (phonons) mediate attraction; spin fluctuations mediate repulsion
2nd electron - charge polarization cloud - 1st electron
2nd electron - spin polarization cloud - 1st electron
spin fluctuations mediate attraction again!
triplet
2nd electron - spin polarization cloud - 1st electron

Trivial stuff: calculations need to be good, and so does the experiment

- 1997 (Cao *et al*) $Sr_3Ru_2O_7$ reported to be magnetic (experimentally)
- 1997 (Hase and Hasegawa) Calculations in the *ideal* structure render a nonmagnetic solution.
- 1998 (Ikeda and Maeno) $Sr_3Ru_2O_7$ reported to be nonmagnetic (experimentally)
- 2001 (Singh and Mazin) $Sr_3Ru_2O_7$ calculated in the *correct* structure is magnetic with 0.8 μ_B per Ru atom.
- 2001 (Grigera *et al*) $Sr_3Ru_2O_7$ shown experimentally to be nonmagnetic, but near a metamagnetic QCP. Quantum critical behavior demonstrated in transport properties.



Other example from our personal experience

We now know that there are other cases where magnetism exists in the calculations, but not in the experiment:

- LiV_2O_4
- Ni_3Ga, Ni_3In
- $(Sr,Ca)RuO_3$(?)
- $SrRhO_3$
- $NaCo_2O_4$
- hexagonal Fe under high pressure

There are cases where magnetism exists both in the experiment and in the calculations, but is suppressed by fluctuations:

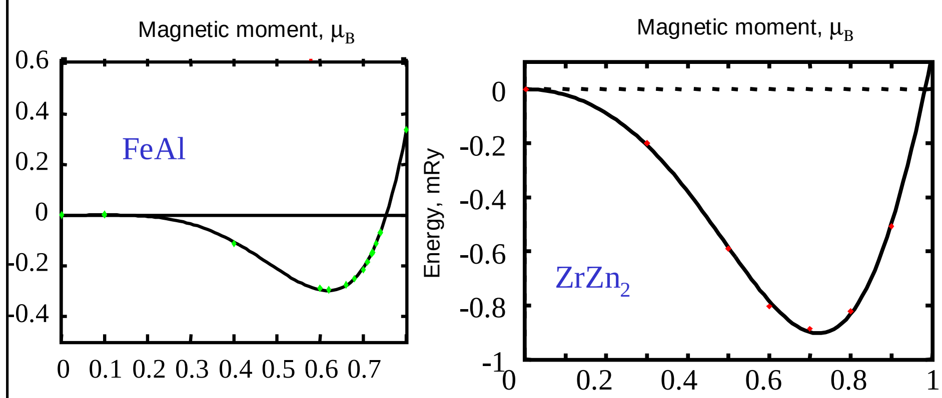
- $ZrZn_2$
- Sc_3In
- Ni_3Al

There are cases where magnetism exists neither in the experiment nor in the calculations, but its magnetic susceptibility is suppressed by fluctuations:

- Pd (exp. QCP in $Pd_{0.98}Ni_{0.02}$)
- Sr_2RuO_4

Fixed spin moment LSDA calculations

$$\Delta E(M) = aM^2 + bM^4 + cM^6 \quad a^{-1}/2 = \chi, \text{ susceptibility}$$



Note that $ZrZn_2$ has a much bigger magnetic energy gain

Can such calculations provide any insight at all?

$$\Delta E(M) = aM^2 + bM^4 + cM^6 \quad a^{-1}/2 = \chi, \text{ susceptibility}$$

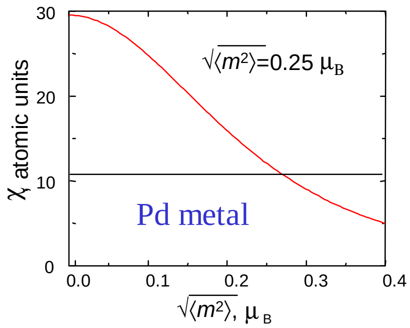
Spin fluctuations renormalize this dependence (Moria, Shimizu, Lonzarich, Yamada….)

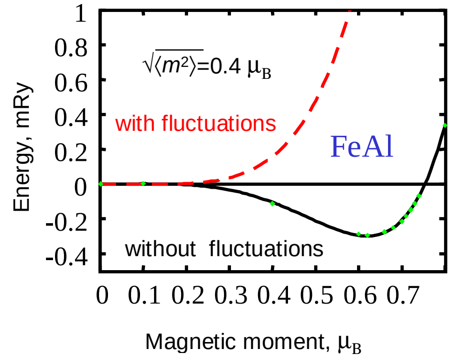
($\langle m^2 \rangle$ is the average amplitude of spin fluctuations)

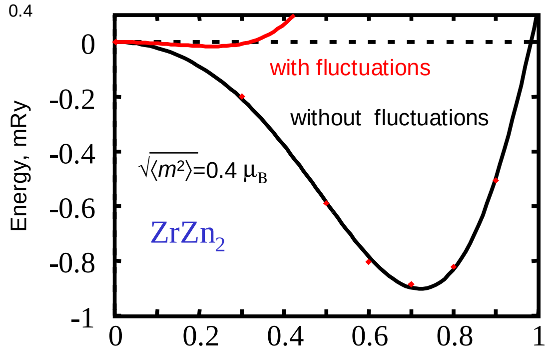
$$a \to a + \frac{10}{3} b \langle m^2 \rangle + \frac{35}{3} c \langle m^2 \rangle^2 \qquad b \to b + 7c \langle m^2 \rangle$$

A possible question: what $\langle m^2 \rangle$ do we need to reproduce experiment?

