Luca de' Medici

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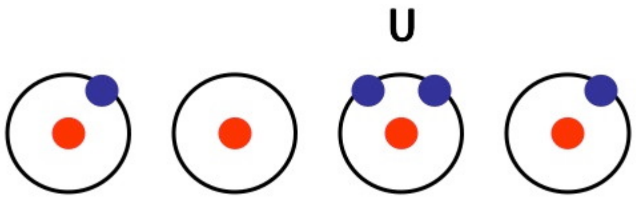
Slave-spin mean field and its application to Iron-based superconductors

20th Mardi Gras Conference - Baton Rouge 14.02.2015



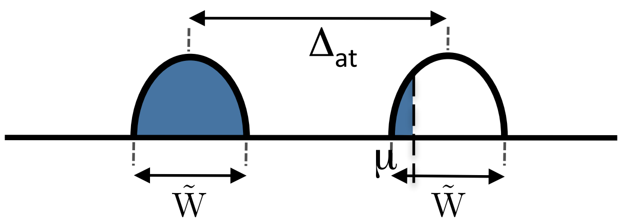
independent electrons → Fermi liquid

- Effective mass
- coherence Temperature
- U very strong ($U>U_c$): Mott Insulator

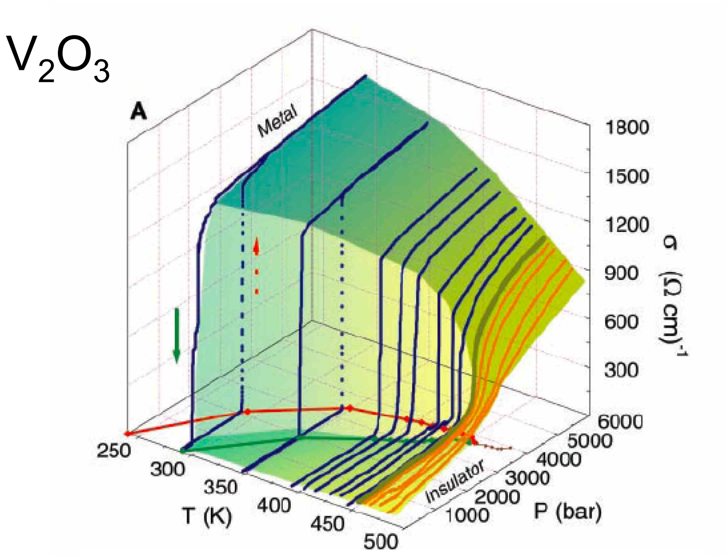
Mott insulators are predicted metallic by DFT

electrons are localized by correlations

(V_2O_3, Fullerenes, Cuprates…)



Spectrum of charge excitations



Limelette et al. Science 2003

The proximity to a Mott state strongly affects the properties of a system:

- reduced metallicity (Z~x)
- mass enhancement
- transfer of spectral weight from low to high energy (e.g. in optical response)
- tendency towards magnetism
- …

Correlated materials: 3d, 4d, 5d, 4f, 5f electrons at the Fermi level

Example: transition metal oxides

Orbital degeneracy is often lifted (partially or totally) by the crystal-field
Several correlated orbitals remain relevant for the low-energy physics

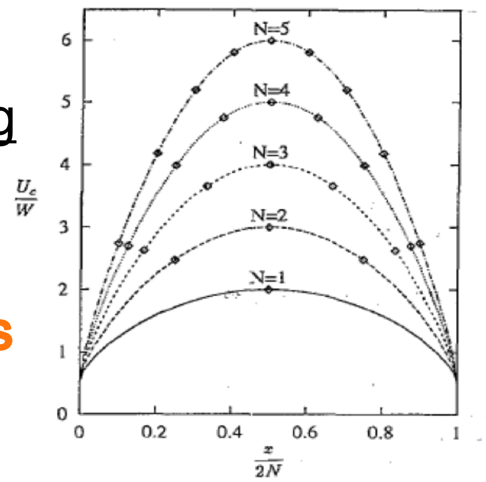
Example for 3d electrons : Iron-SC vs cuprates

The local coulomb interaction is different depending on the electrons occupying the same or a different orbital, and on the mutual spin direction

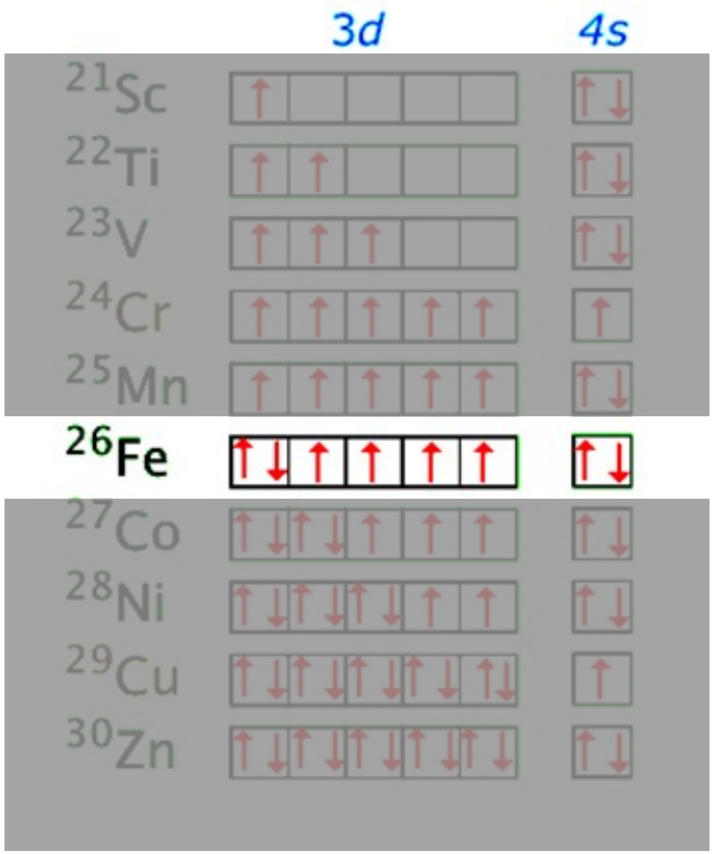
Hund's coupling "J" is a measure of this difference

Mott transition in multi-orbital models,
(Lu '94, Rozenberg '95, Florens et al.'02, …)

- Realized at every integer filling
- Uc grows with degeneracy
- J strongly affects this picture



Aufbau



Hund's Rules

In open shells:

1. Maximize total spin S
2. Maximize total angular momentum T

(3. Dependence on J=T+S, Spin-orbit effects)

$$H = \sum_k H_k^{DFT}$$
$$+U \sum_{i,m} n_{im\uparrow} n_{im\downarrow} + (U-2J) \sum_{i,m>m'\sigma} n_{im\sigma} n_{im'\bar{\sigma}}$$
$$+(U-3J) \sum_{i,m>m'\sigma} n_{im\sigma} n_{im'\sigma} + H_{flip}$$

Many more parameters compared to the one band case: Coulomb and Hund's couplings, several bandwidths, crystal-field splitting…

Difficulty lies in dealing with the localized (atomic) and itinerant nature of electrons on equal footing

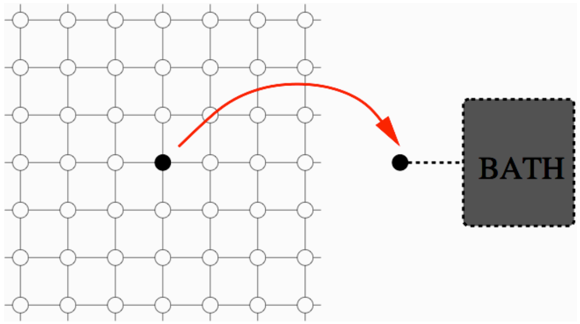
Metzner & Vollhardt '89, Georges & Kotliar '92, Jarrell '92

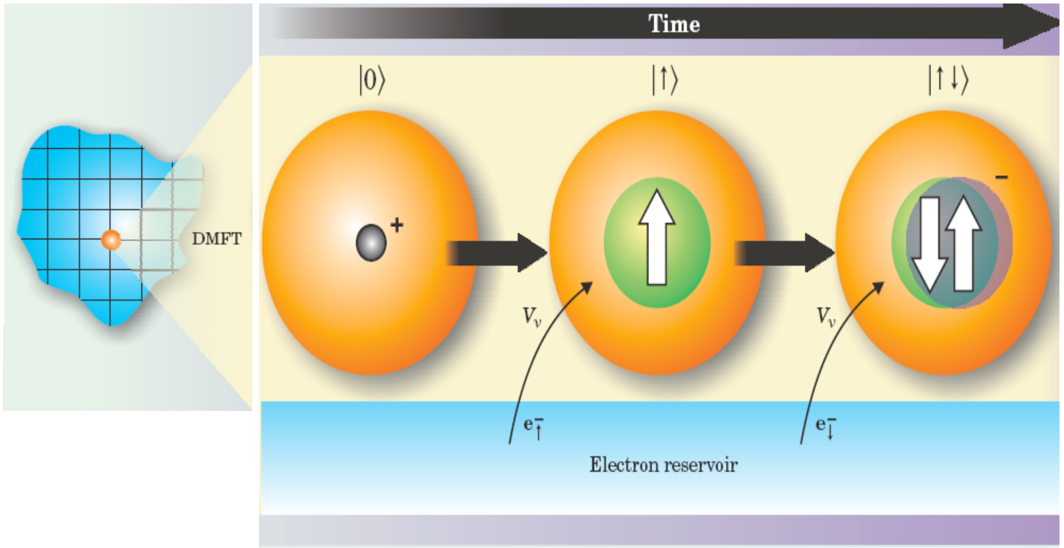
DMFT: use of a self-consistent impurity model to calculate the local correlators (exact in the infinite coordination limit)

Impurity model $$S = -\int_0^\beta \int_0^\beta d\tau d\tau' \sum_{m\sigma} d^\dagger_{m\sigma}(\tau)\mathcal{G}_m^{-1}(\tau-\tau')d_{m\sigma}(\tau') + H_{int}$$

Self-consistency condition

$$\mathcal{G}_m^{-1}(i\omega_n) = i\omega_n - t_m^2 G_m(i\omega_n)$$





Reviews:

DMFT	Georges et al. RMP'96
Cluster DMFT	Maier et al. RMP'05
LDA+DMFT	Kotliar et al. RMP'06

Cheaper alternative: Slave-Spin mean-field

(e.g. as phase diagram surveyor) LdM et al. PRB'05

Recipe:

- Enlarge the local Hilbert space (new variables + constraint)
- Treat the constraint on average
- Decouple the pseudo-fermions from the slave variables (renormalized non-interacting fermionic model)
- Treat the slave variables in a local mean-field

Examples:

- Slave Bosons (Kotliar and Ruckenstein)
- Slave Rotors (Florens and Georges)
- …

- Hilbert Space mapping

$$|0\rangle = |n_f = 0, S^z = -1/2\rangle$$

$$|1\rangle \equiv d^\dagger|0\rangle = |n_f = 1, S^z = +1/2\rangle$$

$$f^\dagger f = S^z + \frac{1}{2}$$

Constraint:
Lagrange multiplier

- Choice of the operators

$$d^\dagger \rightarrow 2S^x f^\dagger, \quad d \rightarrow 2S^x f$$

$$H = -\sum_m t_m \sum_{\langle ij\rangle,\sigma} (d^\dagger_{im\sigma} d_{im\sigma} + h.c.) + H_{int}[d^\dagger, d]$$

$$H = -\sum_m t_m \sum_{\langle ij\rangle,\sigma} 4S^x_{im\sigma} S^x_{jm\sigma} (f^\dagger_{im\sigma} f_{im\sigma} + h.c.) + H_{int}[S]$$

$\mathrm{H}_{\mathrm{int}}$

$$H_{int} = U \sum_{i,m} n_{im\uparrow} n_{im\downarrow} + (U-2J) \sum_{i,m>m'\sigma} n_{im\sigma} n_{im'\bar{\sigma}}$$
$$+(U-3J) \sum_{i,m>m'\sigma} n_{im\sigma} n_{im'\sigma} + H_{flip}$$

$$H_{int} = U \sum_{i,m} (S^z_{im\uparrow} + \frac{1}{2})(S^z_{im\downarrow} + \frac{1}{2}) + (U-2J) \sum_{i,m>m'\sigma} (S^z_{im\sigma} + \frac{1}{2})(S^z_{im'\bar{\sigma}} + \frac{1}{2})$$
$$+(U-3J) \sum_{i,m>m'\sigma} (S^z_{im\sigma} + \frac{1}{2})(S^z_{im'\sigma}) + H_{flip}$$

$$H_{flip} = -J \sum_i \left[S^+_{i1\uparrow} S^-_{i1\downarrow} S^+_{i2\downarrow} S^-_{i2\uparrow} + S^+_{i1\downarrow} S^-_{i1\uparrow} S^+_{i2\uparrow} S^-_{i2\downarrow} \right]$$

Approximation for $\mathrm{H}_{\mathrm{flip}}$

$$-J \sum_i \left[S^+_{i1\uparrow} S^+_{i1\downarrow} S^-_{i2\uparrow} S^-_{i2\downarrow} + S^+_{i2\uparrow} S^+_{i2\downarrow} S^-_{i1\uparrow} S^-_{i1\downarrow} \right]$$

Slave-spins mean-field

$$H_0 = -\sum_m t_m \sum_{<ij>,\sigma} 4S^x_{im\sigma}S^x_{jm\sigma}(f^\dagger_{im\sigma}f_{jm\sigma} + h.c) + H_{int}[S]$$

Mean-field approximation : - decoupling f and S
- static and uniform Lagrange multiplier
- local mean-field on S

<u>Mean-field equations</u>

(Half-filling, $\lambda_m = \varepsilon_m = \mu = 0$
<u>slightly different off-half-filling)</u>

$$H^f_{eff} = \sum_{k,m\sigma} Z_m \varepsilon_{km} f^\dagger_{km\sigma} f_{km\sigma}$$

