Luca de' Medici

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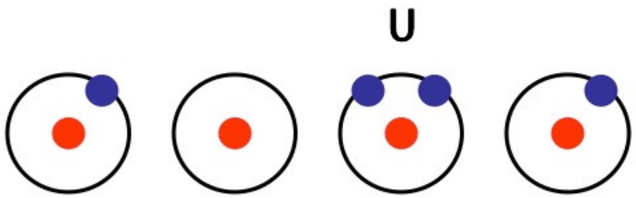
Orbital-selective Mott transitions and their relevance to Iron superconductors

Collège de France, 16.05.2012

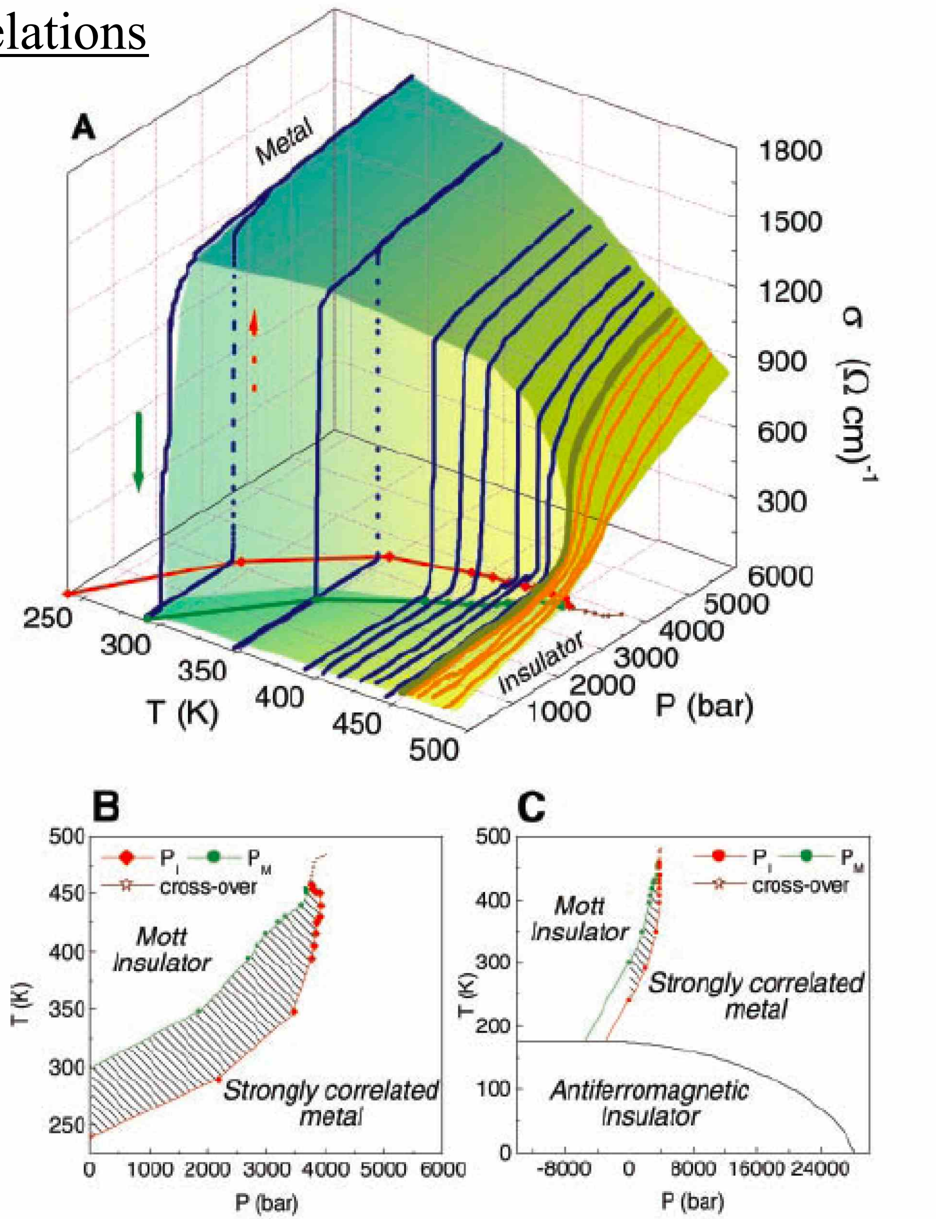
Localization of itinerant electrons by correlations



The proximity to a Mott insulator strongly affects the properties of a system:
- strong spectral weight transfer
- formation of local moments
- large mass enhancement/low coherence temperature

The Mott insulating state has an extensive entropy: instable to ordered phases at low T

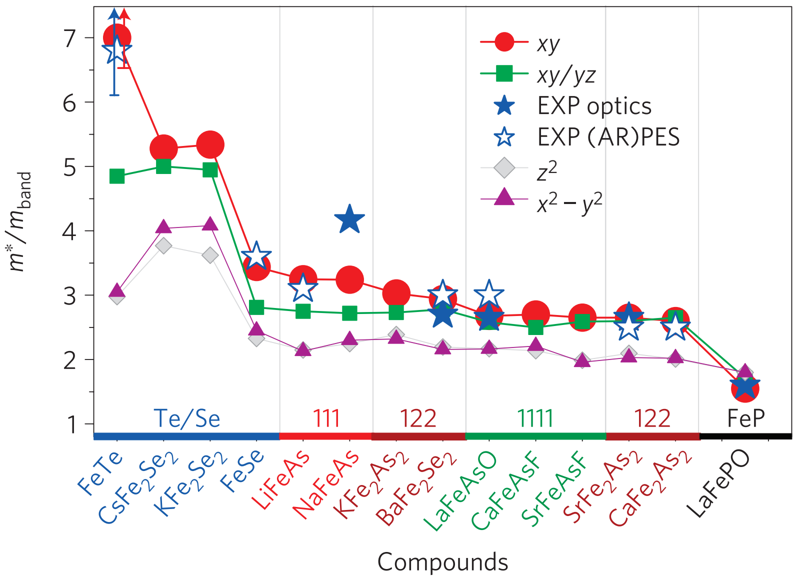
Cuprates have been modeled in terms of proximity to a Mott insulating state



Limelette et al. Science 302, 89 (2003)

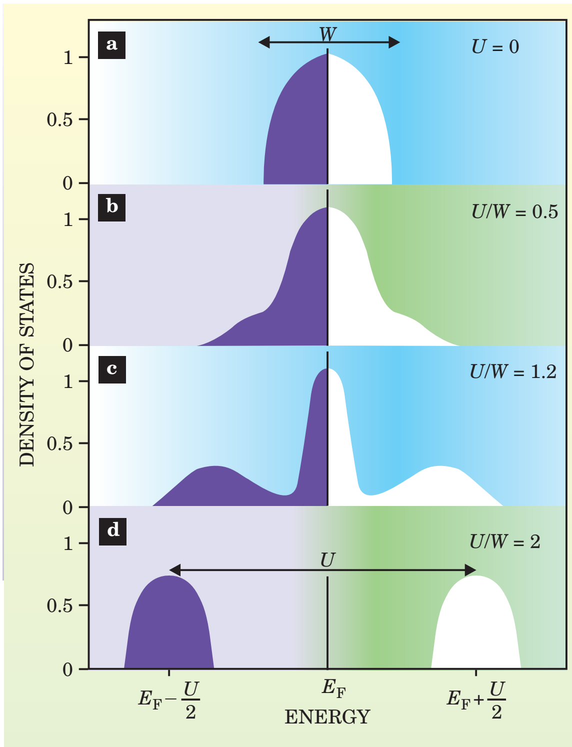
Iron superconductors show in general no Mott insulating state

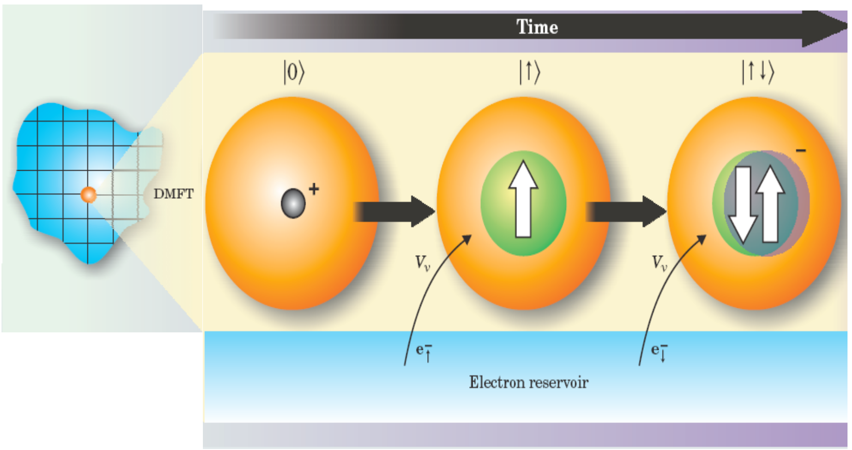
Yin et al., Nat Mat 10, 932 (2011)



Moderate to strong mass enhancements
Correlated physics

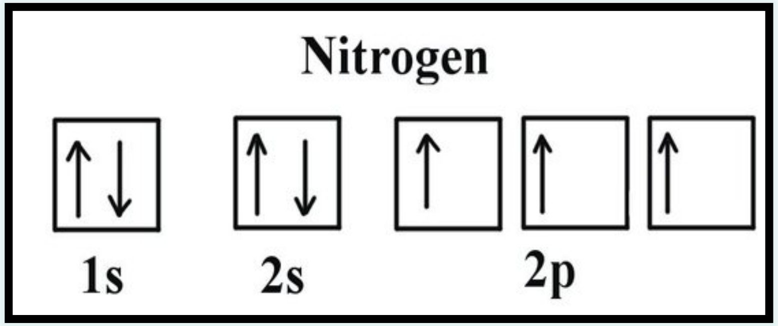
DFT + Dynamical mean-field theory

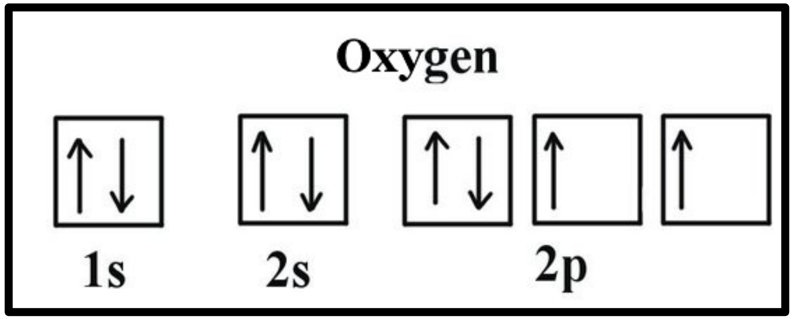




Hund's rules: atoms

Aufbau





<u>Hund's Rules</u>

In open shells:

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

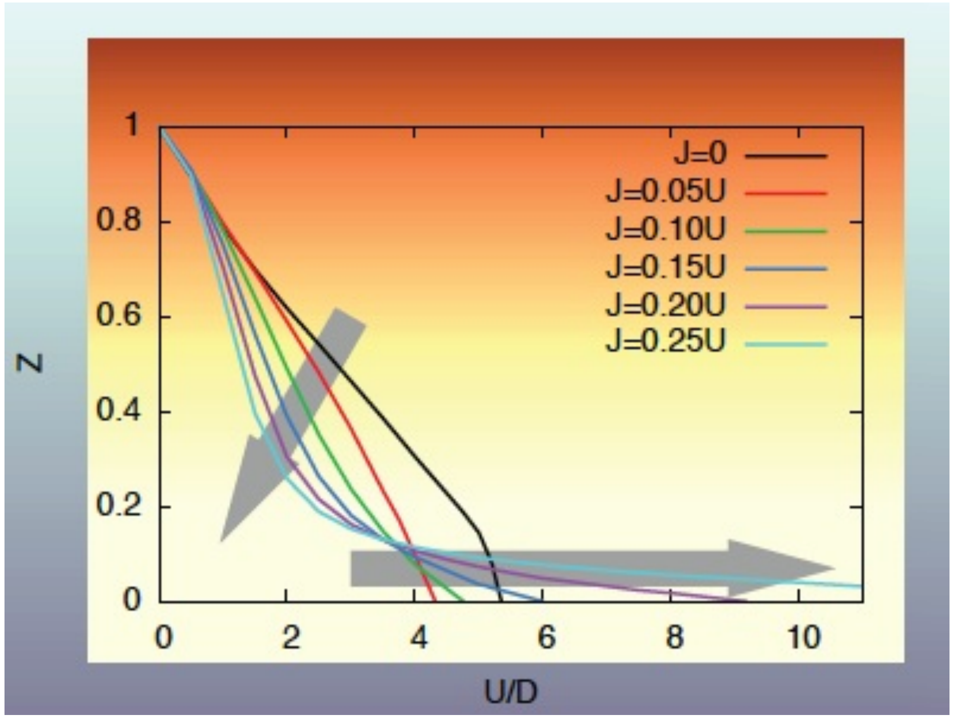
(3. Dependence on J=T+S, Spin-orbit effects)

$$H_{\text{int}} = (U - 3J)\frac{\hat{N}(\hat{N}-1)}{2} - 2J\vec{S}^2 - \frac{1}{2}J\vec{T}^2$$

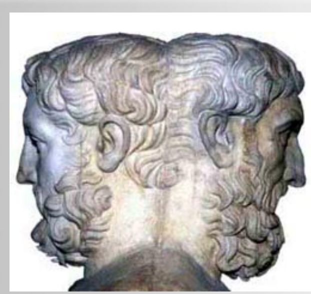
Multi band Hubbard model

J is 'Janus-faced' (has two contrasting effects):

- lowering of coherence Temp (away from single-filling)
- enhancement of the Mott gap (away from half-filling)

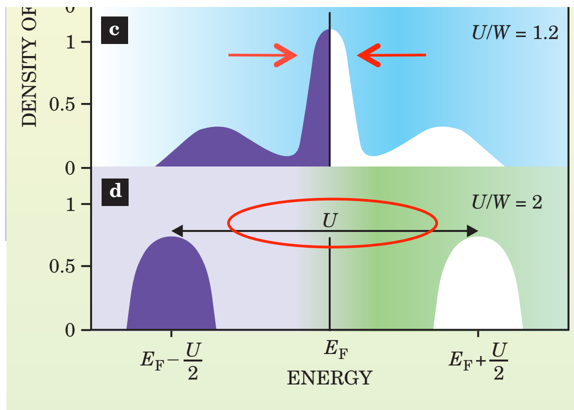


LdM, J. Mravlje, A. Georges, PRL **107**, 256401 (2011)



Janus Bifrons

In ancient Roman religion and mythology, Janus is the god of beginnings and transitions, then also of gates, doors, doorways, endings and time. Most often he is depicted as having two heads [...]

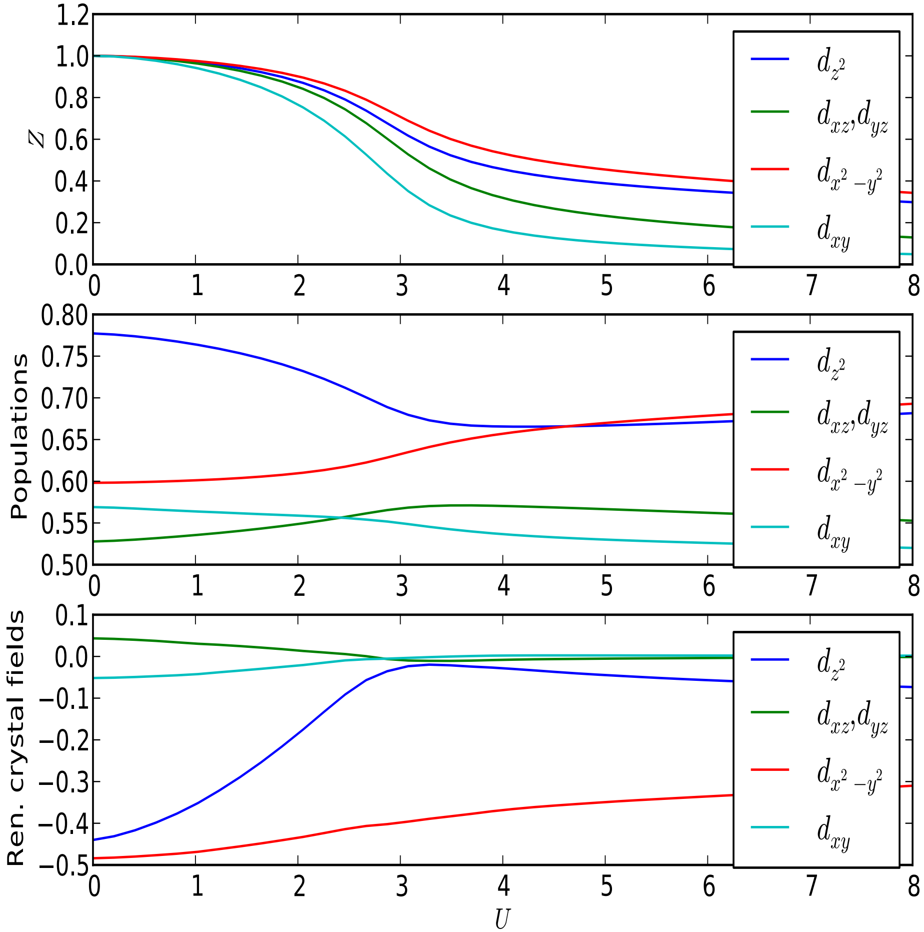


Strong correlations far from a Mott insulator!!

DFT+ 'cheap' mean fields

N. Lanatà, H. Strand, G. Giovannetti, LdM and M. Capone (unpublished)

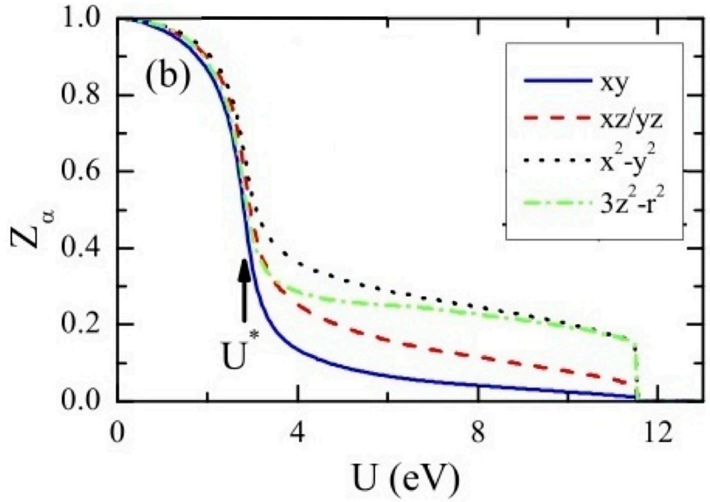
FeSe, J/U=0.224



LDA+Gutzwiller

R. Yu and Q. Si, ArXiv:1202.6115

LaFeAsO, J/U=0.25



LDA+Slave Spins

Slave-spins:
LdM, A. Georges and S. Biermann, PRB 72, 205124 (2005)
S. R. Hassan and LdM, PRB 81, 35106 (2010)

