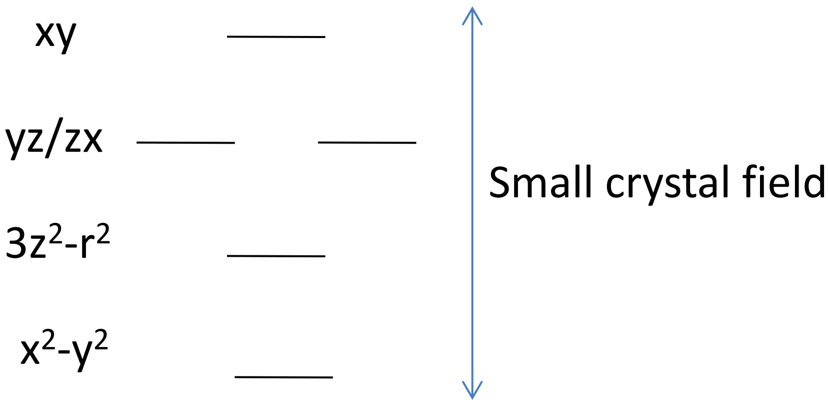
Iron superconductors as multi-orbital systems



The 5 Fe d-orbitals
are necessary to describe
the electronic properties

Focus on electronic filling

- **Parent compounds** ($BaFe_2As2$,LaFeAsO,LiFeAsFeSe,FeTe …) : **6 electrons in 5 orbitals**
  mass enhancement **~3** in As compounds,larger in chalcogenides

- **Doping with holes:**

  KFe2As2, RbFe2As2, CsFe2As2: **5.5 electrons in 5 orbitals**
  large mass enhancements (up to **10** or larger in some orbitals)
  BaMn2As2: **5electrons** in 5 orbitals. **Insulator**

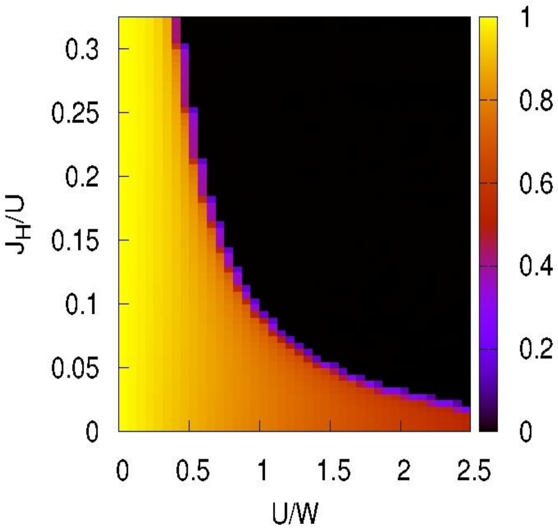
- **Doping with electrons**: BaCo2As2: **7 electrons in 5 orbitals**
  mass enhancement ~**1.2**

Iron superconductors: Focus on electronic filling

Quasiparticle weight Z (inverse of mass enhancement)As a function of interactions U, JH

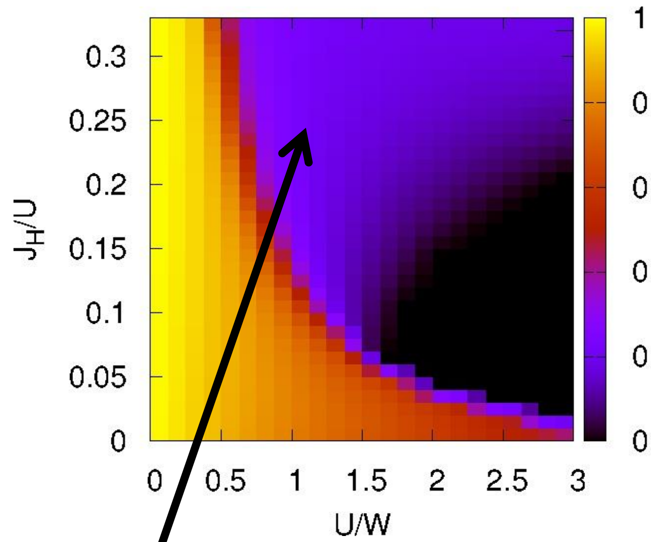
Degenerate 5 orbital model (all orbitals are equivalent) Slave-spin calculation

5 electrons in 5 orbitals
(highly hole-doped)