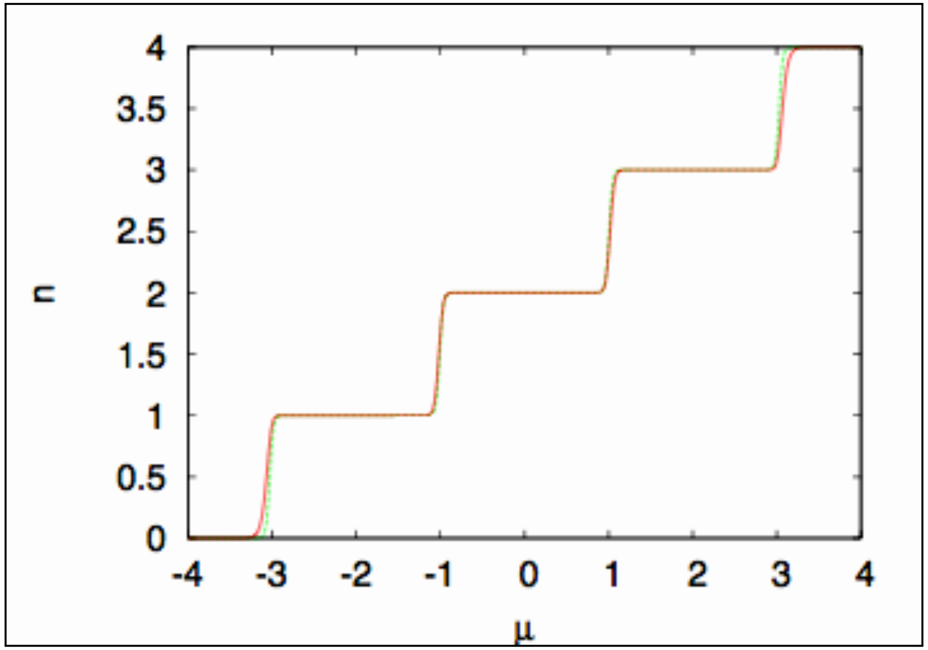
$$H_s = \sum_{m\sigma} 2h_m S^x_{m\sigma} + H_{int}[\vec{S}_{m\sigma}]$$

$$h_m = 4\langle S^x_{m\sigma}\rangle \frac{1}{\mathcal{N}} \sum_k \varepsilon_{km} \langle f^\dagger_{km} f_{km}\rangle$$

$$Z_m = 4\langle S^x_{m\sigma}\rangle^2$$

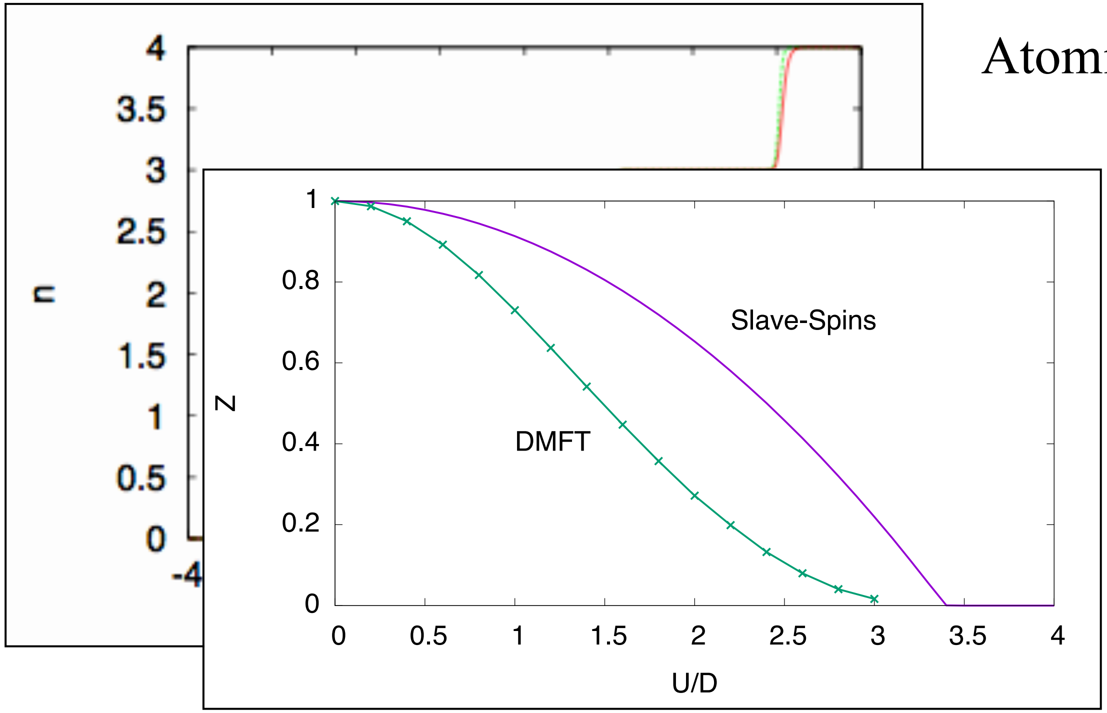
$$\langle n^f_{im\sigma}\rangle = \langle S^z_{im\sigma}\rangle + \frac{1}{2}$$

Benchmarks



Atomic limit: Coulomb staircase

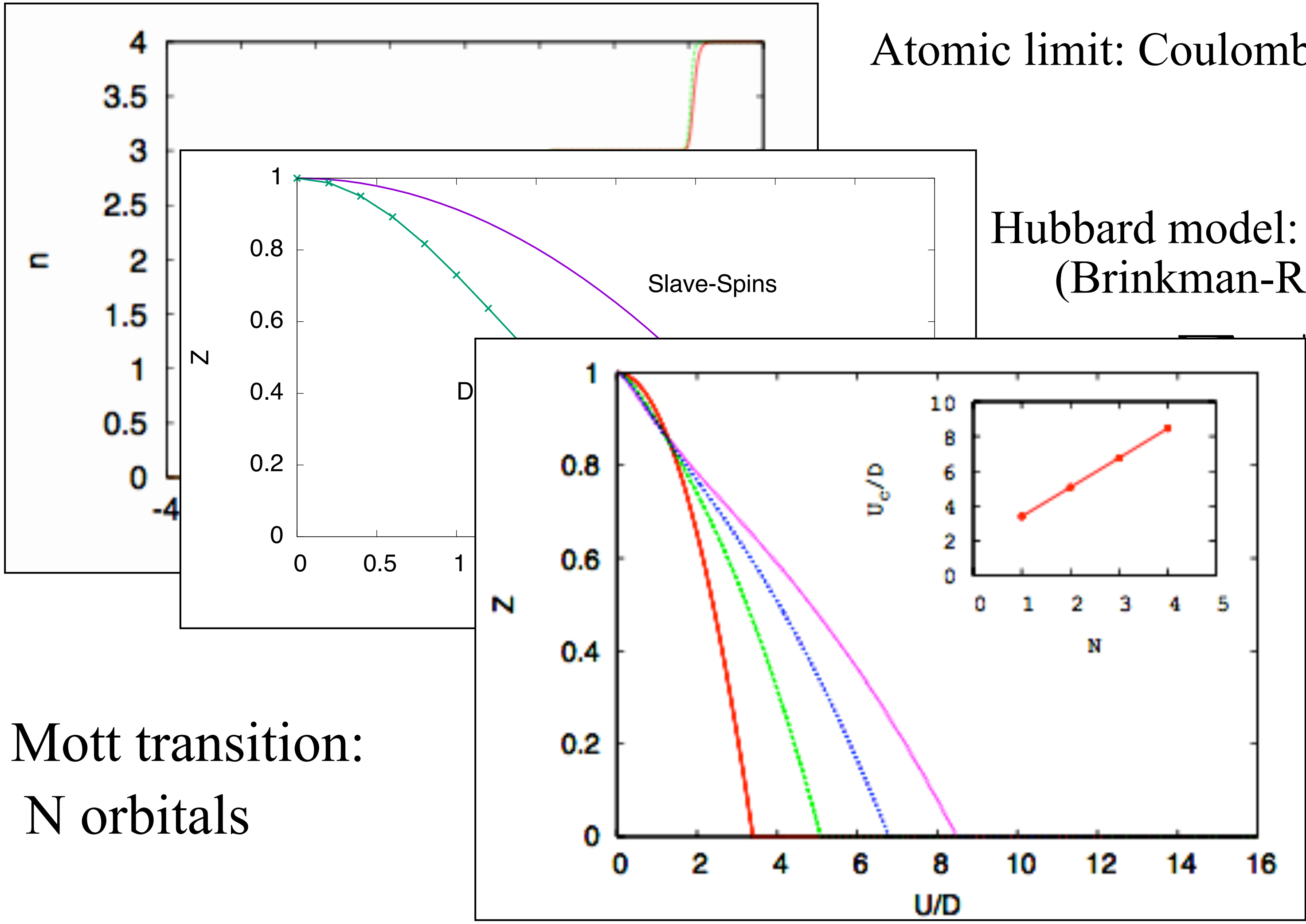
Benchmarks



Atomic limit: Coulomb staircase

Hubbard model: Mott transition
(Brinkman-Rice scenario)

$$H = -t \sum_{\langle ij \rangle, \sigma} (d^{\dagger}_{i\sigma} d_{i\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



Atomic limit: Coulomb staircase

Hubbard model: Mott transition
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$$\ldots_{\sigma} d_{i\sigma} + h.c.)$$

$$U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Mott transition:
N orbitals

Benchmarks

Atomic limit: Coulomb staircase

Hubbard model: Mott transition
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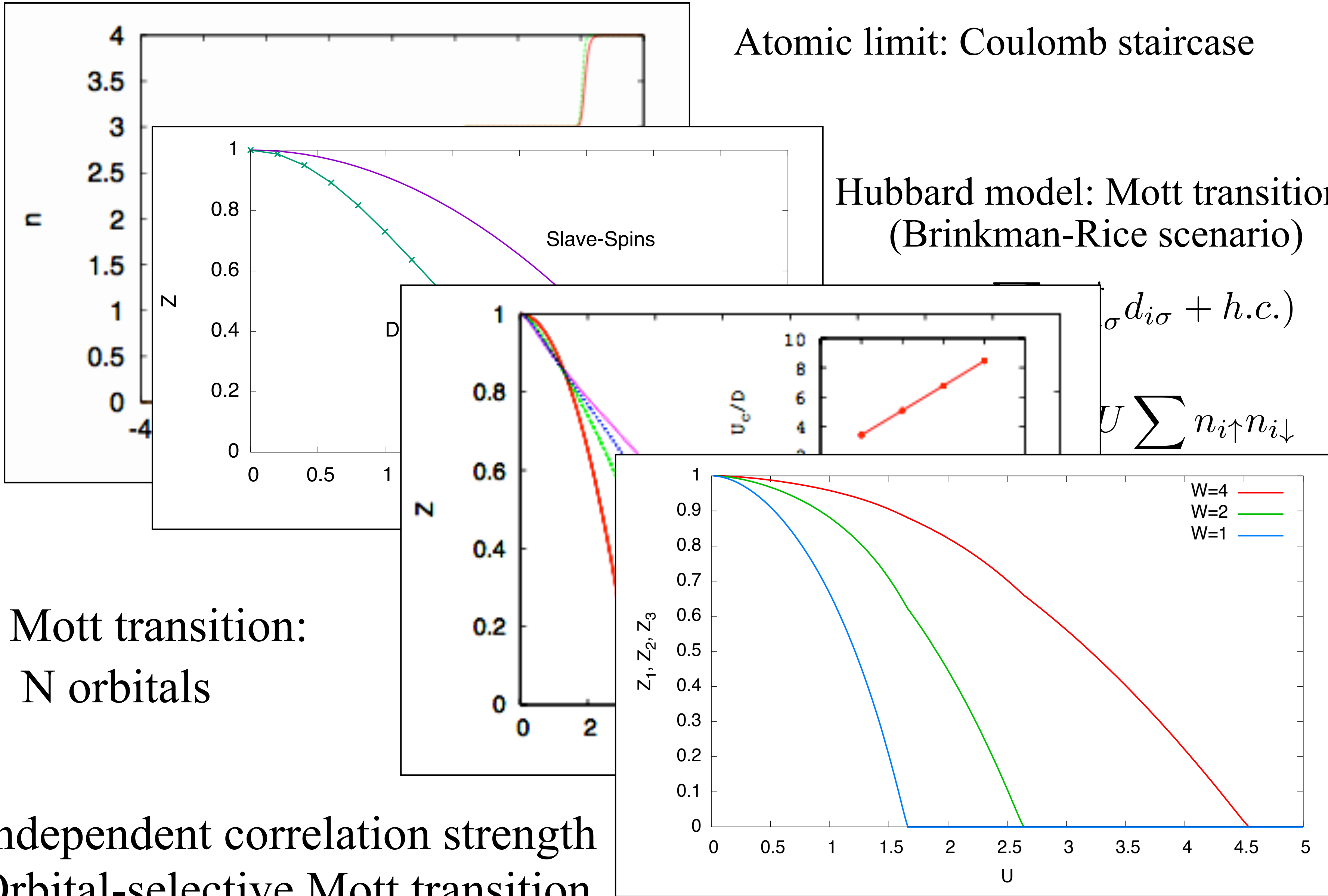


Mott transition:
N orbitals

Independent correlation strength
Orbital-selective Mott transition

Generalization off half-filling

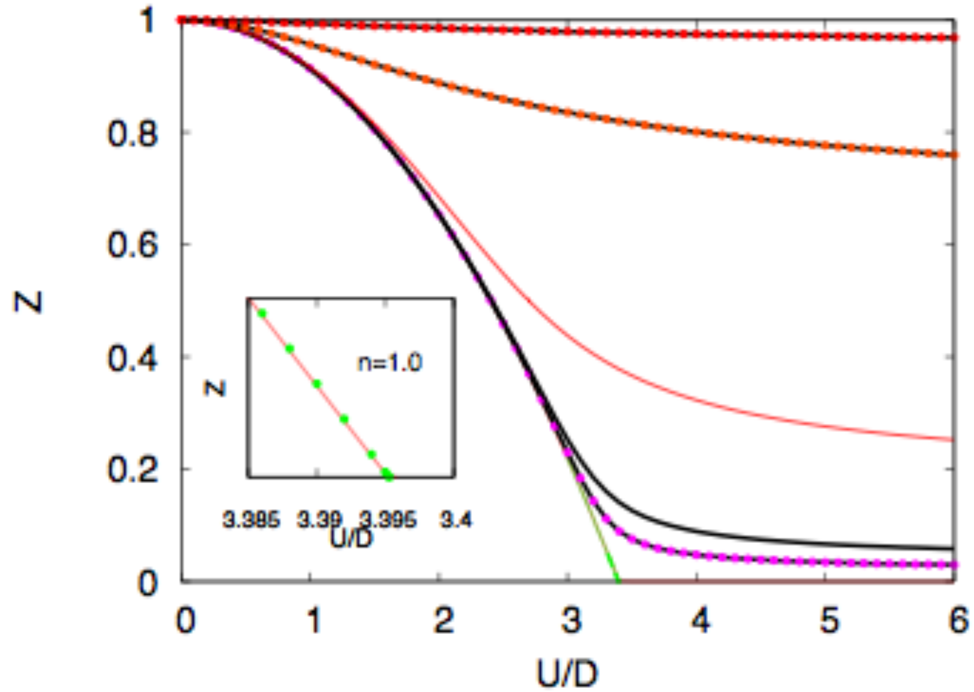
$d \rightarrow 2S^x f$ Is no longer a good choice (bad non-interacting limit)

Good choice:

$$d \rightarrow Sf$$

$$S = cS^+ + S^-$$

$$c = \frac{1}{\sqrt{n(1-n)}} - 1$$



Coincident in one-band models with Slave Bosons mean-field (Gutzwiller approximation)

Comparison with similar techniques

Number of non-physical states in the enlarged Hilbert space:

Slave Bosons: ∞

Slave Spin: finite

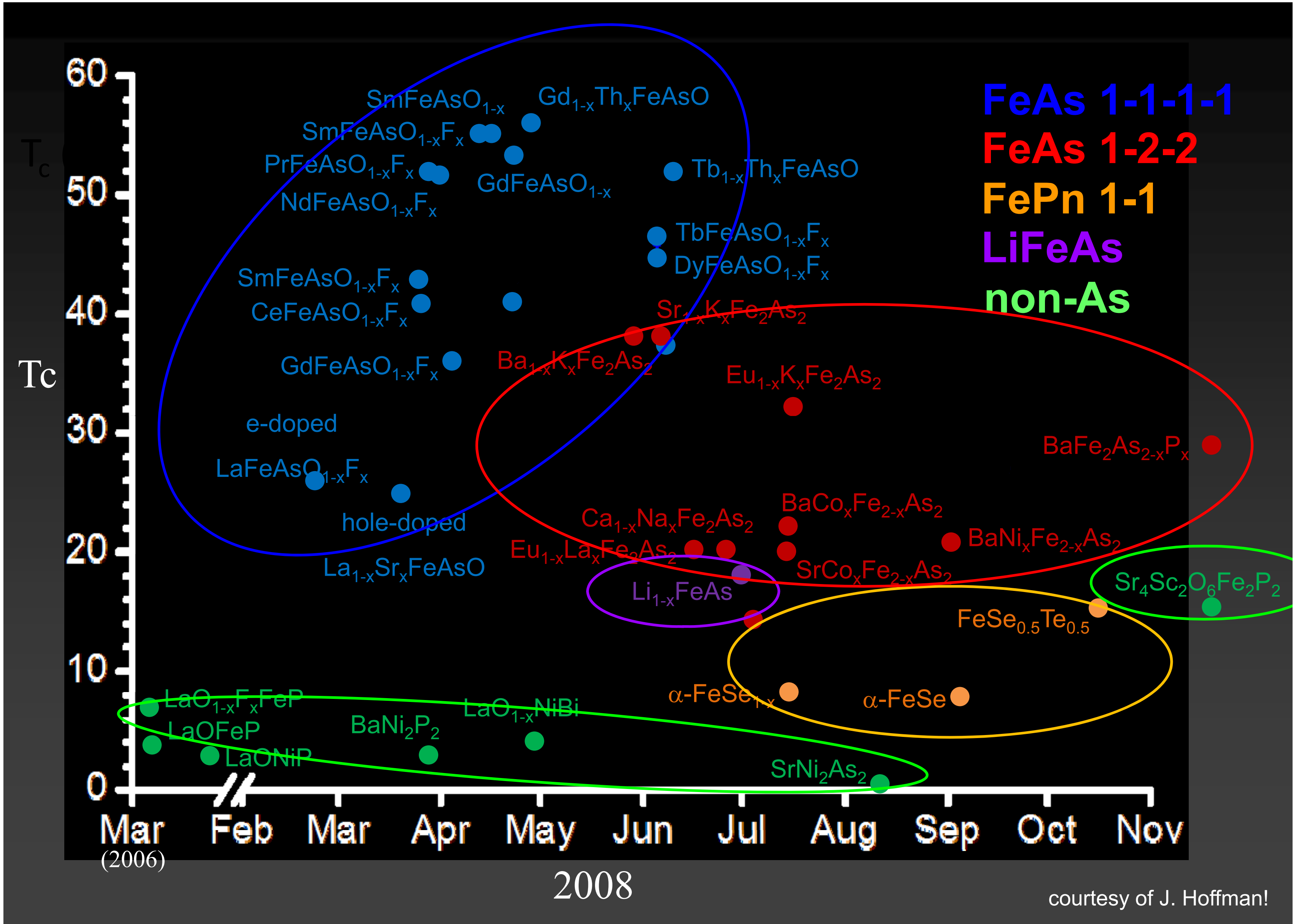
Slave Rotors: ∞

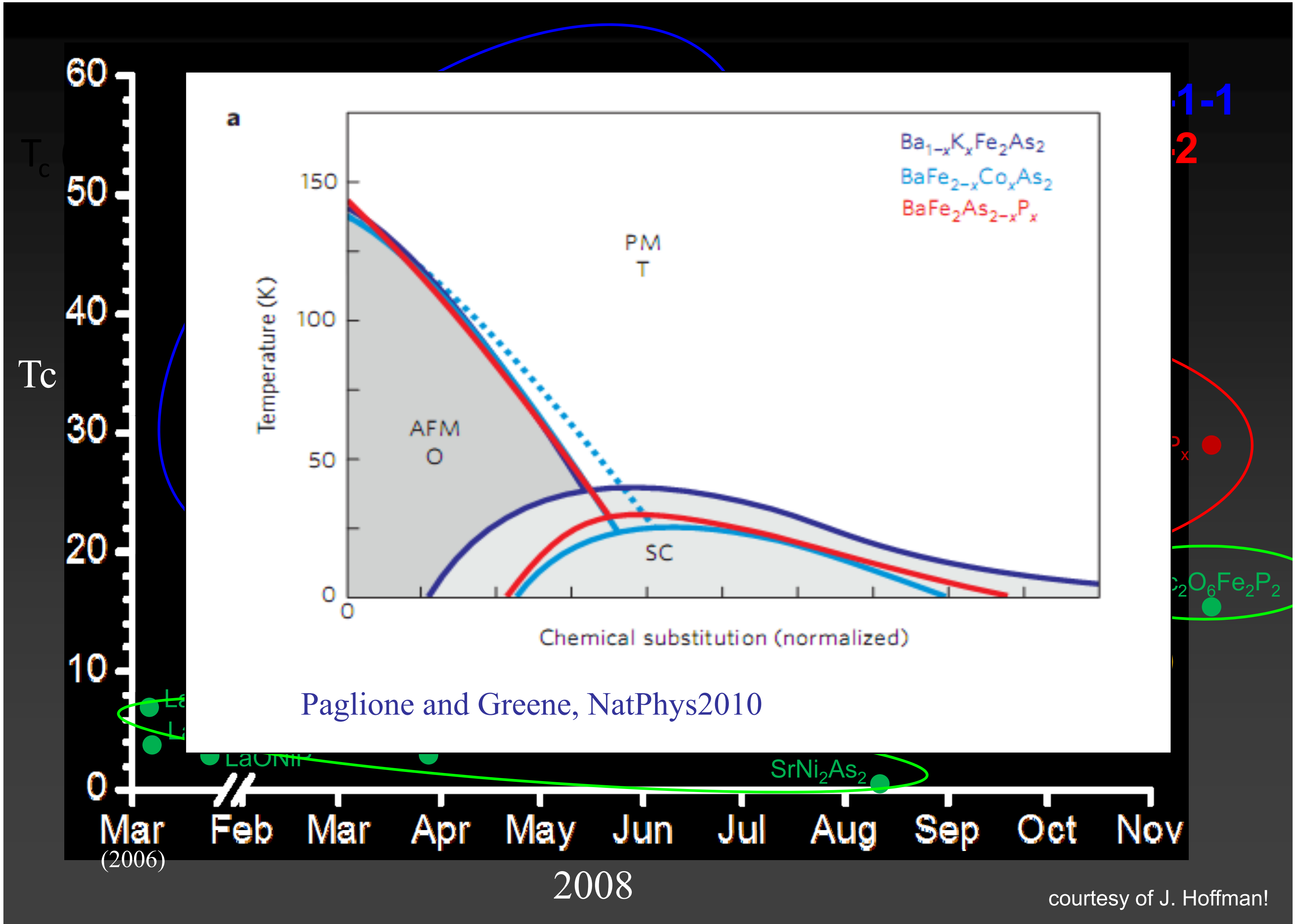
Number of auxiliary variables:

Slave Bosons: 2^{2N}

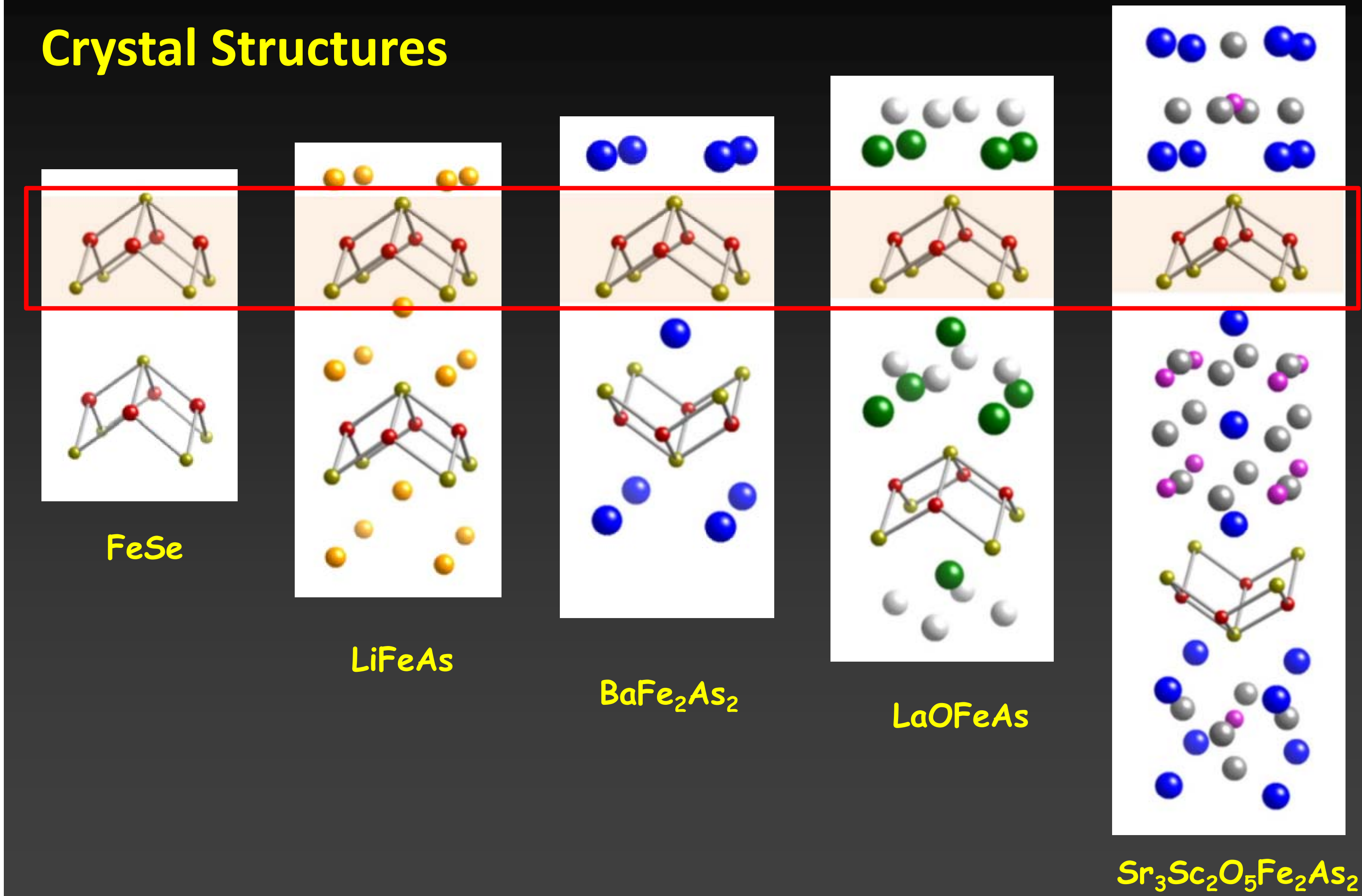
Slave Spin: 2N

Slave Rotors: 1 (only for totally degenerate systems)


FeAs 1-1-1-1
FeAs 1-2-2
FePn 1-1
LiFeAs
non-As
Tc
60
50
40
30
20
10
0
Mar
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
(2006)
2008
SmFeAsO1-x
Gd1-xThxFeAsO
SmFeAsO1-xFx
PrFeAsO1-xFx
GdFeAsO1-x
Tb1-xThxFeAsO
NdFeAsO1-xFx
TbFeAsO1-xFx
DyFeAsO1-xFx
SmFeAsO1-xFx
CeFeAsO1-xFx
Sr1-xKxFe2As2
GdFeAsO1-xFx
Ba1-xKxFe2As2
Eu1-xKxFe2As2
e-doped
BaFe2As2-xPx
LaFeAsO1-xFx
hole-doped
Ca1-xNaxFe2As2
BaCoxFe2-xAs2
BaNixFe2-xAs2
Eu1-xLaxFe2As2
La1-xSrxFeAsO
SrCoxFe2-xAs2
Li1-xFeAs
Sr4Sc2O6Fe2P2
FeSe0.5Te0.5
α-FeSe1-x
α-FeSe
LaO1-xFxFeP
LaO1-xNiBi
LaOFeP
BaNi2P2
LaONiP
SrNi2As2
courtesy of J. Hoffman!


a
Temperature (K)
150
100
50
0
Ba$_{1-x}$K$_x$Fe$_2$As$_2$
BaFe$_{2-x}$Co$_x$As$_2$
BaFe$_2$As$_{2-x}$P$_x$
PM
T
AFM
O
SC
Chemical substitution (normalized)
Paglione and Greene, NatPhys2010
Tc
60
40
30
20
10
SrNi$_2$As$_2$
Mar
(2006)
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
2008
courtesy of J. Hoffman!

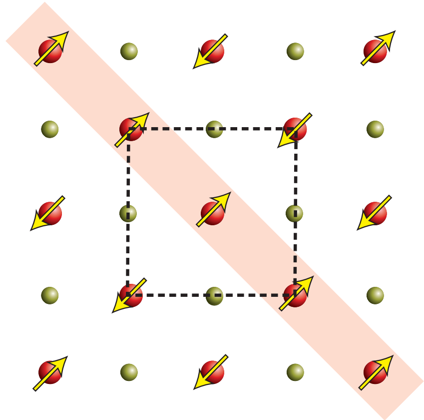
Crystal Structures

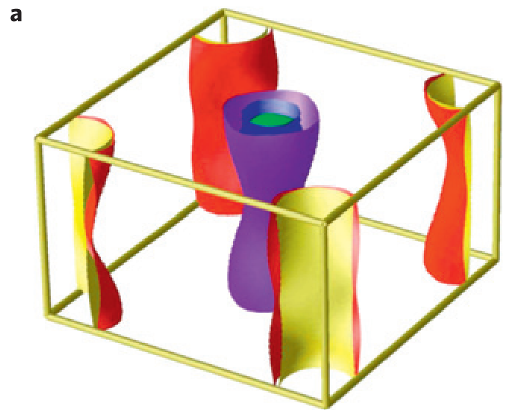


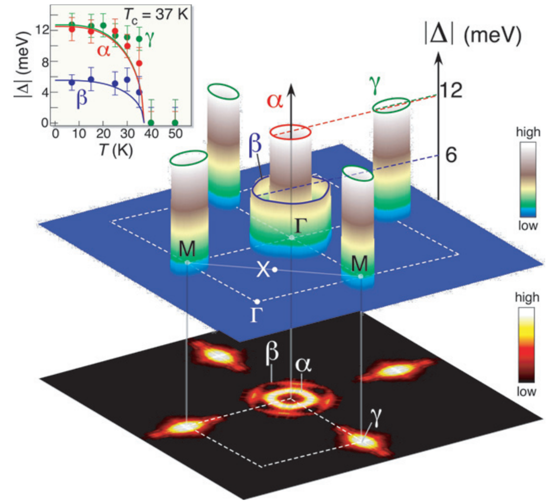
Paglione/Greene review (2010)

Iron-based superconductors

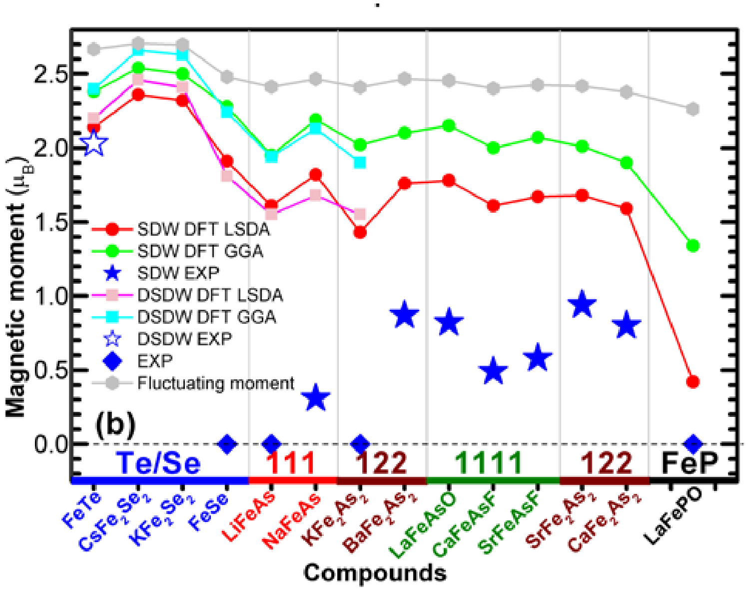
Paglione and Greene, NatPhys2010



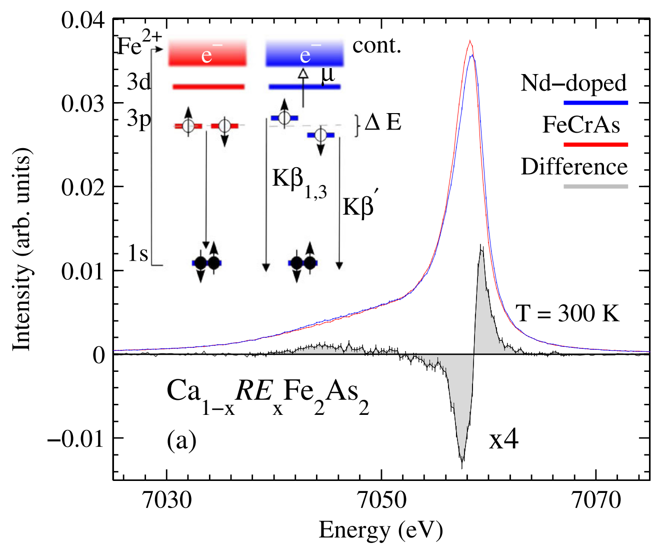




Ding et al. EPL 2008



Yin et al. NatMat2011



Gretarsson et al. PRL2013

Correlations in Iron SC?