Orbital selective physics

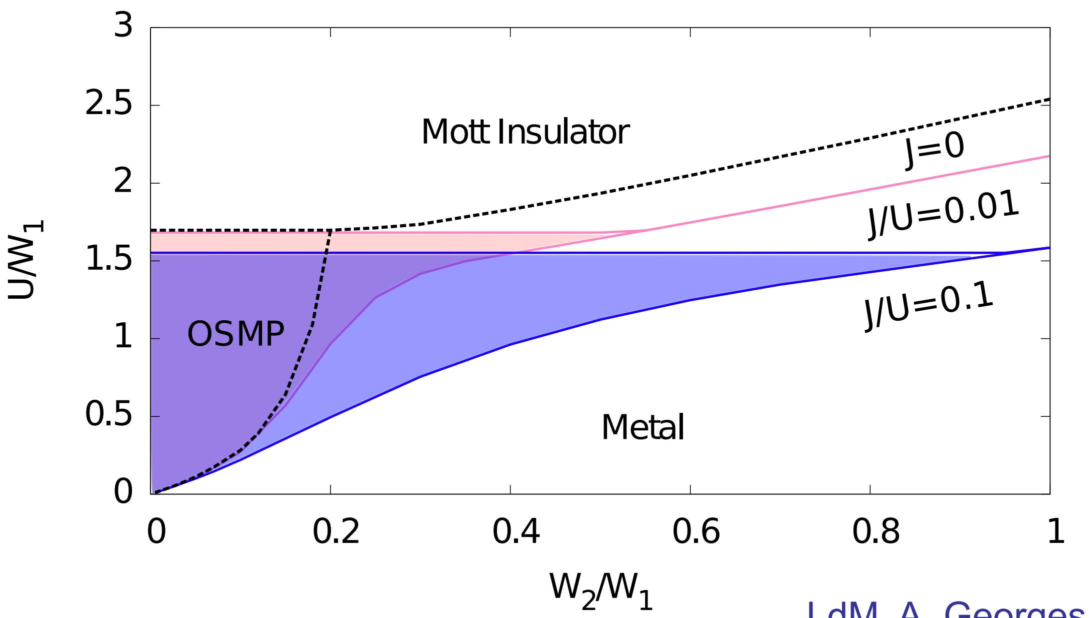
Orbital-selective Mott transition (OSMT)

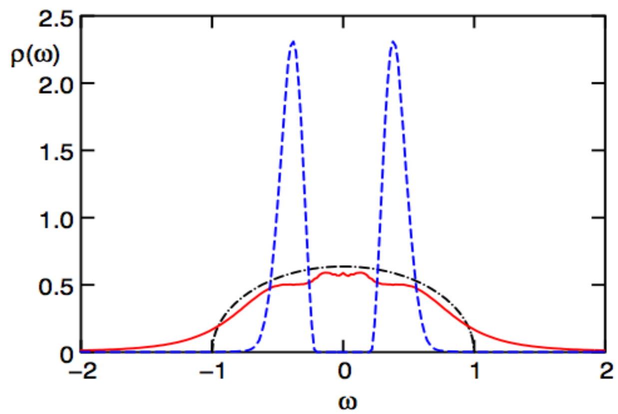
- Coexisting itinerant and localized conduction electrons
- Metallic resistivity and free-moment magnetic response
- non Fermi-liquid physics of the intinerant electrons

Possibly relevant for:
$Ca_{2-x}Sr_xRuO_4$, $BaVS_3$, LiV_2O_4, α-Fe, Fe-Superconductors, …

Anisimov et al., Eur. Phys. J. B 25, 191 (2002)
Koga et al., Phys. Rev. Lett. 92, 216402 (2004)
For a review:
M. Vojta J. Low Temp. Phys. 161, 203 (2010)

Two-orbital Hubbard model with different bandwidths

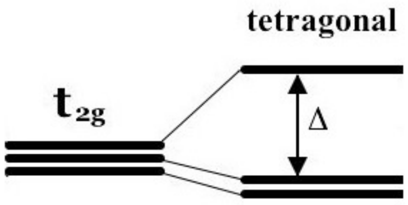


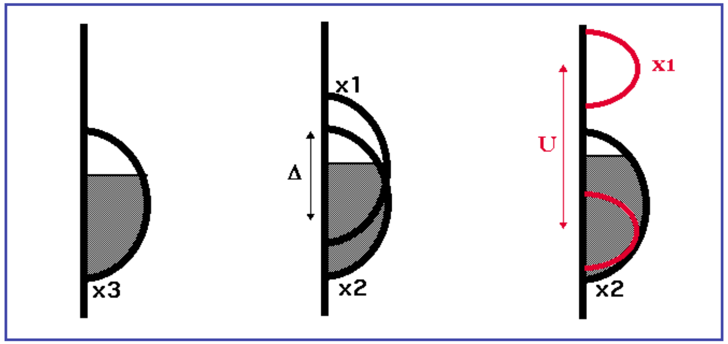


J favors the OSMT

LdM, A. Georges and S. Biermann, PRB 72, 205124 (2005)

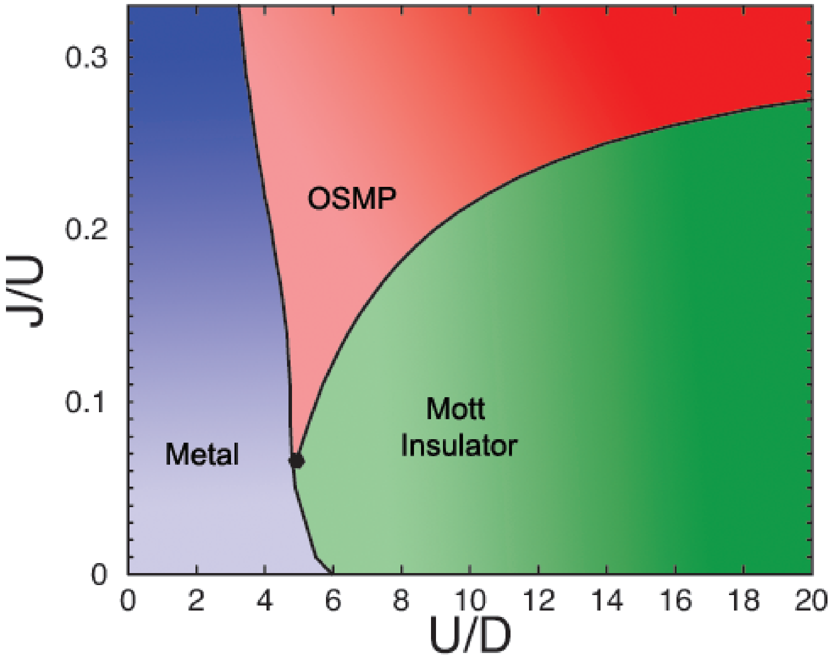
OSMT in systems with the same bandwidth





3 bands of the same width

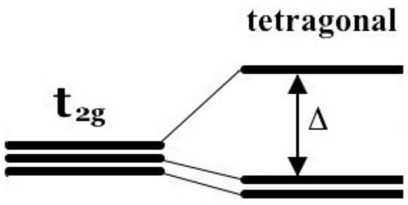
Crystal-field (one band up)
+ Hund's coupling

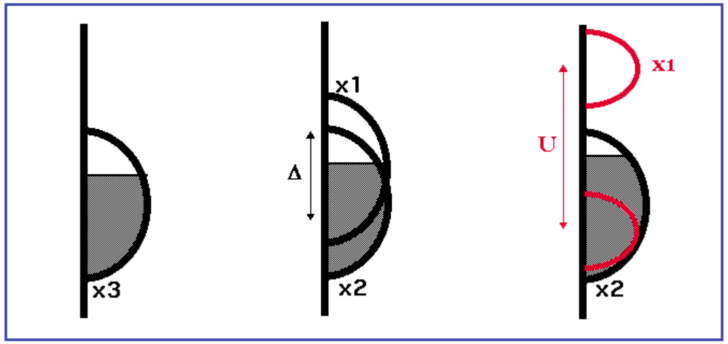


OSMT region widens with J

LdM, S.R. Hassan, M. Capone, X. Dai, **PRL**102, 126401 (2009)

OSMT in systems with the same bandwidth





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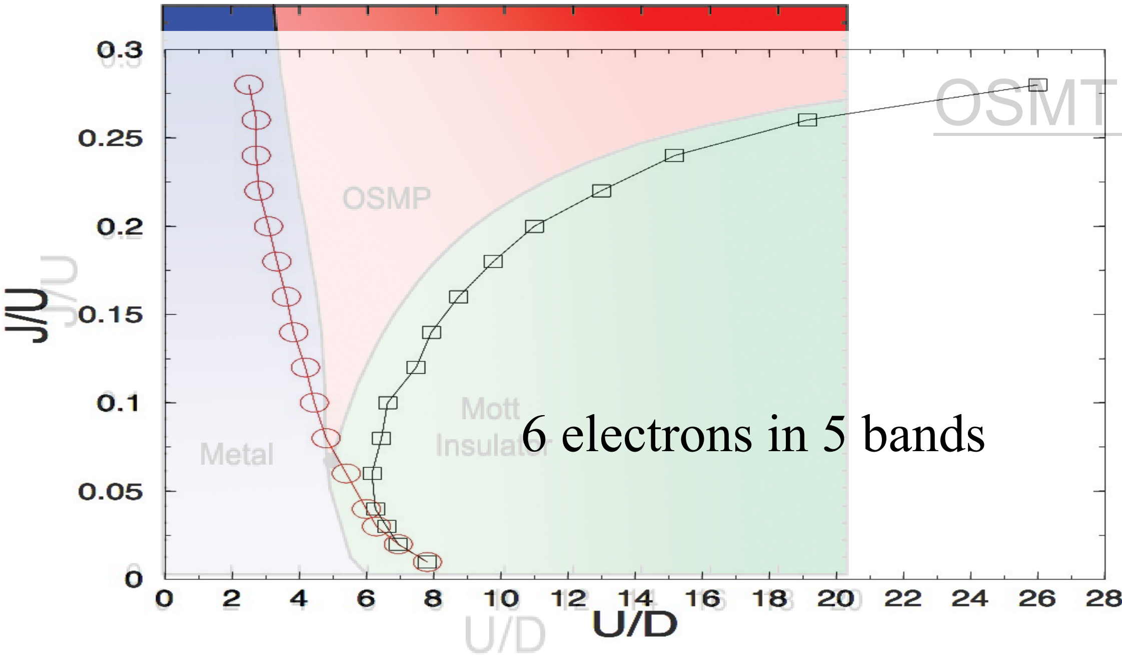