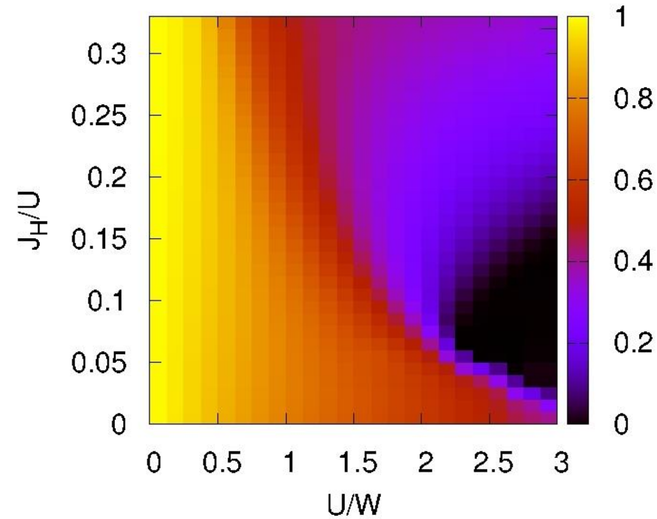
Half-filling

6 electrons in 5 orbitals
(parent compount)



Strongly correlated metal
Correlations dominated by
The proximity to a half-filled
Mott insulator

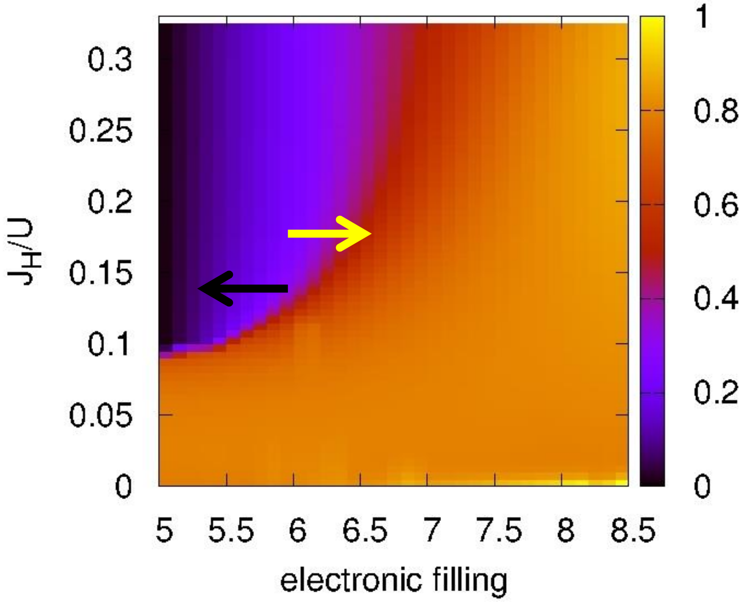
7 electrons in 5 orbitals
(highly electron doped)

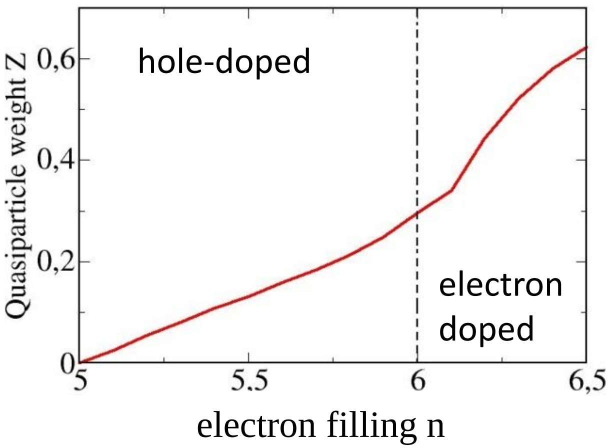


Fanfarillo,EB, in preparation

Iron superconductors: Focus on electronic filling

Quasiparticle weight Z

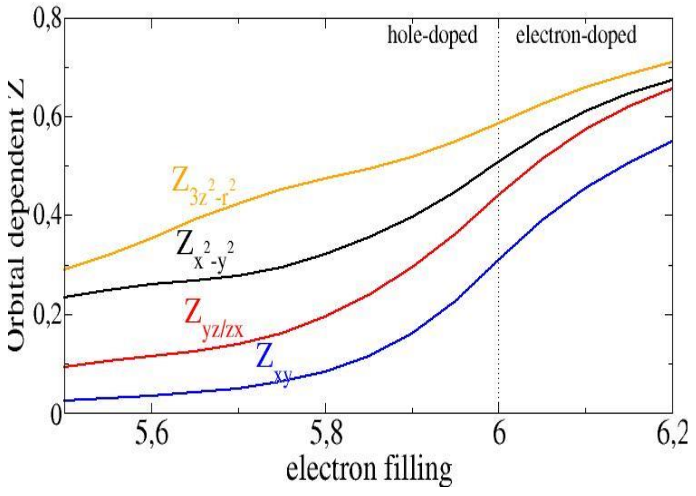




Strong doping dependence
electron-hole asymmetry

Correlations become larger with hole doping as the system approaches a Mott insulating state

In real systems orbitals are not equivalent
Mass enhancement different for different orbitals



Calderon et al, PRB 90, 115128 (2014)