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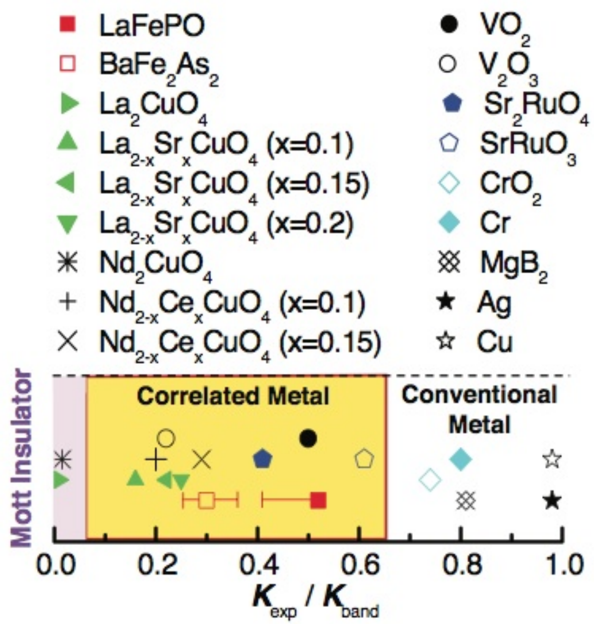
Contrasting evidences for correlation strength

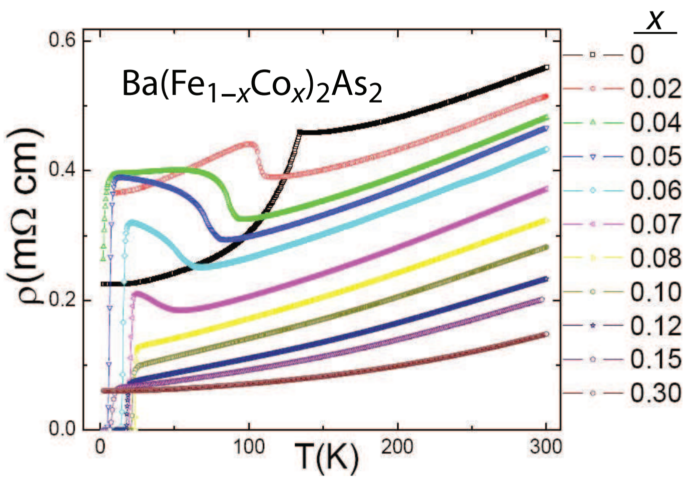
weak
- no Mott insulator in the phase diagram
- no detection of prominent Hubbard bands
- moderate correlations from Optics

strong
- bad metallicity
- strong sensitivity to doping
- local vs itinerant magnetism

<u>Weak-coupling vs Strong-coupling scenarios</u>

Qazilbash et al. NatPhys2009





Fang et al. PRB80 (2009)
Rullier-Albenque et al. PRL103 (2009)

Specific heat (mJ/ mol K^2)

LaFePO	7
$Ba(Co_xFe_{1-x})_2As_2$	15-20
$Ba_{1-x}K_xFe_2As_2$	50
$FeSe_{0.88}$	9.2
KFe_2As_2	69-102
$K_{0.8}Fe_{1.6}Se_2$	6

Review: Stewart, RMP (2011)

Modeling Iron-based superconductors: Hund's coupling

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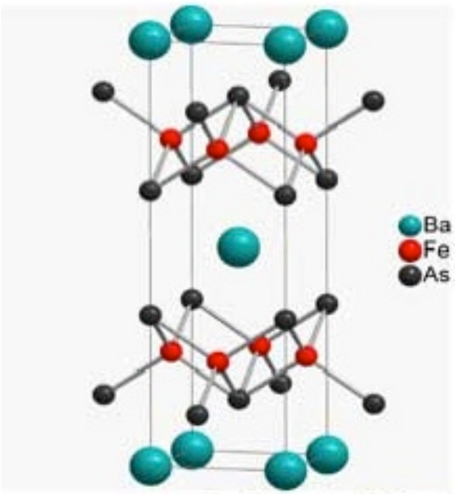
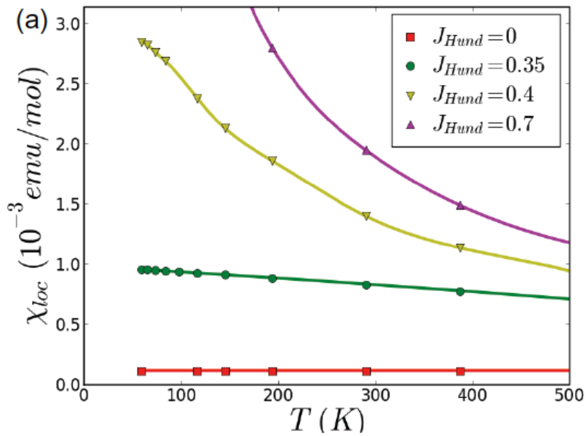


$BaFe_2As_2$

- cubic
- multi-orbital: 5 bands (Fe 3d) at the Fermi level
  n=6 conduction electrons
- Partially lifted degeneracy
- Not a very large U but strong Hund's coupling J
  W~4eV, U~2-4eV, J~0.5eV

Theory:
'Hund's metals'

Haule and Kotliar, NJP 11 (2009)



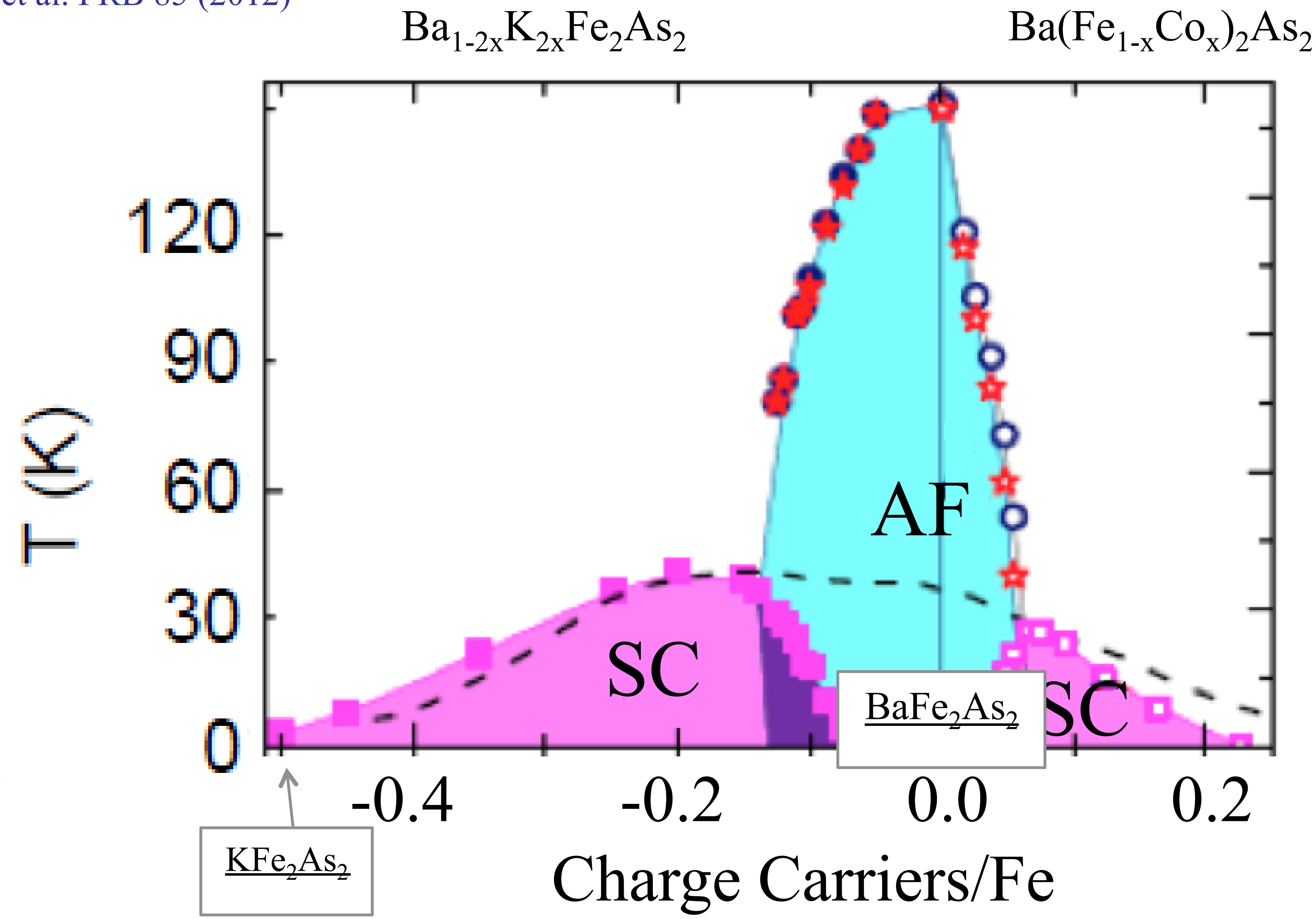
$$H = \sum_k H_k^{DFT}$$

$$+U\sum_{i,m} n_{im\uparrow}n_{im\downarrow} + (U' - \frac{J}{2})\sum_{i,m>m'} n_{im}n_{im'}$$

$$-J\sum_{i,m>m'}\Big[2\mathbf{S}_{im}\cdot\mathbf{S}_{im'} + (d^\dagger_{im\uparrow}d^\dagger_{im\downarrow}d_{im'\uparrow}d_{im'\downarrow} + h.c.)\Big]$$

(U'=U-2J)

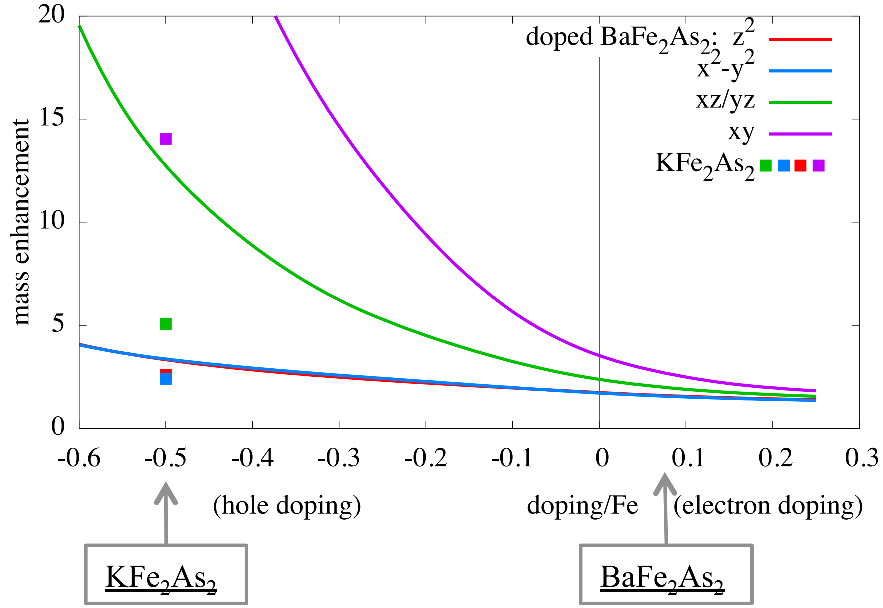
Avci et al. PRB 85 (2012)



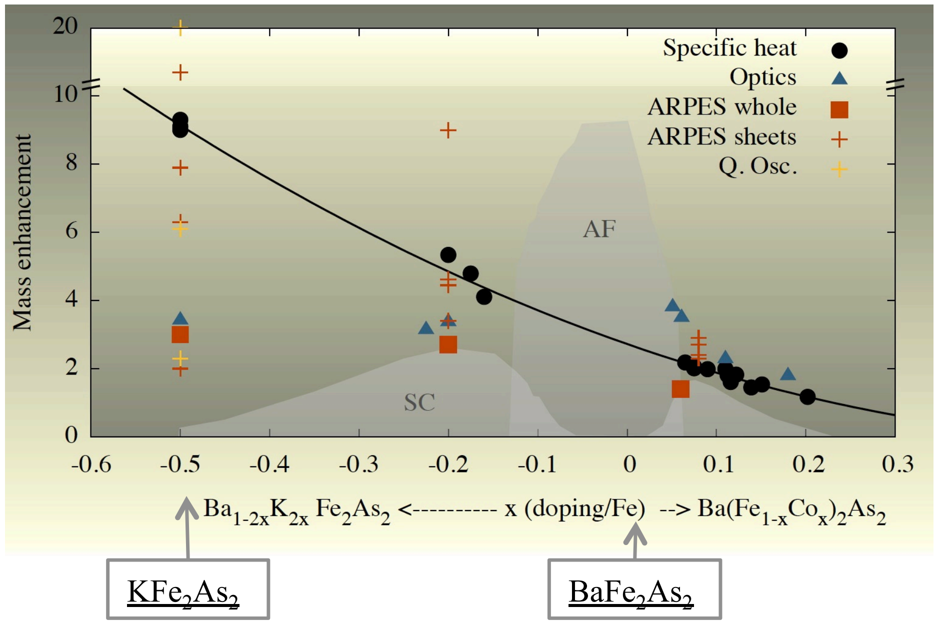
mass enhancements

LdM, G. Giovannetti, M. Capone, PRL 2014

Theory (LDA+Slave-spins)