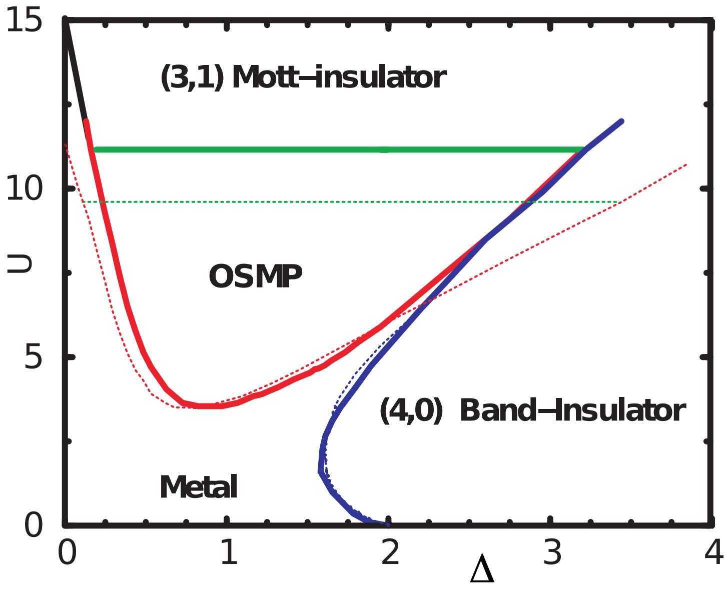
OSMT region widens with J

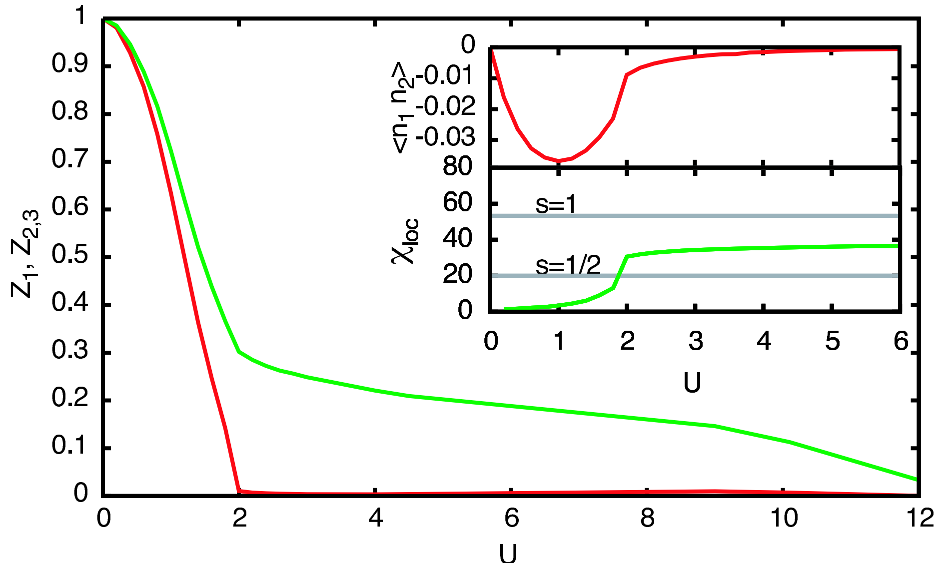
Is it the remaining degeneracy, which plays the role of a larger bandwidth?

LdM, S.R. Hassan, M. Capone, X. Dai, **PRL**102, 126401 (2009)

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

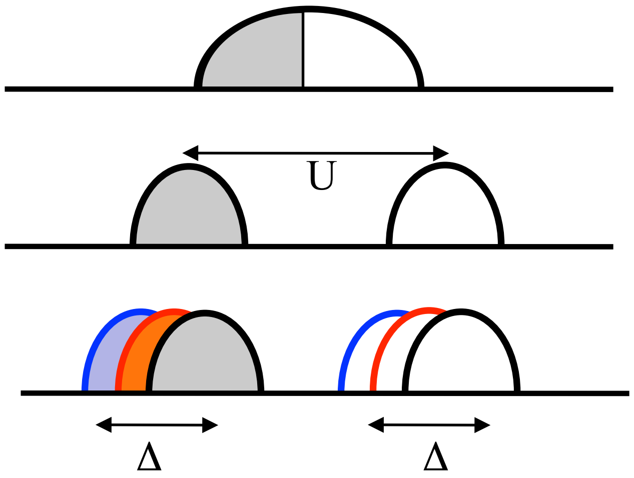
OSMT in a 3-band model with equal bandwidths and a symmetric crystal field splitting





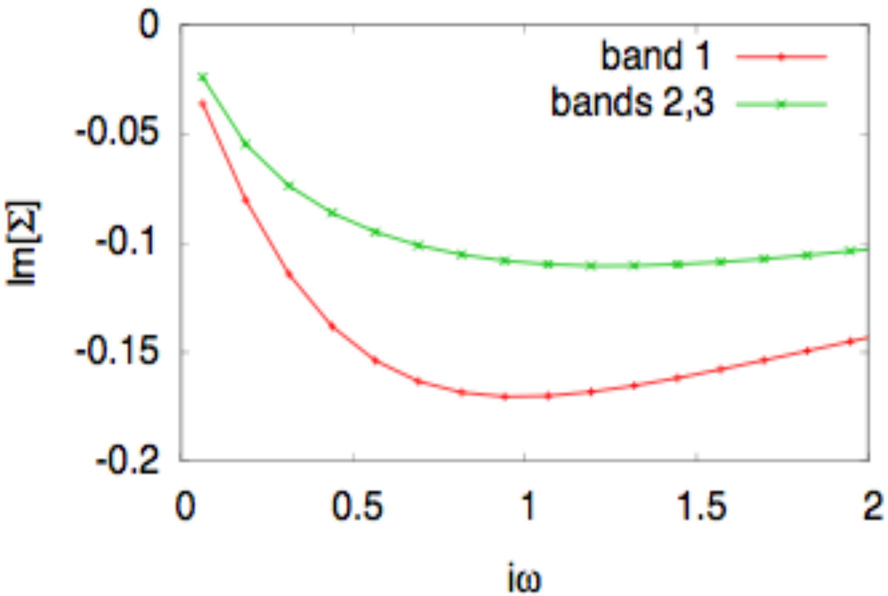
Crucial: Hund's coupling suppresses the orbital fluctuations, rendering the orbitals independent from one-another

Hund's coupling acts as a **band-decoupler**

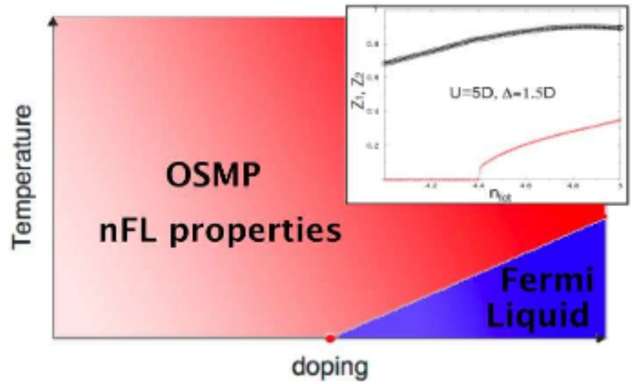


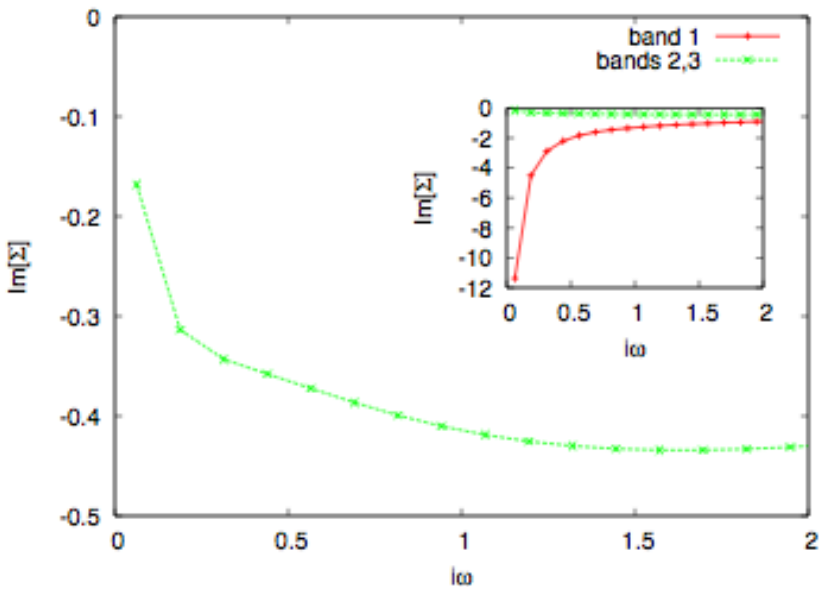
LdM, S.R. Hassan, M. Capone, X. Dai, **PRL**102, 126401 (2009)
LdM, Phys. Rev. B 83, 205112 (2011)
Werner and Millis, Phys. Rev. Lett.99, 126405 (2007)