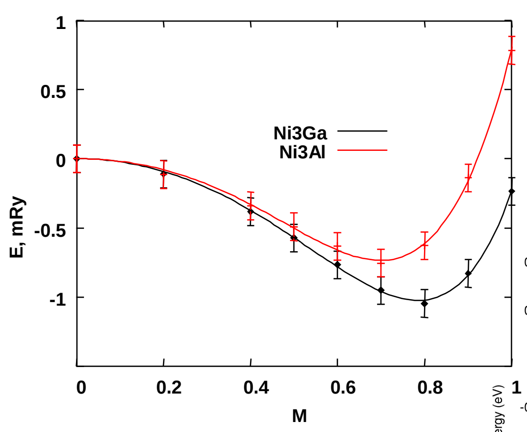
Examples:





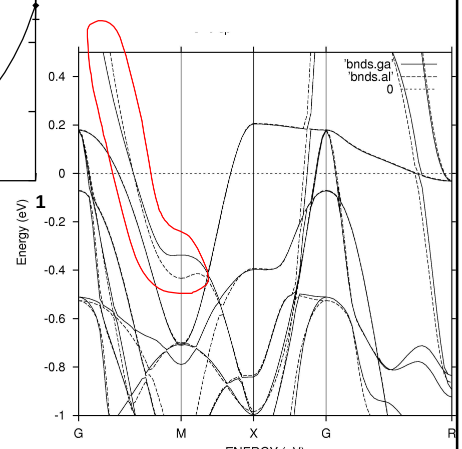


In these examples, we determined the average amplitude of spin fluctuations, by comparing the calculated and the experimental magnetic properties



Ni_3Al *is* magnetic ($M=0.2\ \mu_B$)

Ni_3Ga *is not* magnetic



To bring things to agreement with the experiment, one needs at least 12% larger spin fluctuations in Ni_3Ga

Superconductivity near QCP

Berk-Schrieffer-Fay-Appel weak coupling theory, 1966-1980

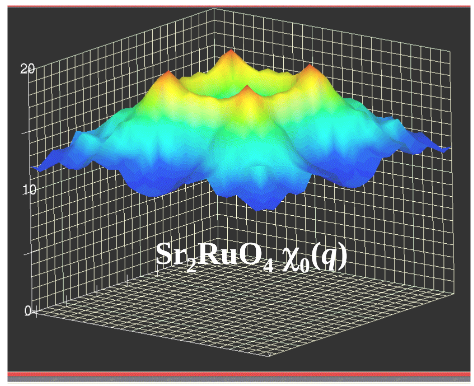
for triplet (p-wave) superconductivity

$V(q)=I(q)^2\chi_0(q)/[1-I(q)^2\chi_0^2(q)]$

for singlet (d-wave) superconductivity

$V(q)=-I(q)/[1-I(q)^2\chi_0^2(q)]$

where the magnetic coupling $I(q)$ and spin susceptibility $\chi_0(q)$ can be extracted from electronic structure calculations.



Direct (quantitative) approaches to QC:

Dynamical Mean Field Theory?
Extended Dynamical Mean Field Theory?
FLEX?

Lichtenstein and Chioncel, DMFT

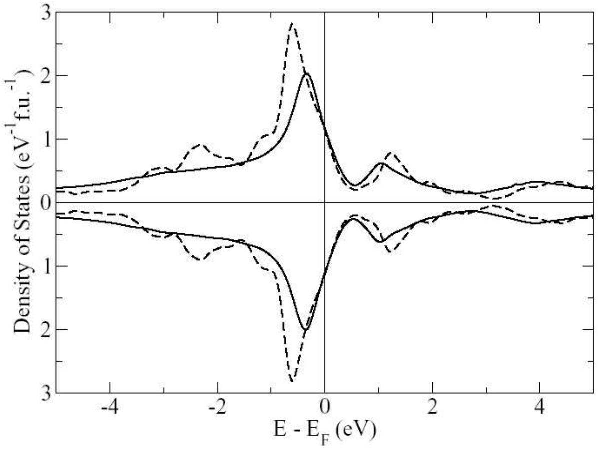


FIG. 3: FeAl density of states, $D(E)$, in DMFT (solid line) compared with the nonmagnetic LDA. The DMFT solution

+: DMFT includes fluctuations (also spin fluctuations) -> suppresses magnetism.

-: Fluctuations are local (should be at q~0) Fluctuations driven by U, not I and J.

Extended DMFT?

$$H = \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_{ij,\sigma} t_{ij} c_{i\sigma}^{+} c_{j\sigma} \quad \ldots + \tfrac{1}{2} \sum_{ij} J_{ij} m_i m_j$$

$$H = \tfrac{1}{4} \sum_i I m_i^2 + \sum_{ij,\sigma} t_{ij} c_{i\sigma}^{+} c_{j\sigma}$$

+: Fluctuations are q-dependent.
Fluctuations are driven by I (Hund) and J - appropriate for weak itinerant magnets like *e.g.* $ZrZn_2$.
-: q-dependence only in J, while in reality most of q-dependence comes from χ_0 (*i.e.*, t_{ij})

$$\chi(q,\omega) = \frac{\Pi(\omega)}{1 - J(q)\Pi(\omega)} \qquad \chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - I\chi_0(q,\omega)}$$

in any event substantial improvement over DMFT!

I believe that weakly correlated itinerant magnets are more challenging and more exciting system than strongly correlated localized systems. I urge our DMFT- and other gurus to take a closer look at the matter. And...