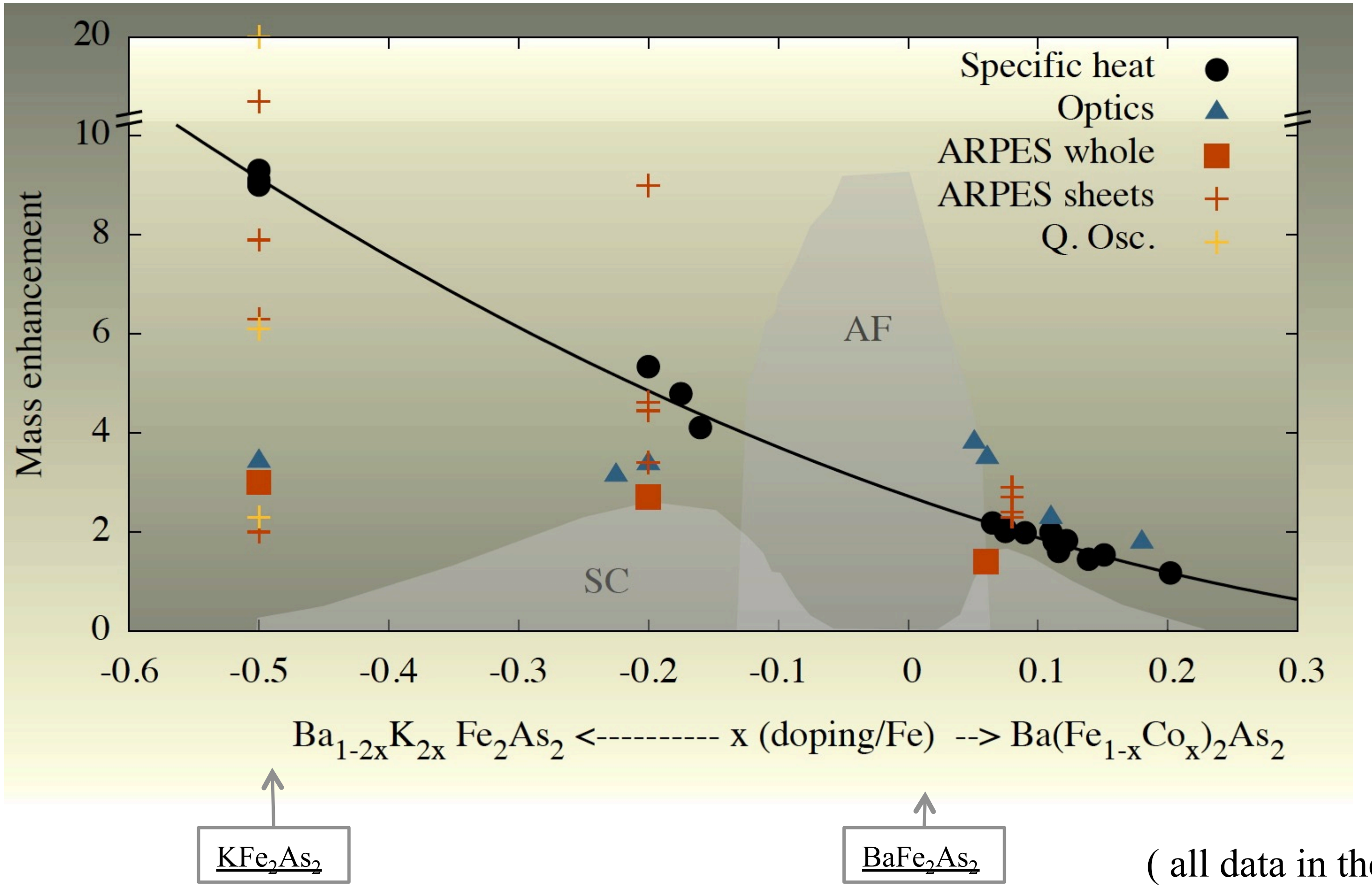
Experimental data
(high-T tetragonal phase)



Selective correlation strength: strongly *and* weakly correlated electrons

Many other theoretical works showing orbital-dependent correlations (DFT+..) : Ishida et al., Aichhorn et al., Shorikov et al., Craco, Laad et al., Werner et al., Yin et al., Backes et al. (DMFT), Misawa Imada (VQMC) Bascones et al. (Hartree-Fock), Ikeda et al. (FLEX), Yu Si (slave spins), Lanatà et al. (Gutzwiller), Calderon et al. (slave-spins), etc.

Correlations: experimental mass enhancements in Ba-122



(all data in the high-T tetragonal phase)

Sommerfeld coefficient $$\gamma \sim N^*(E_F) = \sum_\alpha (m^*/m_b)_\alpha N_b^\alpha(E_F)$$

Optics: Drude contribution $$D^* = \sum_\alpha (m_b/m^*)_\alpha D_b^\alpha$$

References in: LdM, G. Giovannetti, M. Capone, PRL2014

Optics: beware of interband transitions! Calderon et al., PRB2014

Orbital-dependent correlation strength

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mass enhancements

LdM, G. Giovannetti, M. Capone, PRL 2014

Theory (LDA+Slave-spins)

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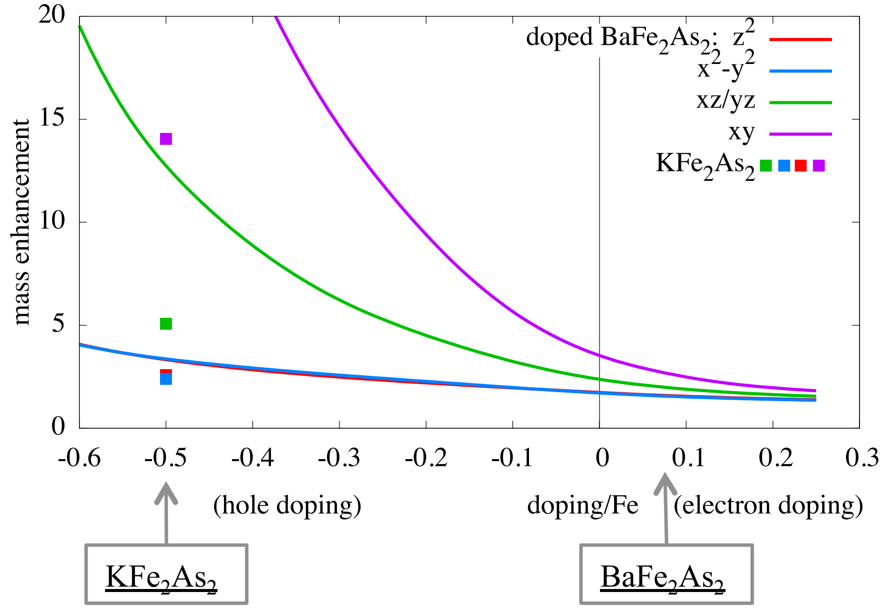
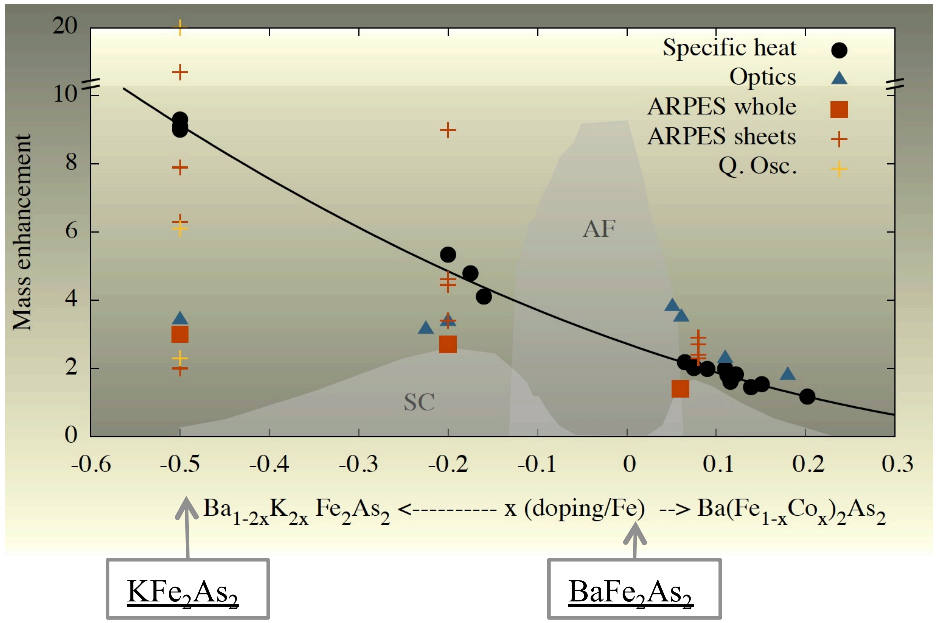
(high-T tetragonal phase)





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Heavy-fermionic behaviour in KFe_2As_2

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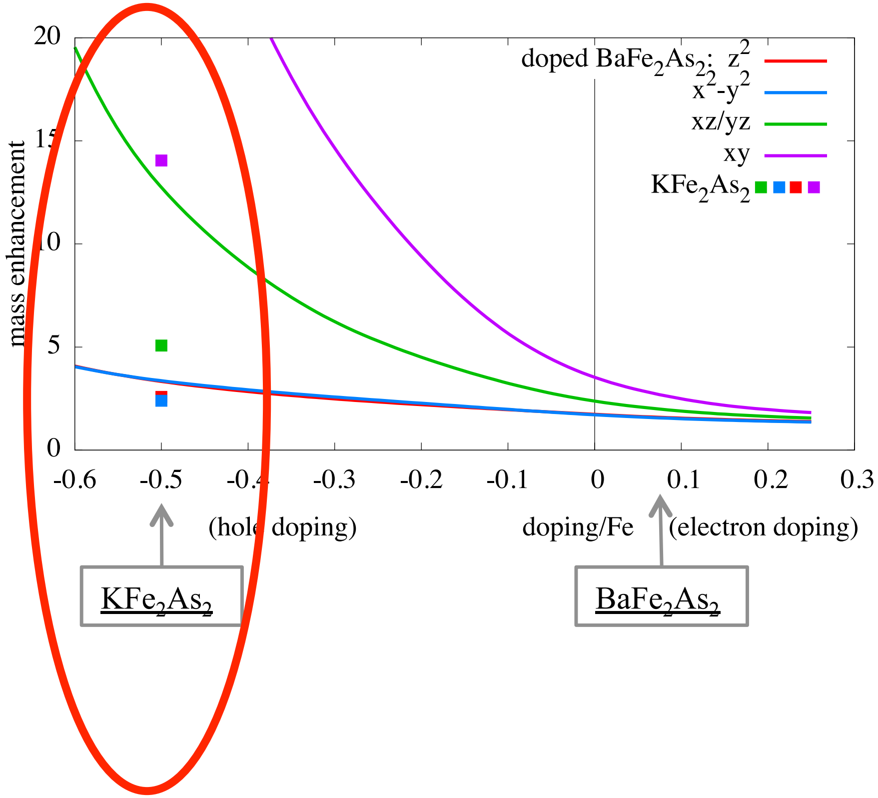
mass enhancements

LdM, G. Giovannetti, M. Capone, PRL 2014

Theory (LDA+Slave-spins)



PRL **111,** 027002 (2013) PHYSICAL REVIEW LETTERS week ending 12 JULY 2013

Evidence of Strong Correlations and Coherence-Incoherence Crossover in the Iron Pnictide Superconductor KFe_2As_2

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[2]*INAC/SPSMS, CEA Grenoble, 38054 Grenoble, France*
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[4]*Ames Laboratory US-DOE, Ames, Iowa 50011, USA*
[5]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*
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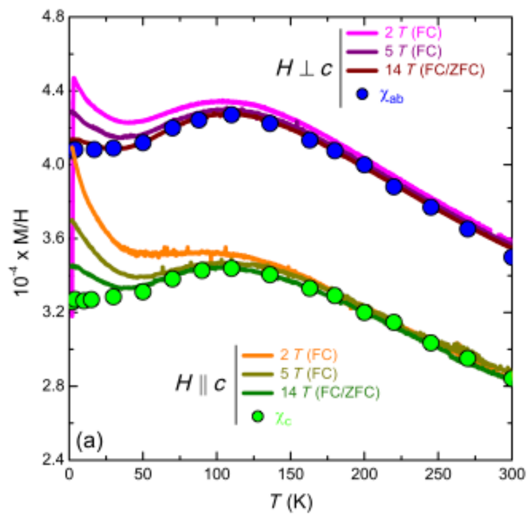
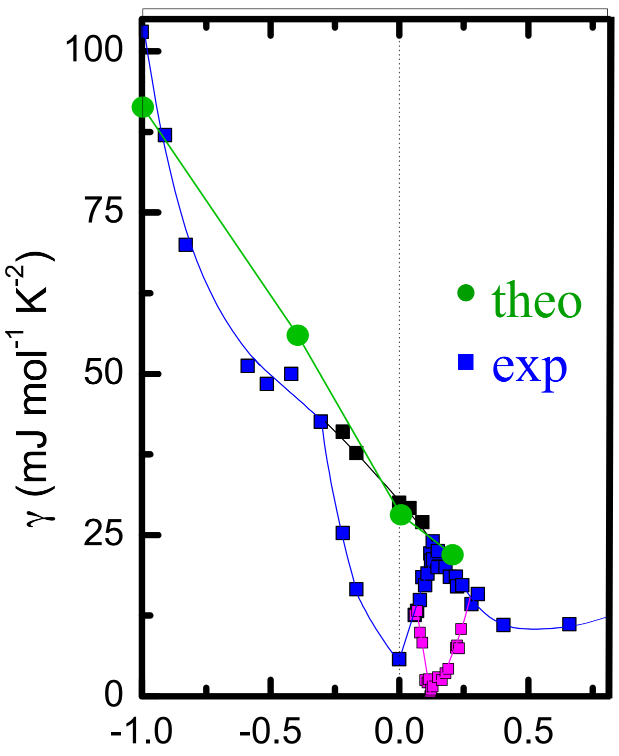
(Received 15 January 2013; published 9 July 2013)

Using resistivity, heat-capacity, thermal-expansion, and susceptibility measurements we study the normal-state behavior of KFe_2As_2. Both the Sommerfeld coefficient ($\gamma \approx 103$ mJ mol^{-1} K^{-2}) and the Pauli susceptibility ($\chi \approx 4 \times 10^{-4}$) are strongly enhanced, which confirm the existence of heavy quasiparticles inferred from previous de Haas–van Alphen and angle-resolved photoemission spectroscopy experiments. We discuss this large enhancement using a Gutzwiller slave-boson mean-field calculation, which shows the proximity of KFe_2As_2 to an orbital-selective Mott transition. The temperature dependence of the magnetic susceptibility and the thermal expansion provide strong experimental evidence for the existence of a coherence-incoherence crossover, similar to what is found in heavy fermion and ruthenate compounds, due to Hund's coupling between orbitals.