Non Fermi-liquid properties of the OSMP

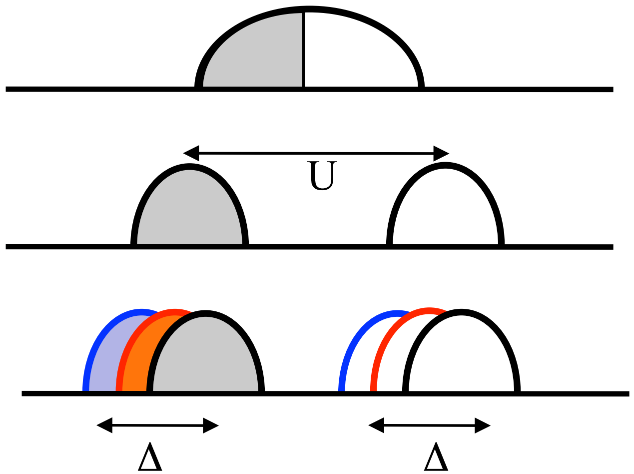


Metallic phase



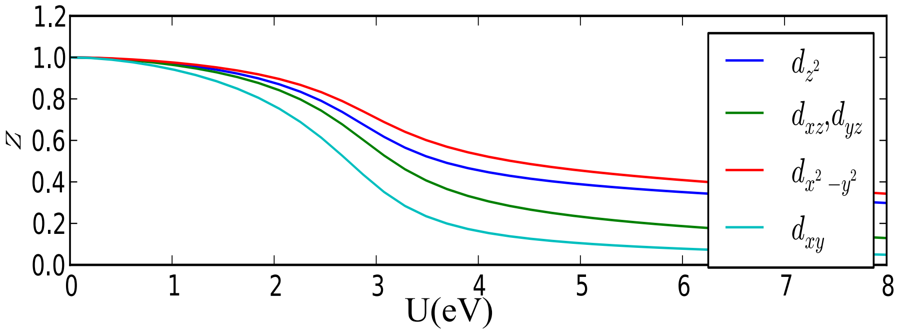


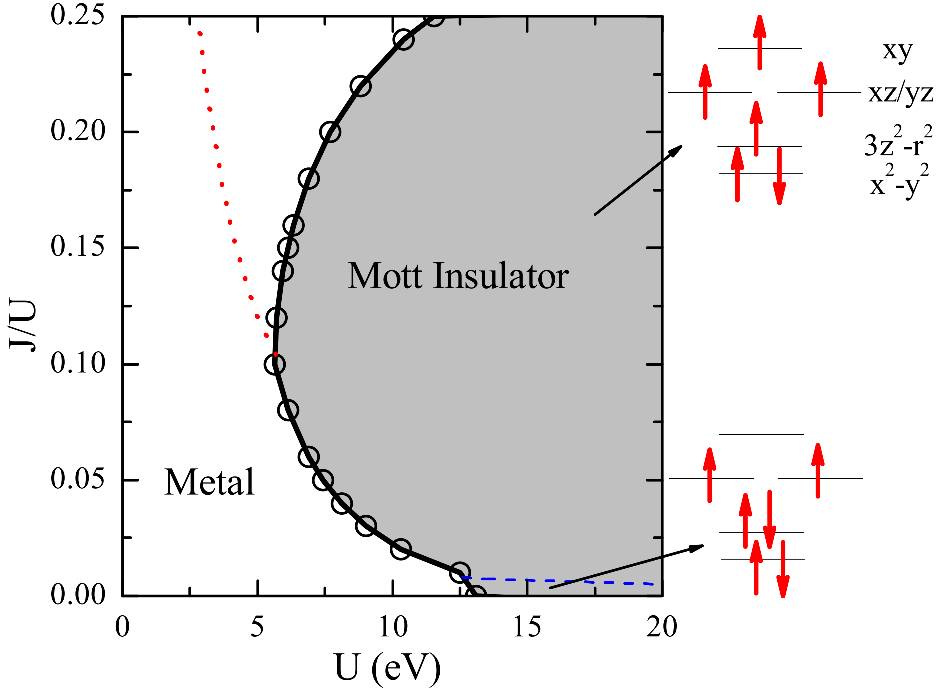
OSMP



Back to realistic calculations (ab-initio +MF)

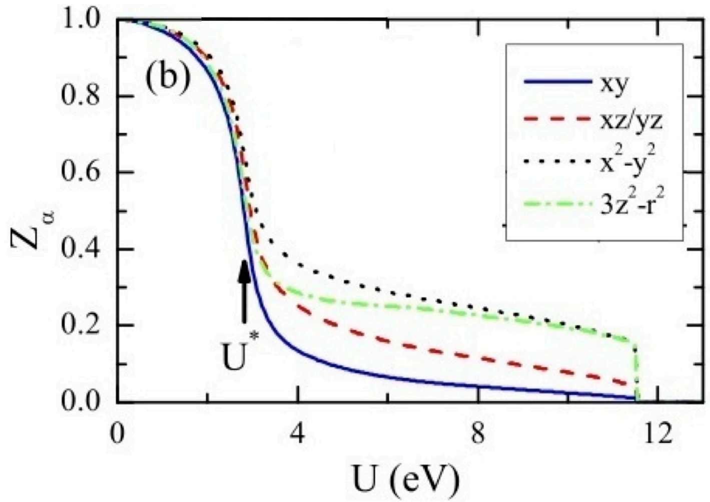
FeSe, J/U=0.224





N. Lanatà, H. Strand, G. Giovannetti, LdM and M. Capone (unpublished)

LaFeAsO, J/U=0.25



R. Yu and Q. Si, ArXiv:1202.6115

Proximity to an OSMT

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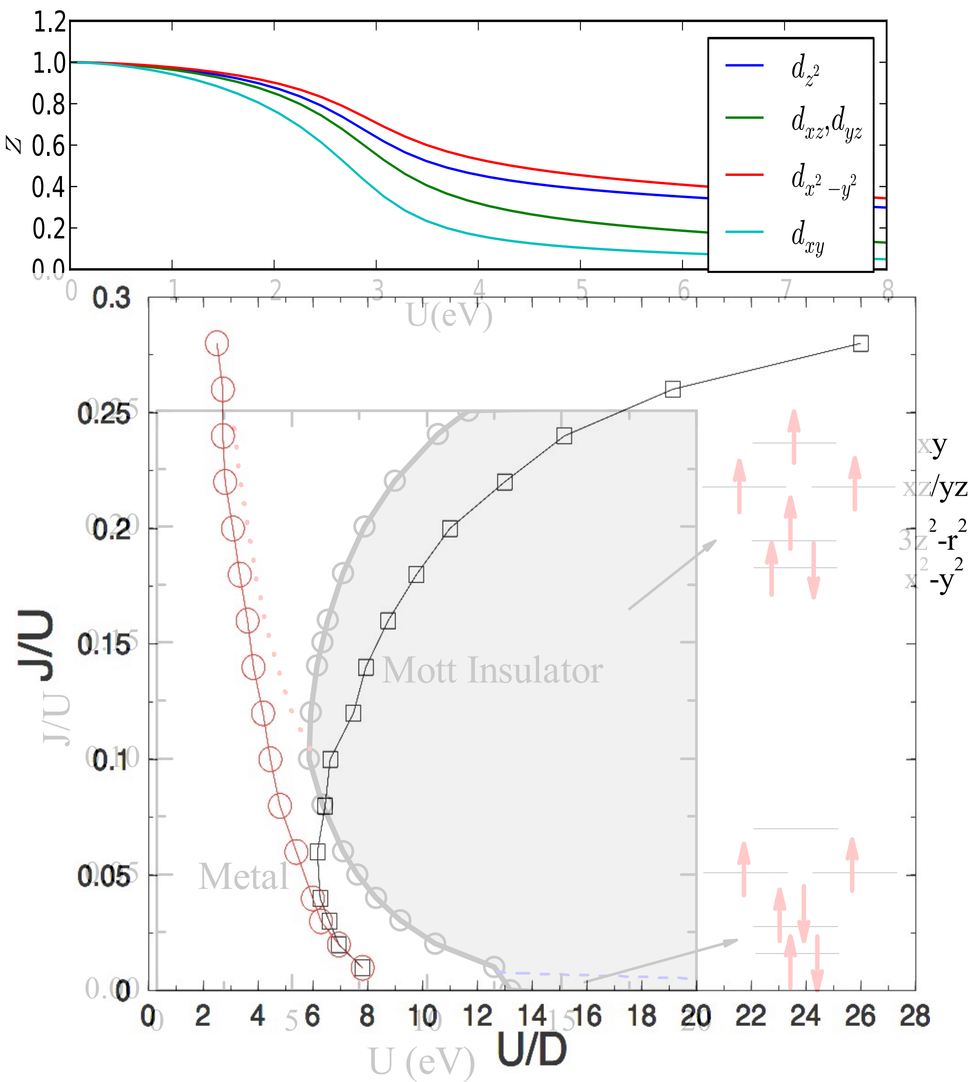

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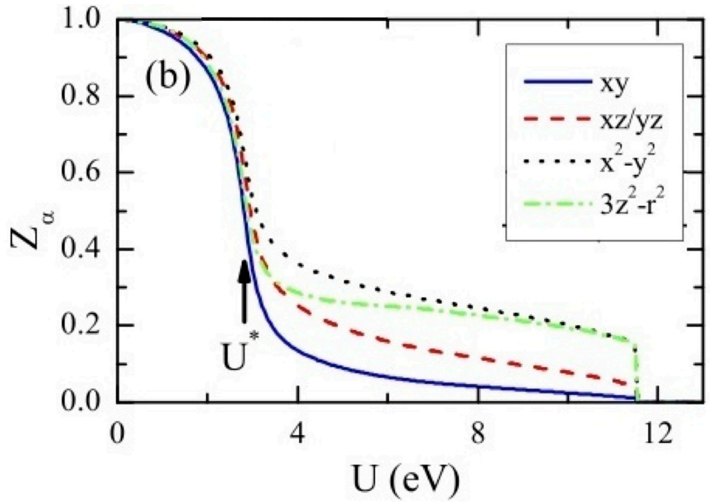