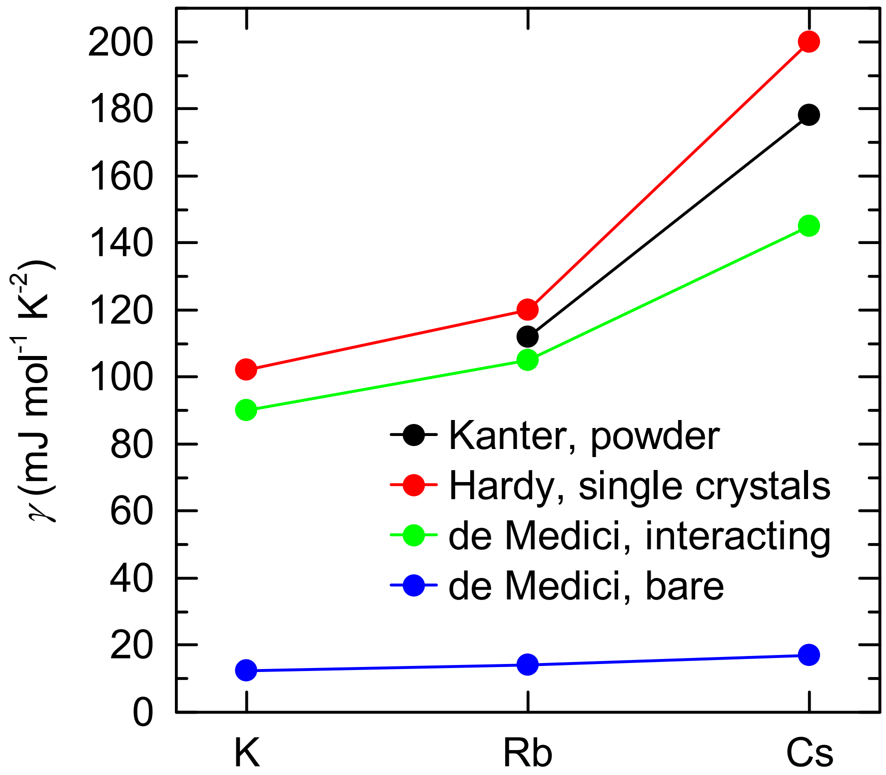


Heavy-fermionic behavior: theory vs experiment

$Ba_{1-x}K_xFe_2As_2$



AFe_2As_2 (A= K, Rb, Cs)



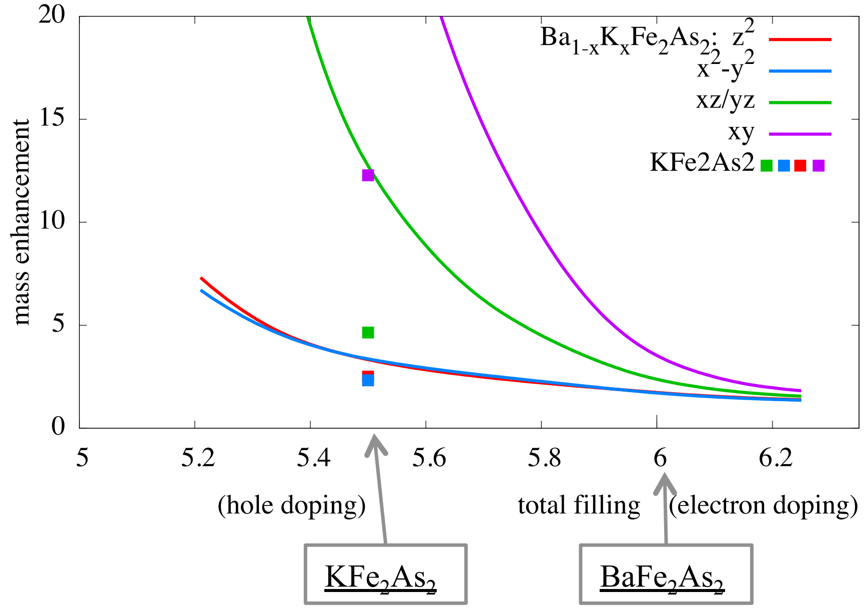
Experiments from Meingast's group in Karlsruhe. F. Hardy et al. unpublished

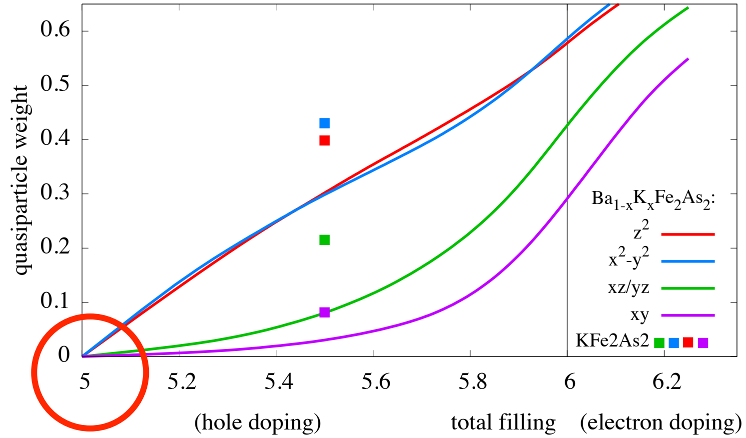
Mott insulating state at half-filling

mass enhancements

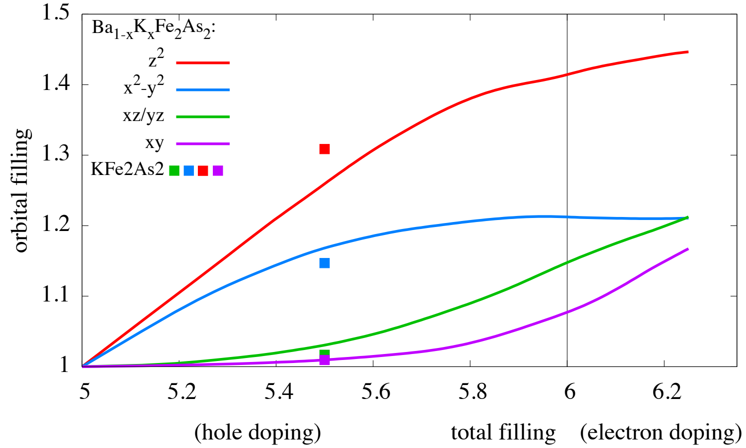
LdM, G. Giovannetti, M. Capone, PRL 2014

Theory (LDA+Slave-spins)





Mott Insulator

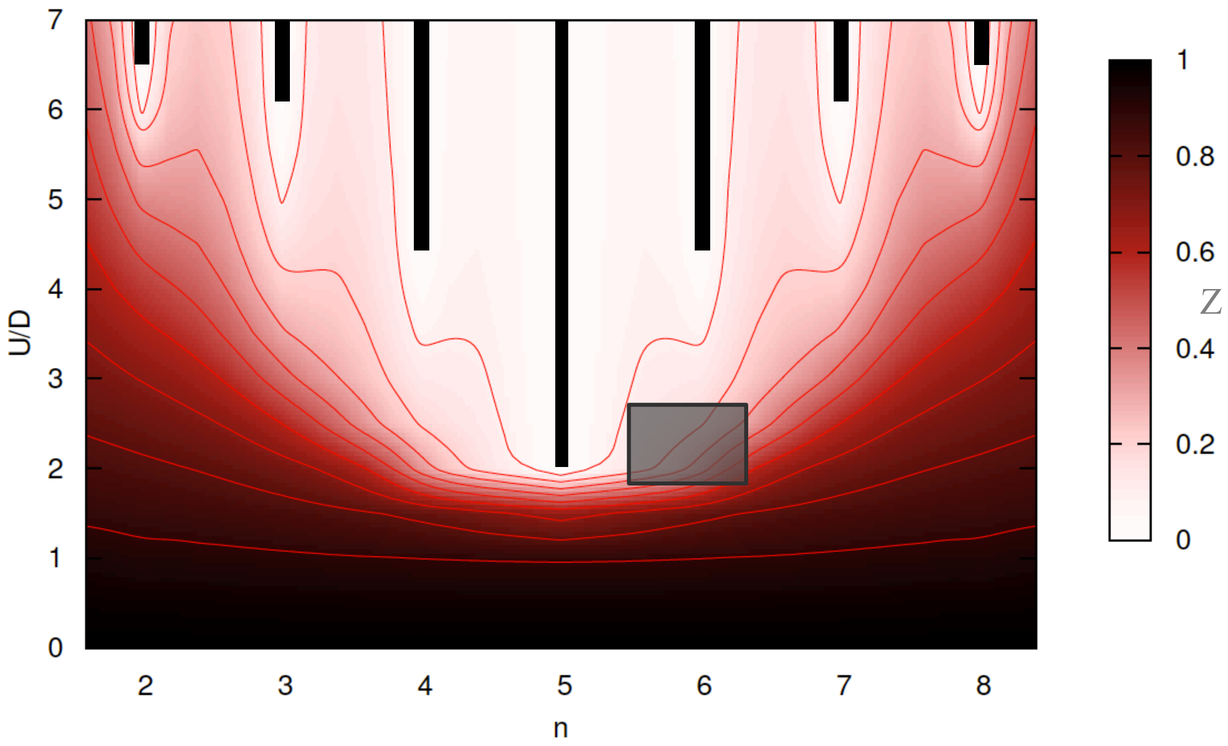


Slave-spin mean field (LdM et al., PRB 72 (2005))

J/U=0.15

J/U=0.20

J/U=0.25



Mott Gap: E(n+1)+E(n-1)-2E(n)

- half-filling: ~U+(N-1)J
- other filling: ~U-3J

LdM, PRB **83** (2011)
LdM, J. Mravlje, A. Georges, PRL **107** (2011)

For a review:
"Strong Correlations from Hunds' Coupling"
A. Georges, LdM, J. Mravlje,
Ann Rev Cond. Mat. 4, 137 (2013)

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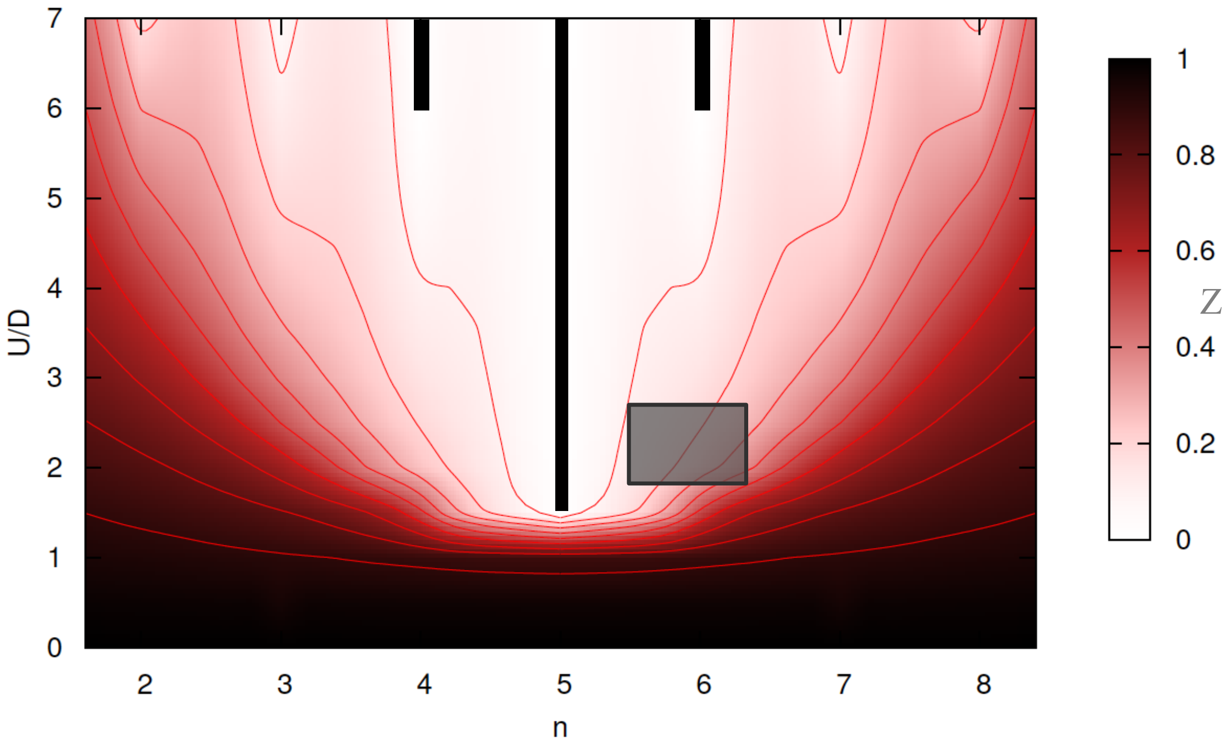

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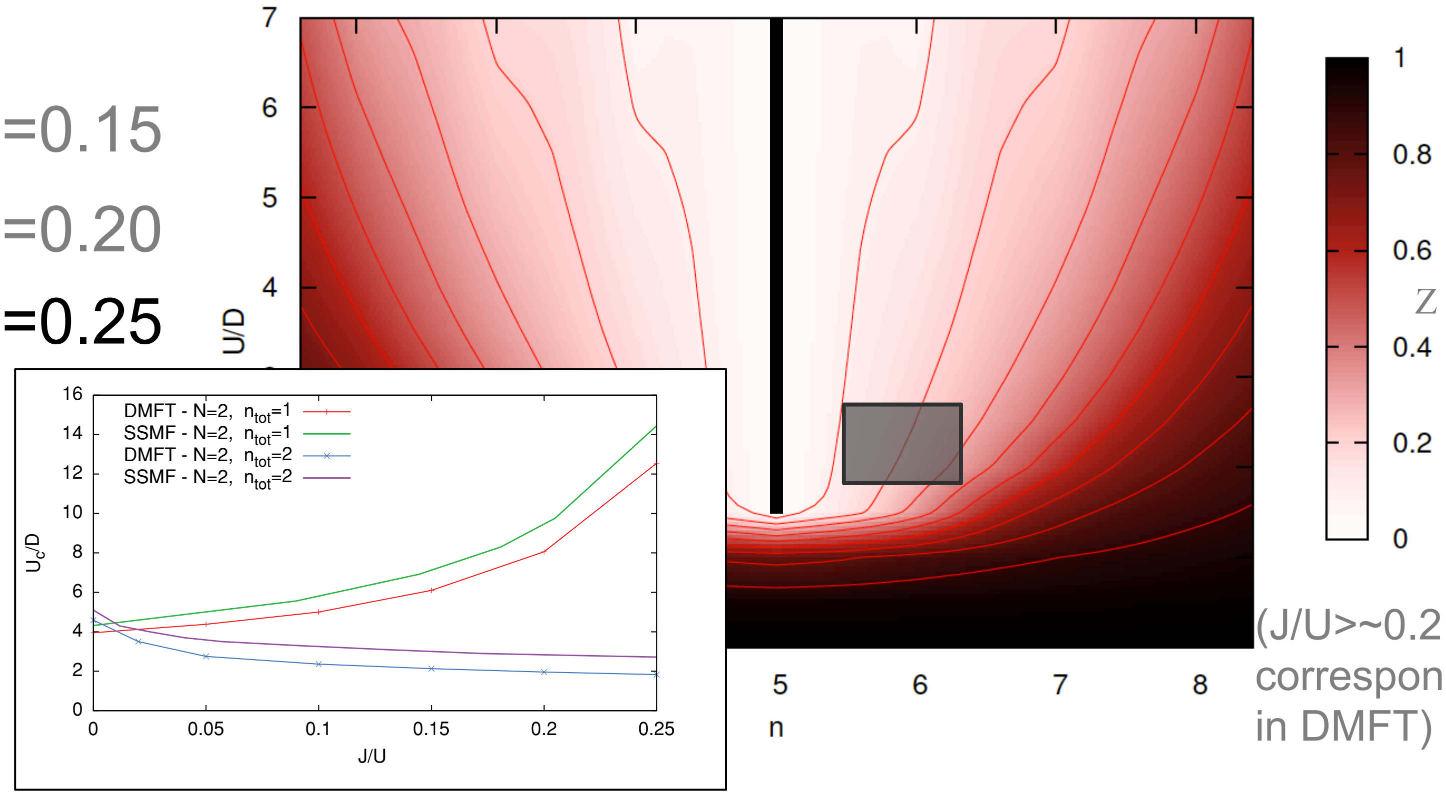


(J/U>~0.2 in Slave-spins corresponds to J/U=0.15 in DMFT)

Mott Gap: E(n+1)+E(n-1)-2E(n)

- half-filling: ~U+(N-1)J
- other filling: ~U-3J

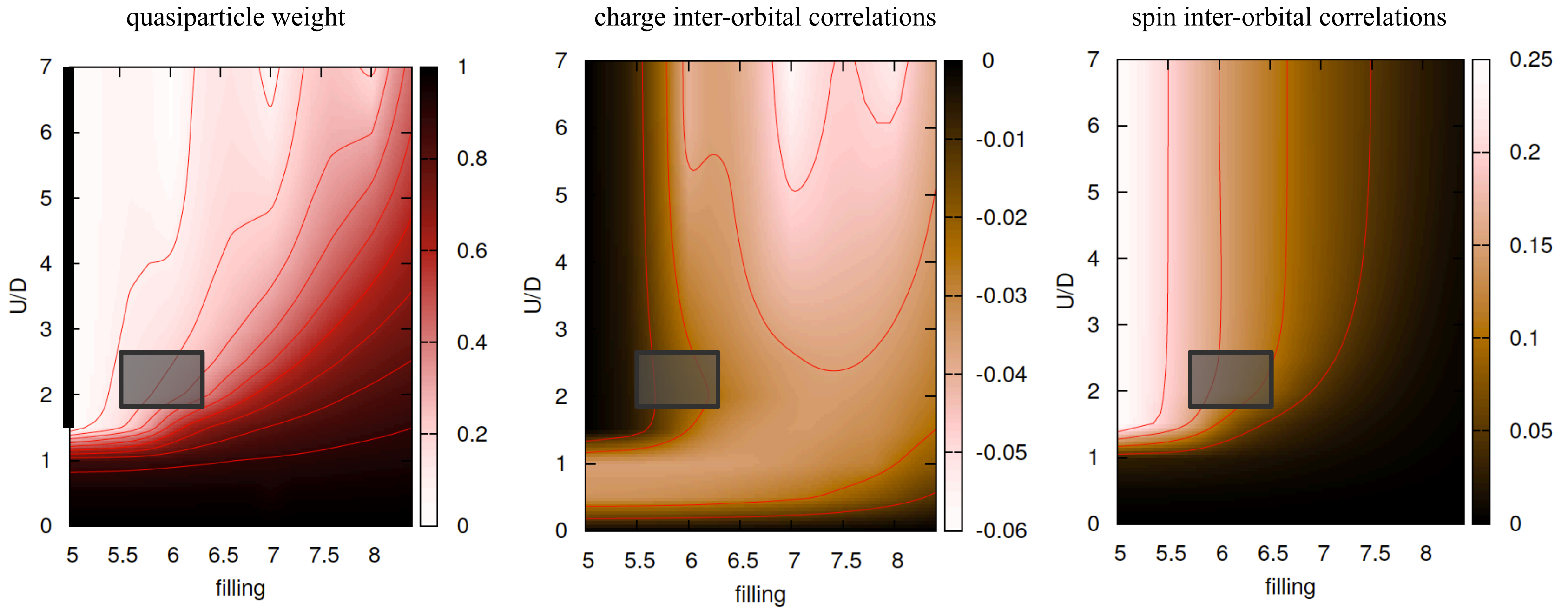
For a review:
"Strong Correlations from Hunds' Coupling"
A. Georges, LdM, J. Mravlje,
Ann Rev Cond. Mat. 4, 137 (2013)

LdM, PRB **83** (2011)
LdM, J. Mravlje, A. Georges, PRL **107** (2011)

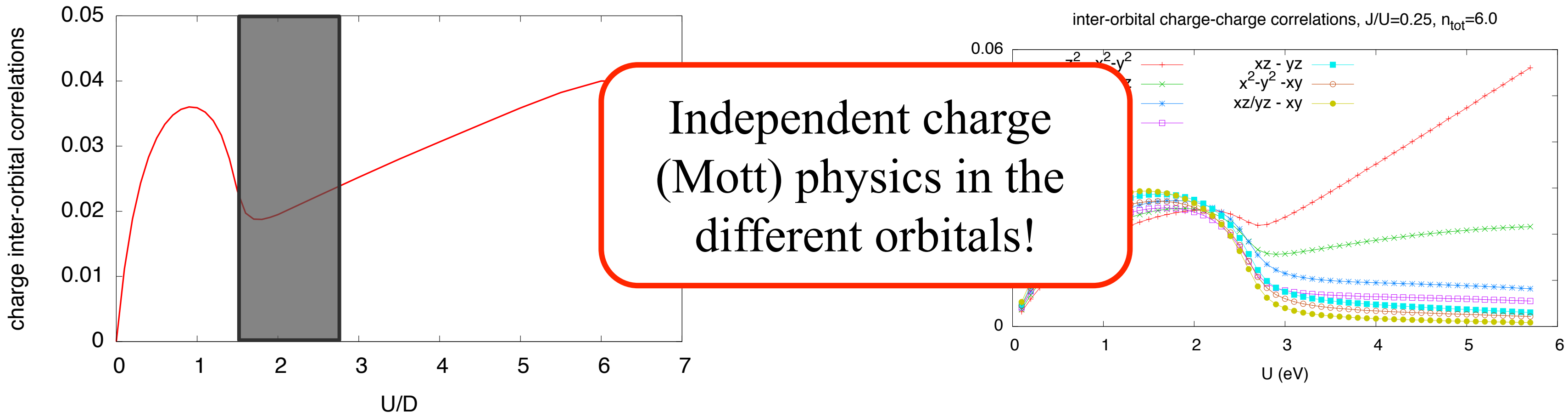
Degenerate 5-band Hubbard model

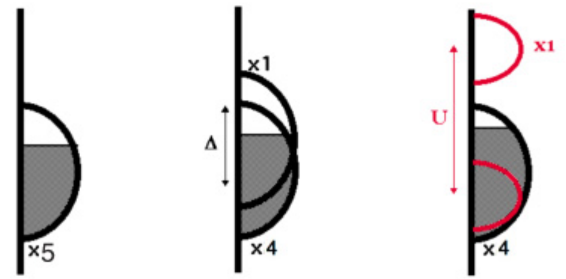
'Near' half-filling:

- local inter-orbital spin correlations are enhanced (high-spin locking)



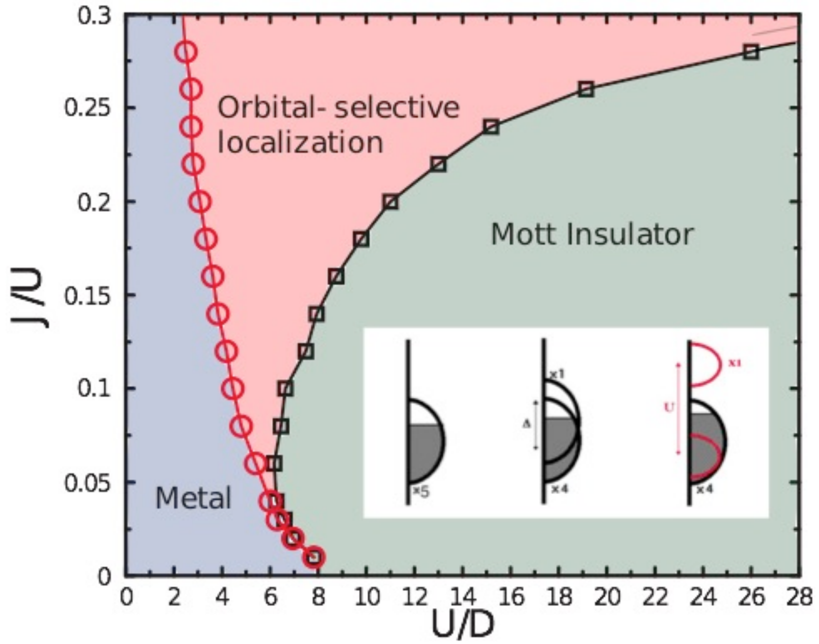
- local inter-orbital charge correlations are suppressed





5 bands of the same width
N=6 (half-filling+1)

Crystal-field (one band up)
+ Hund's coupling



LdM, S.R. Hassan, M. Capone, JSC **22**, 535 (2009)

Orbital-selective Mott transition

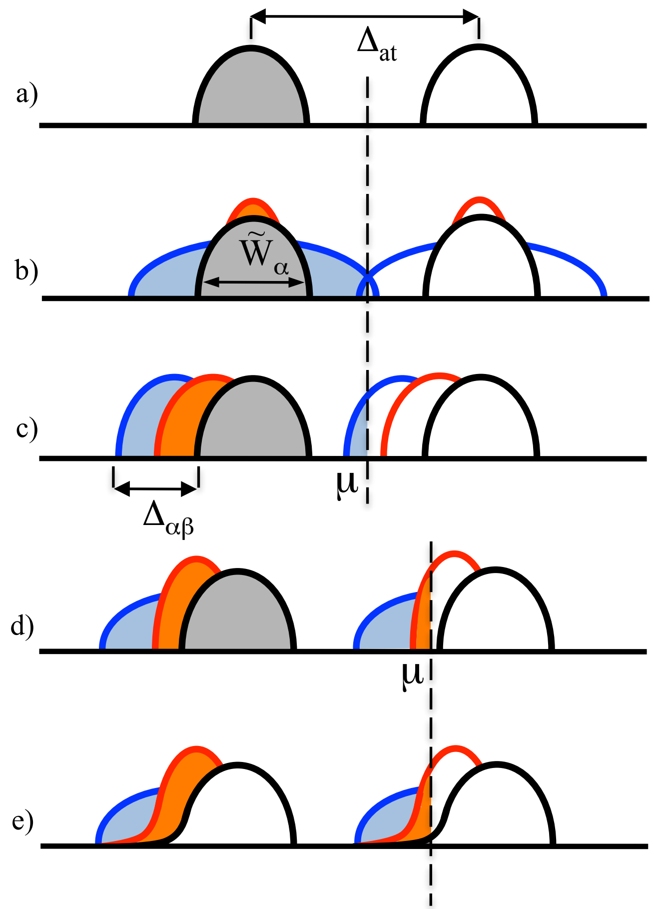
•Coexisting itinerant and localized conduction electrons
• Metallic resistivity and free-moment magnetic response
• non Fermi-liquid physics of the intinerant electrons

Anisimov et al., Eur. Phys. J. B 25 (2002)
Koga et al., Phys. Rev. Lett. 92 (2004)
For a review:
M. Vojta J. Low Temp. Phys. 161 (2010)

J favors the OSMT

(OSMT is the extreme case. More generally J favors a differentiation in the correlation strength for each orbital)

Hund's coupling as an orbital decoupler

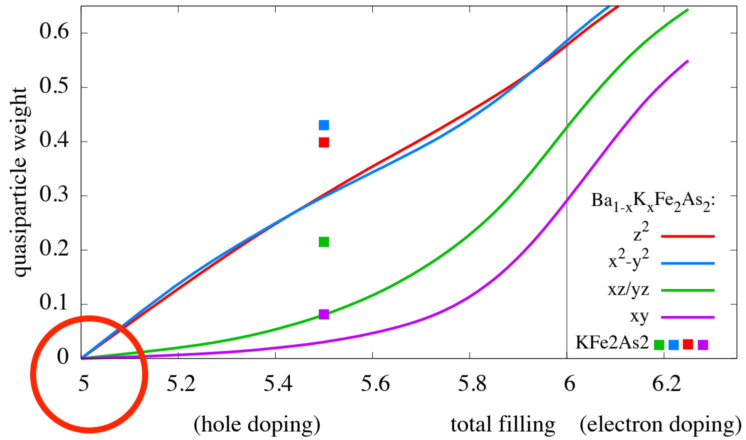


Hund's coupling suppresses the inter-orbital correlations, rendering the charge excitations in the different orbitals independent from one-another, i.e. acting as an **orbital-decoupler for Mott-physics**

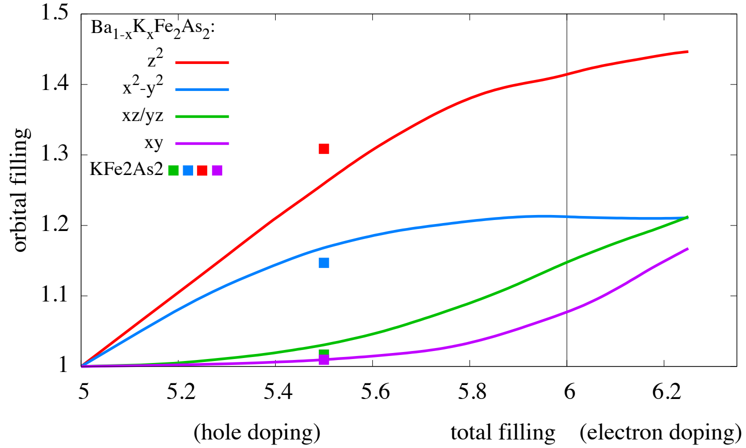
LdM, S.R. Hassan, M. Capone, X. Dai, PRL**102** (2009)
LdM, Phys. Rev. B **83** (2011)
Werner and Millis, Phys. Rev. Lett. **99** (2007)

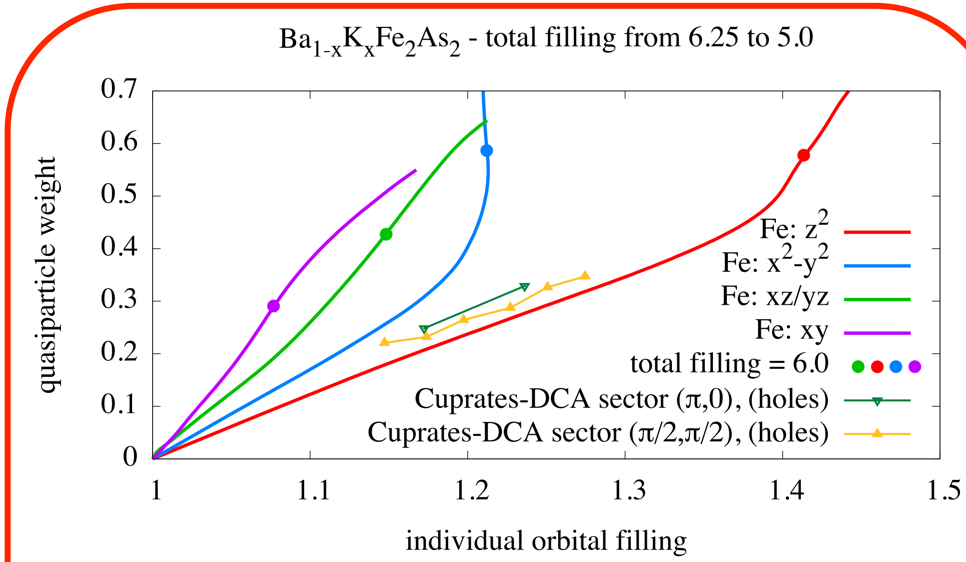
Selective Mottness in iron-SC: doped $BaFe_2As_2$ (DFT+SSpins)

Luca de' Medici



Mott Insulator





Strikingly linear behaviour, when plotting Z against the individual orbital populations
Same as for cuprates!

Mottness

Orbital-Selective correlation strength

Selective Mottness!