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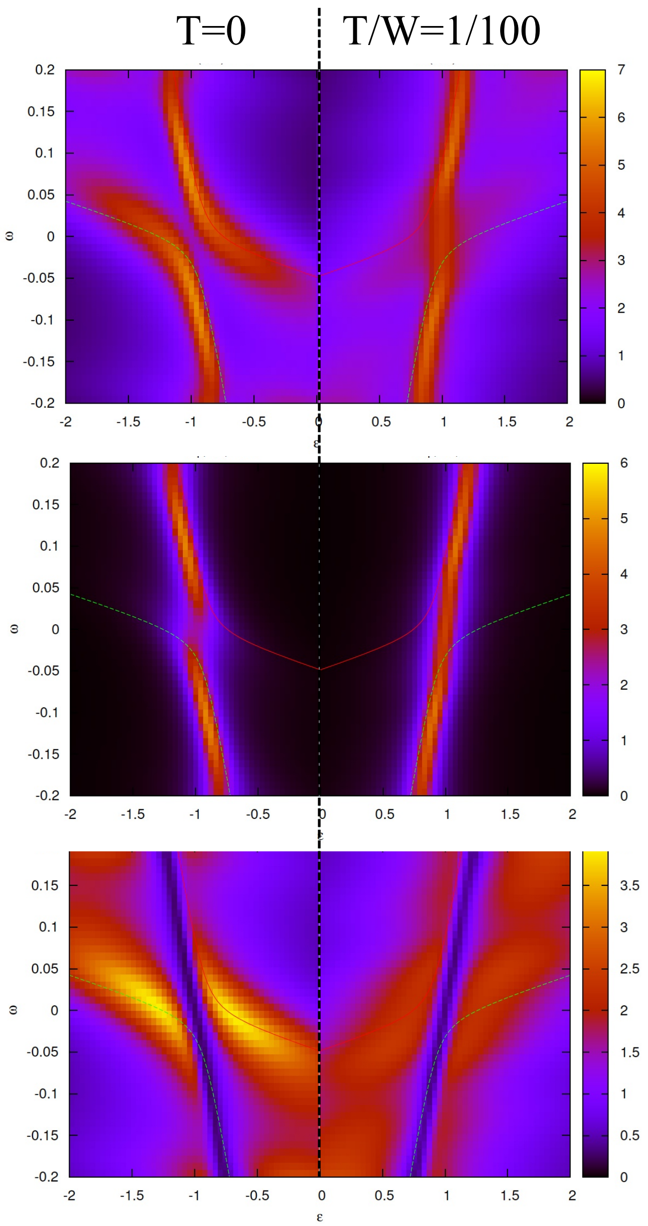
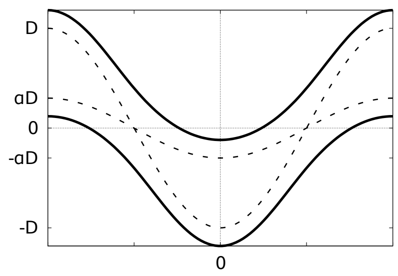
Proximity to an OSMT

Orbital selective coherence temperature

Luca de' Medici - LPS Orsay

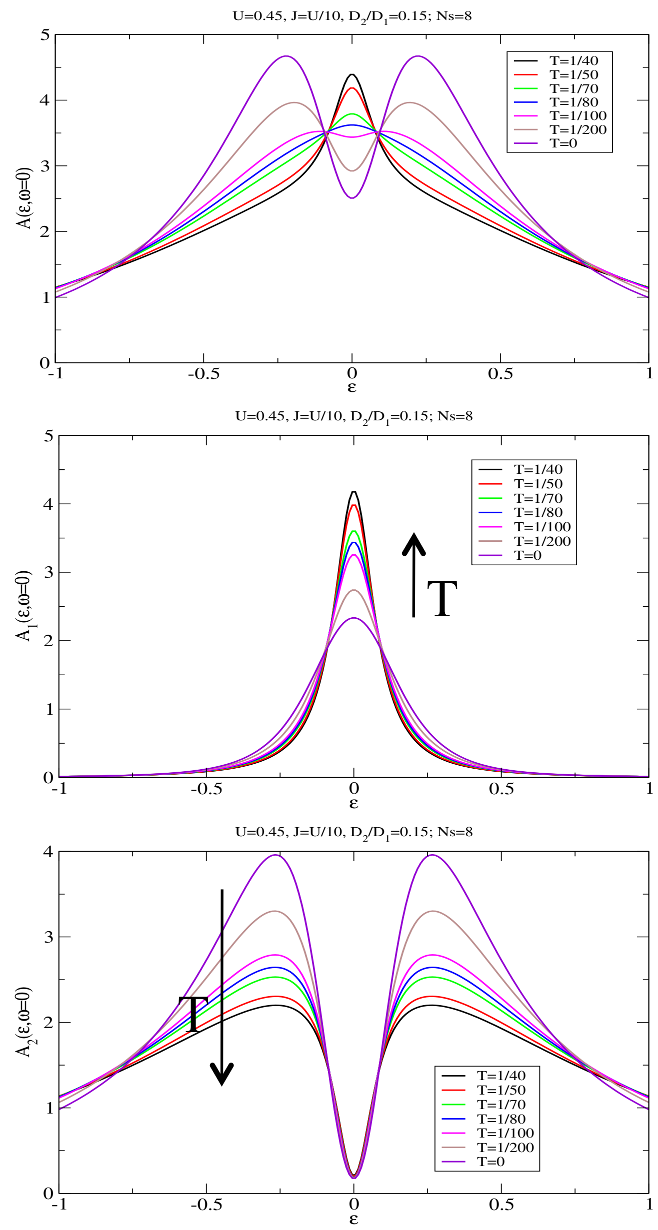




Total A(k,ω)
(ARPES)

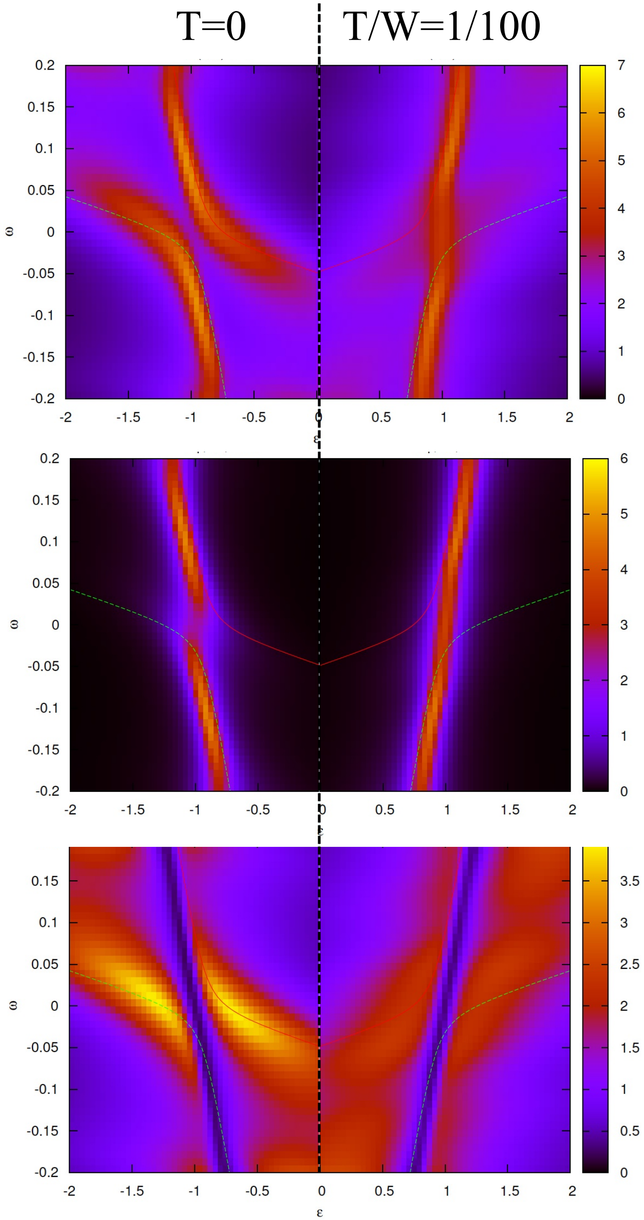
Orbital 1
(wide band)

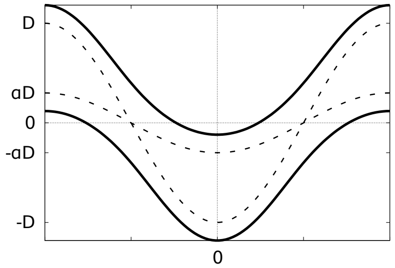
Orbital 2
(narrow band)