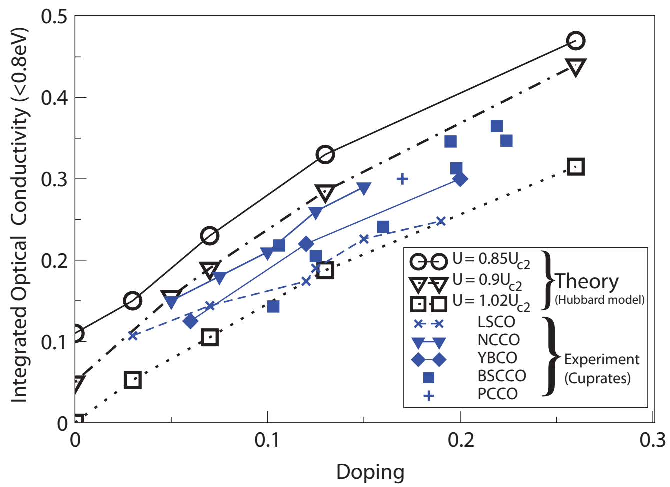
Each orbital behaves as a doped Mott insulator

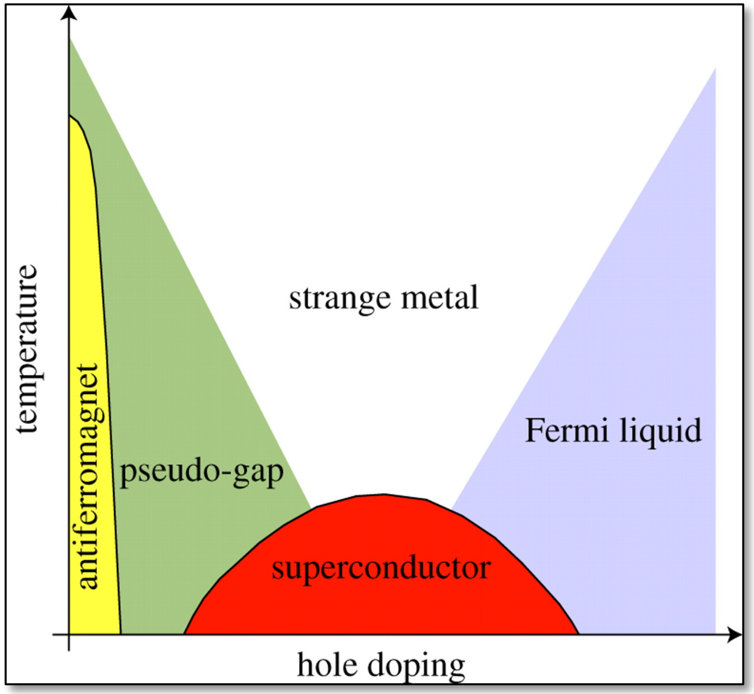
orbital decoupling, and influence of the n=5 Mott insulator

Similar evidences from
LDA+DMFT: Ishida et al., PRB **81** (2010), Werner et al. NatPhys '12
Variational MC: Misawa et al.,PRL **108** (2012)

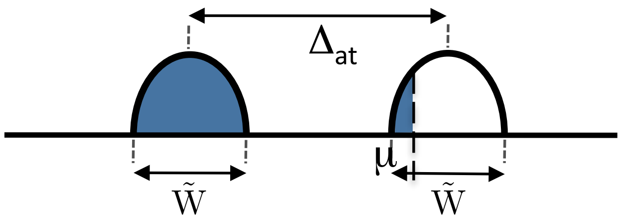
Cuprates: Mottness

Comanac et al. Nat.Phys. 2008





'Mottness'



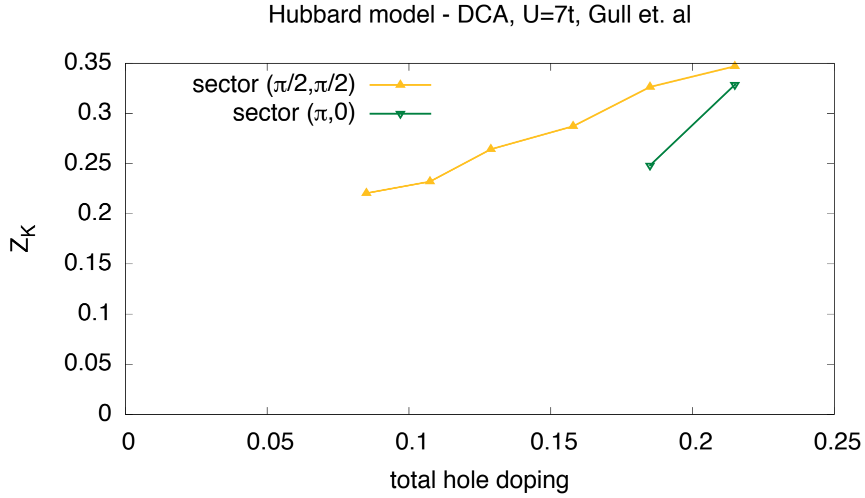
Spectrum of charge excitations

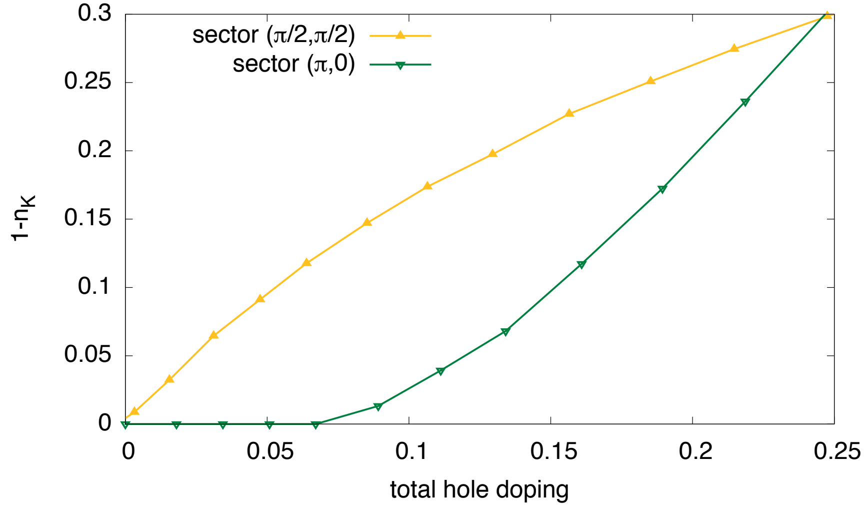
The proximity to a Mott state strongly affects the properties of a system:

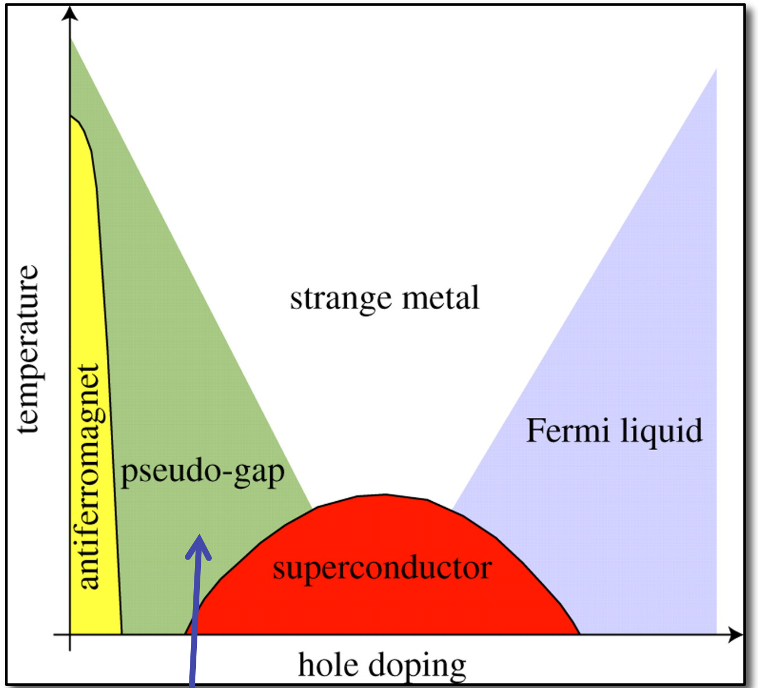
- reduced metallicity (Z~x)
- mass enhancement
- transfer of spectral weight from low to high energy (e.g. in optical response)
- tendency towards magnetism
- …

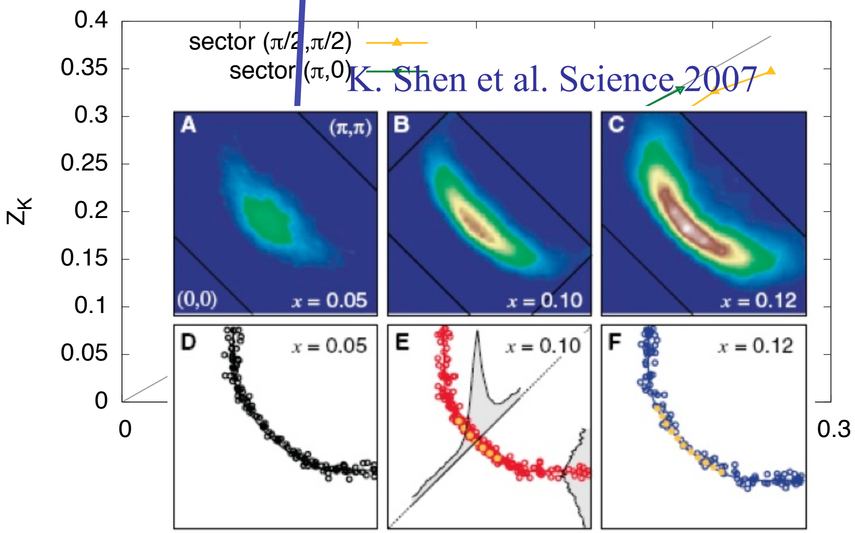
Cuprates: Pseudogap as Selective Mottness

Luca de' Medici



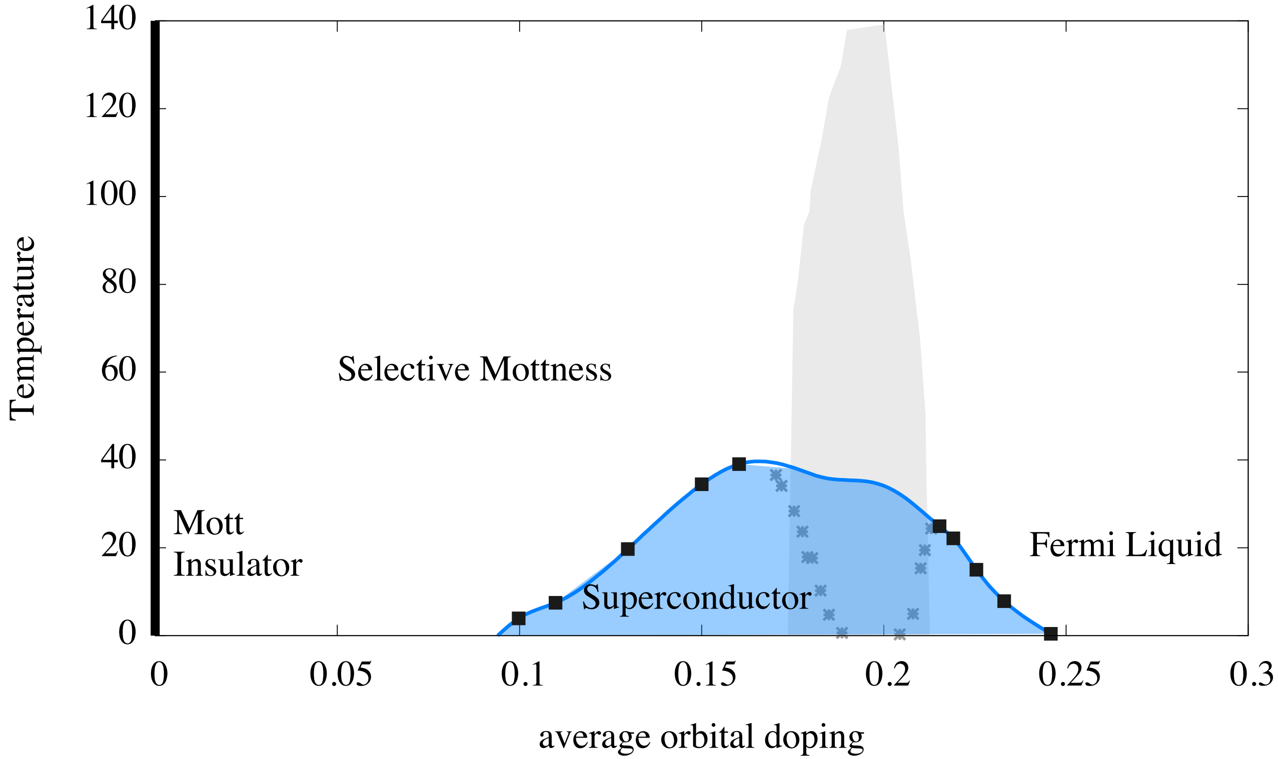


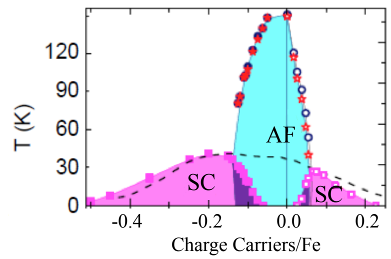


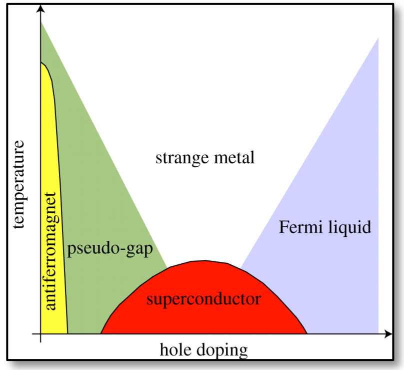


DCA calculation from: Gull et al.
Phys Rev. B 82, 155101 (2010)

Tentative common phase diagram for Cuprates and Iron-SC







When plotted against the average orbital doping the experimental phase diagram of iron-SC closely resembles the one for cuprates! (suppressing magnetism)

- a superconducting dome at 20% doping from a Mott insulator
- a phase with selective Mottness in between the two
- a good Fermi-liquid at higher dopings

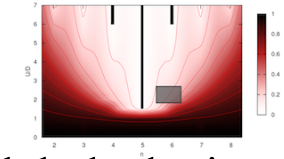
Is then **selective Mottness important for superconductivity?**

A. Hackl and M. Vojta, New J. Phys.11 (2009)
Kou et al. Europhys. Lett. 88 (2009)
Yin W-G et al. Phys. Rev. Lett. 105 (2010)
You Y-Z et al., Phys. Rev. Lett.107 (2011)

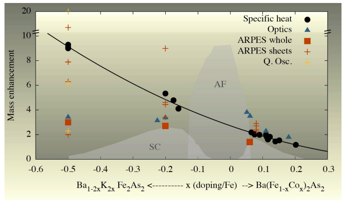
Conclusions:

Luca de' Medici

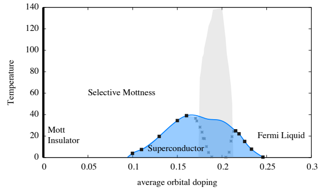
Iron superconductors: Hund's coupling J has a key-role in tuning correlations



- Overall coherence reduced. Mott transition at n=6 pushed far.
- Phase diagram dominated by Mott transition at n=5 (half-filling).
- Filling of the conduction bands is a key variable: correlations increase with hole doping
- J acts as an "**orbital-decoupler**": suppresses inter-orbital charge correlations and favors **orbital selective Mottness**



i.e. coexistence of **strongly *and* weakly correlated** electrons in most of the phase diagram (KFe2As2 heavy fermion)



Analogy with the pseudogap phase in the cuprates

A common phase diagram?

LdM, G. Giovannetti, M. Capone, PRL 112, 177001 (2014)

Perspective in book chapter:

LdM, "Weak *and* strong correlations in Iron superconductors", in "**Iron-based superconductivity**", Springer series in materials science, vol 211, pp409-441

LdM, S.R. Hassan, M. Capone, X. Dai, PRL **102**, 126401 (2009)
LdM, S.R. Hassan, M. Capone, JSC **22**, 535 (2009)
LdM, PRB **83**, 205112 (2011)
A. Georges, LdM, J. Mravlje, Annual Reviews Cond. Mat. 4, 137 (2013)

Slave-spins can be a useful guidance for heavier computational methods