E. Winograd and LdM (unpublished)

Orbital selective coherence temperature





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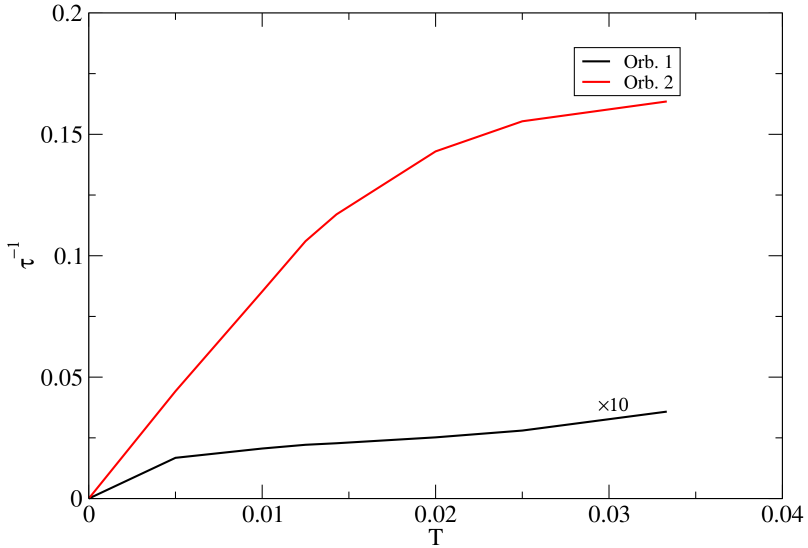
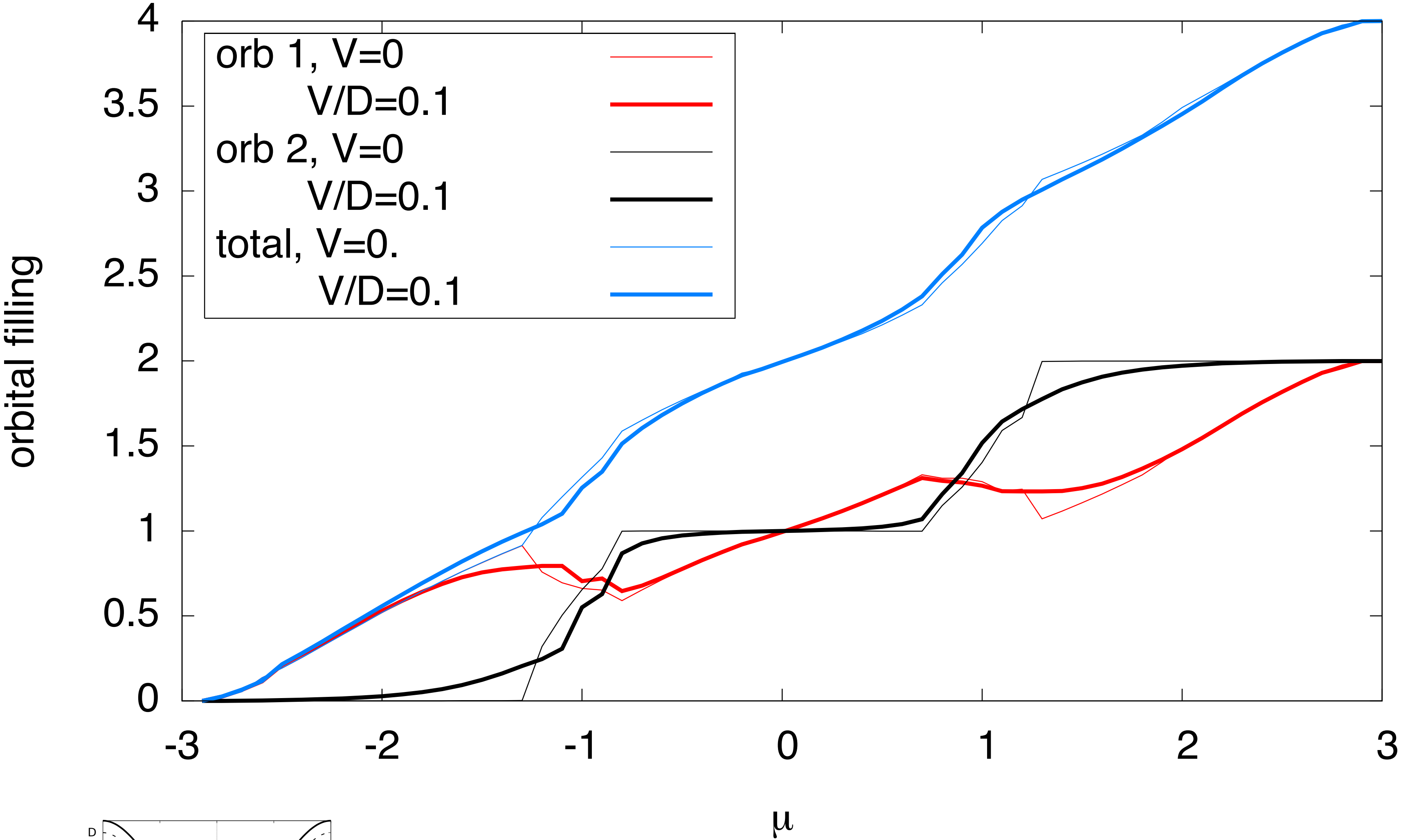
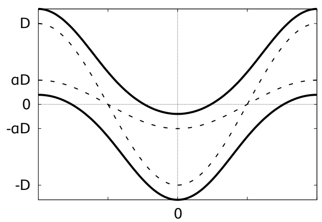


E. Winograd and LdM (unpublished)

OSMT + hybridization = pseudogap





large U (OSMP)

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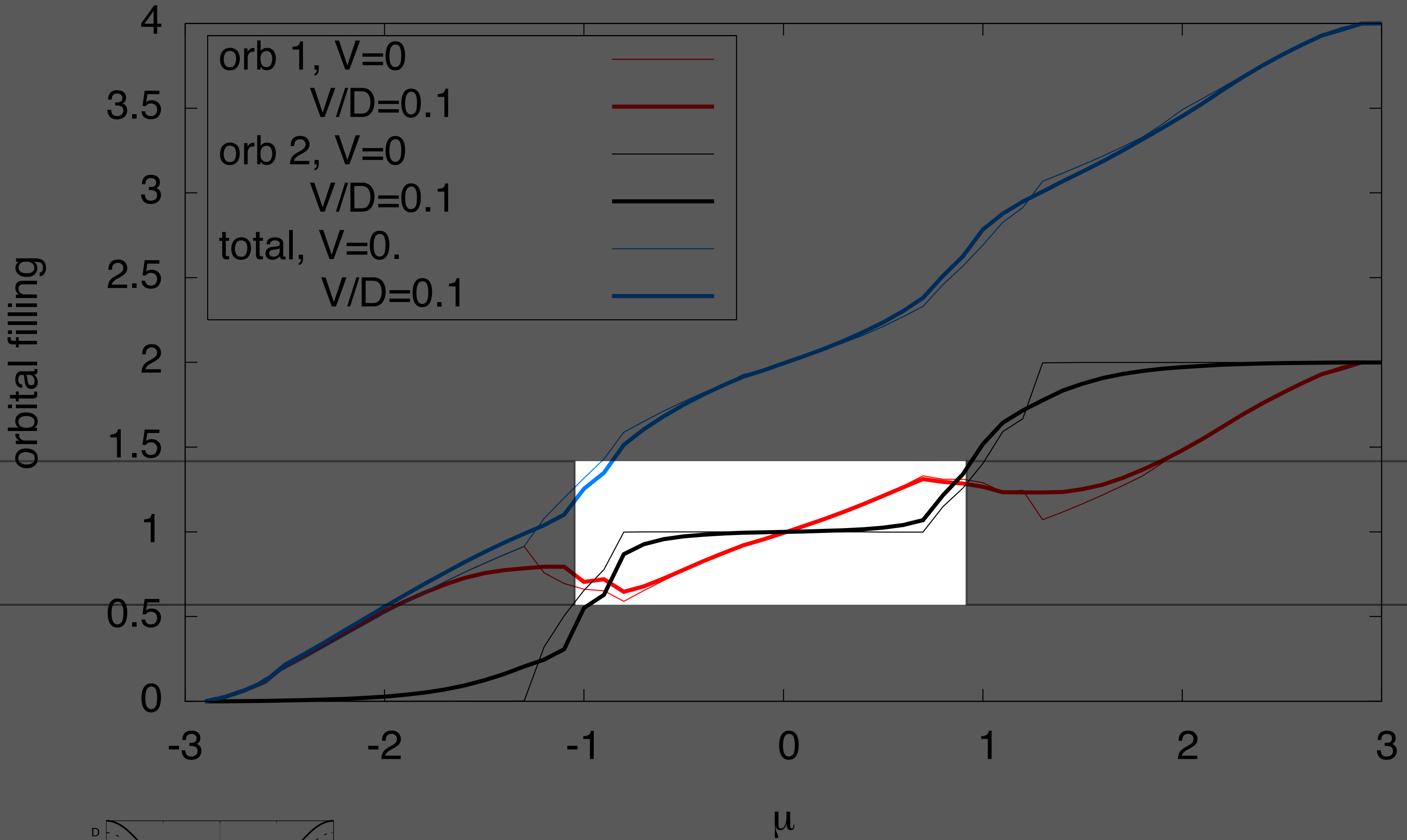
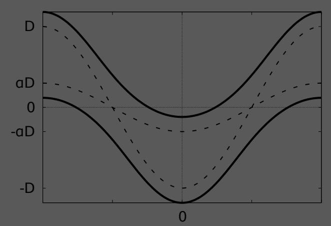
OSMT + hybridization = pseudogap



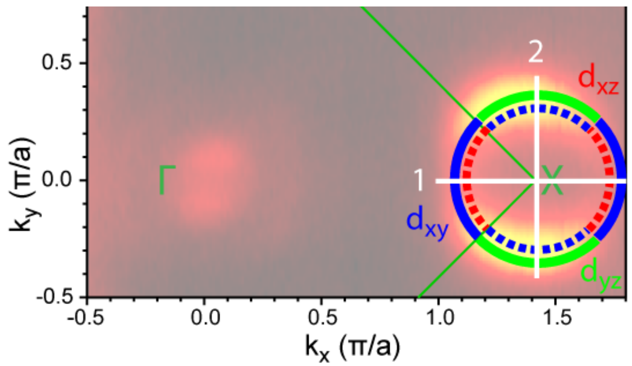


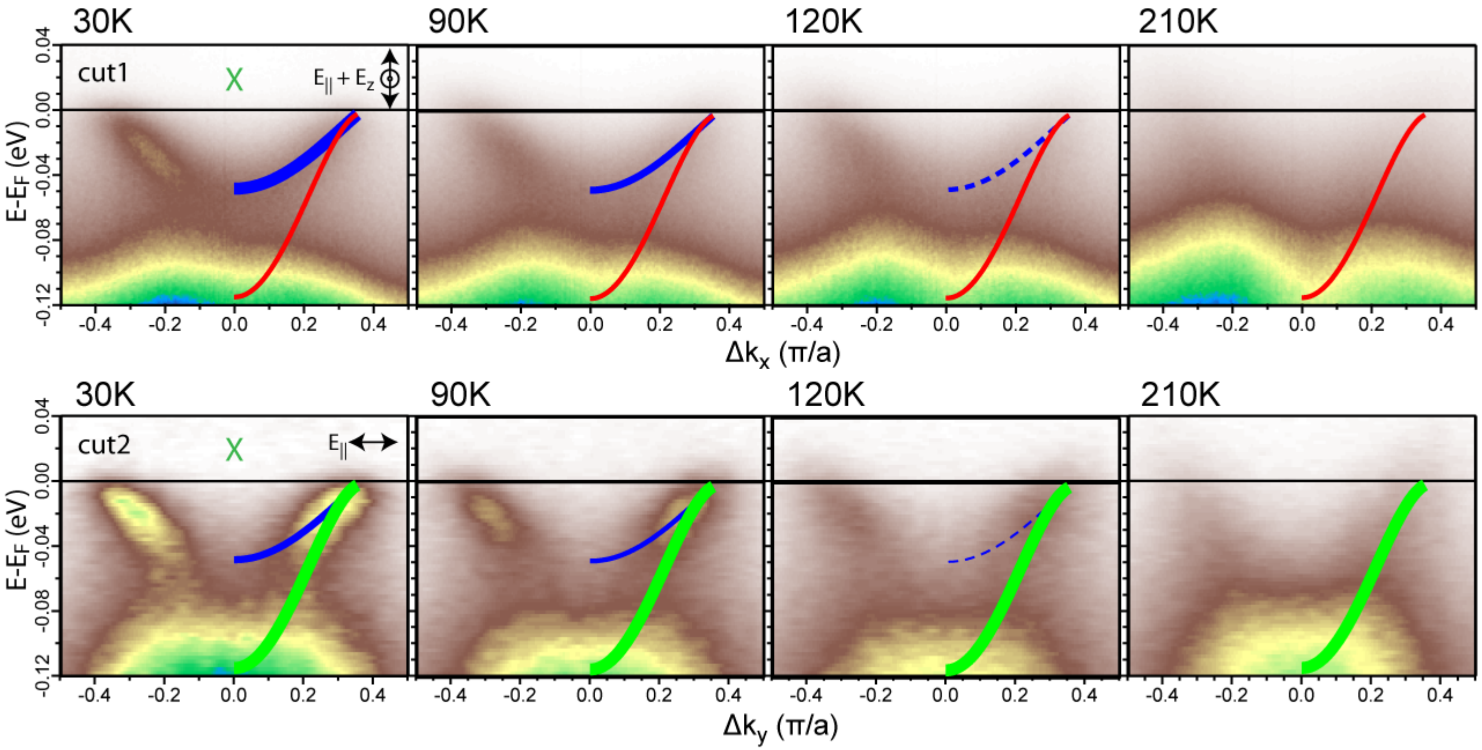
large U (OSMP)

E. Winograd and LdM (unpublished)

Angle-resolved Photoemission Data (Shen's group Stanford)

$A_xFe_{2-y}Se_2$ (A=K,Rb)





M. Yi et al. (unpublished 2012)

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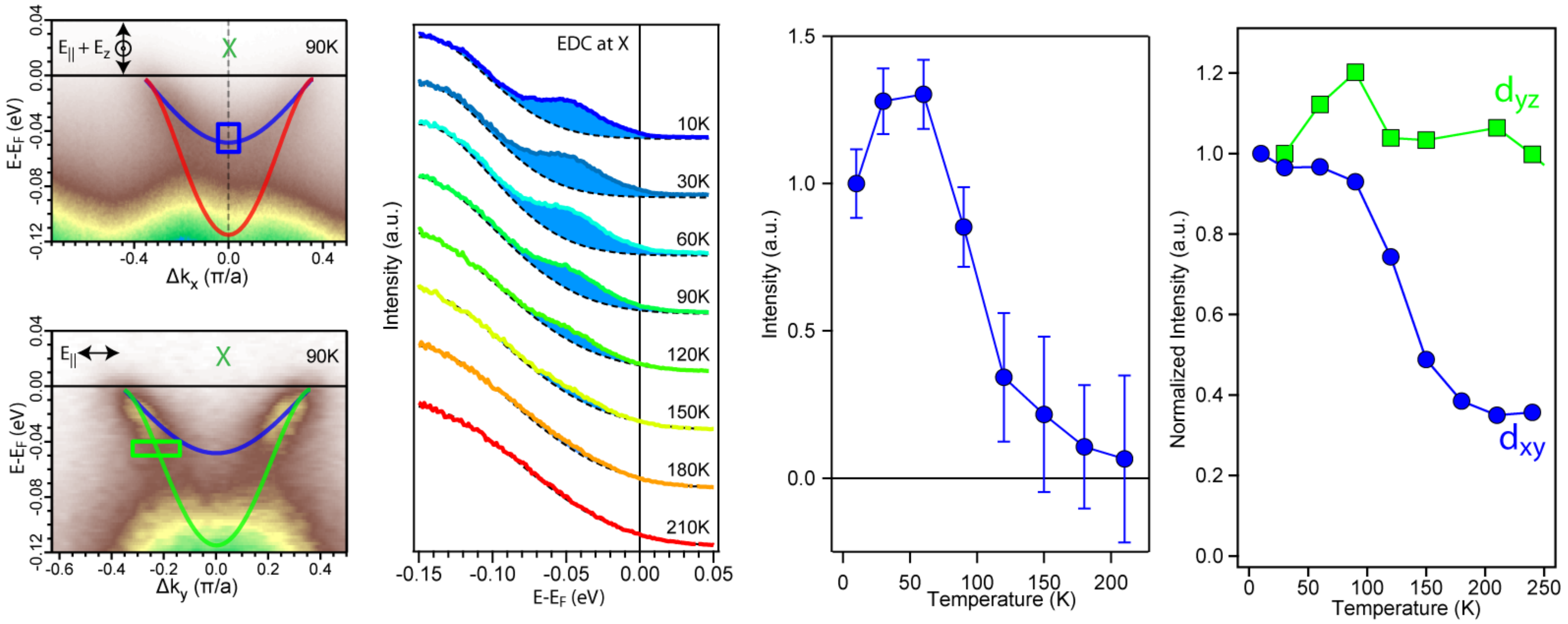


- d_{xy} spectral weight diminishes with temperature.
- d_{xz}/d_{yz} spectral weight does not diminish in the same temperature window.

temperature-induced Orbital-Selective Mott Transition

M. Yi et al. (unpublished 2012)

Other experimental evidences

- EPR-NMR, Arçon et al., Phys. Rev. B 82, 140508 (2010)

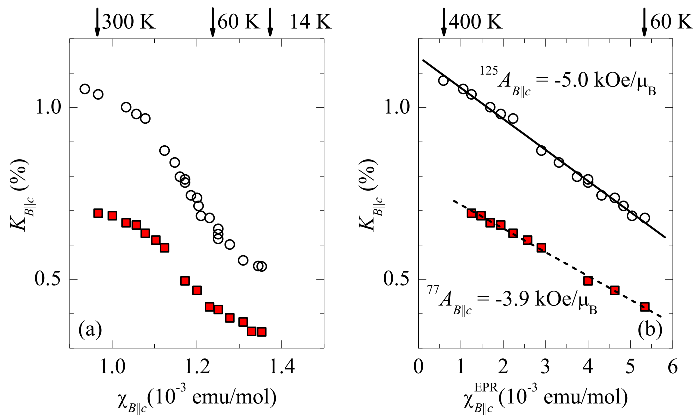


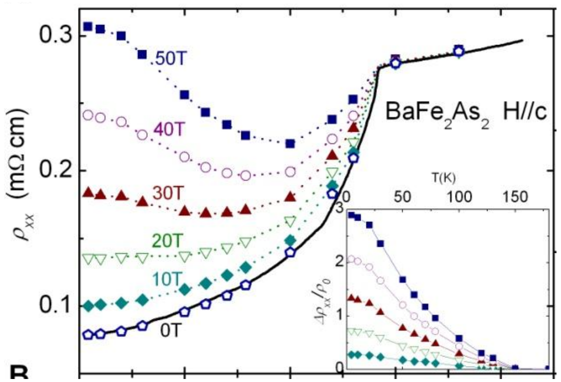
FIG. 3. ^{125}K and ^{77}K Knight shifts versus (a) bulk susceptibility, $\chi_{B||c}$ and (b) χ_{EPR} with temperature as an implicit parameter.

$FeSe_{0.42}Te_{0.58}$
Knight shift scales with local (EPR) and not bulk susceptibility

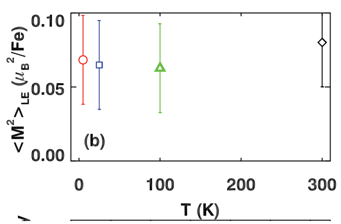
- Neutrons, Xu et al, Phys. Rev. B 84, 052506 (2011)

$FeSe_{0.65}Te_{0.35}$
Integrated magnetic spectral weigth up to 12meV shows little change with T

- Magnetoresistance , Yuan H-Q et al. ArXiv:1102.5476

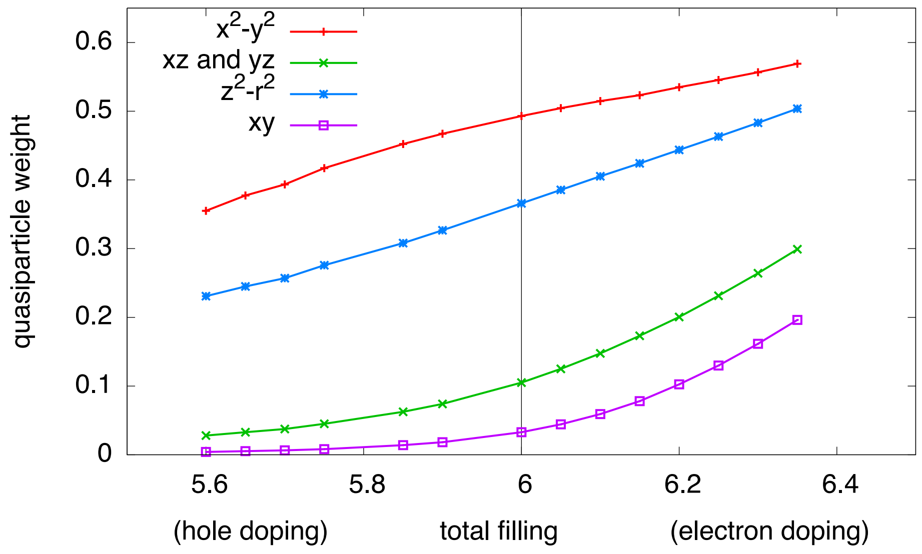


Magnetic transition insensitive to large magnetic fields: magnetism of local origin.
Also: two-component Hall resistance analysis

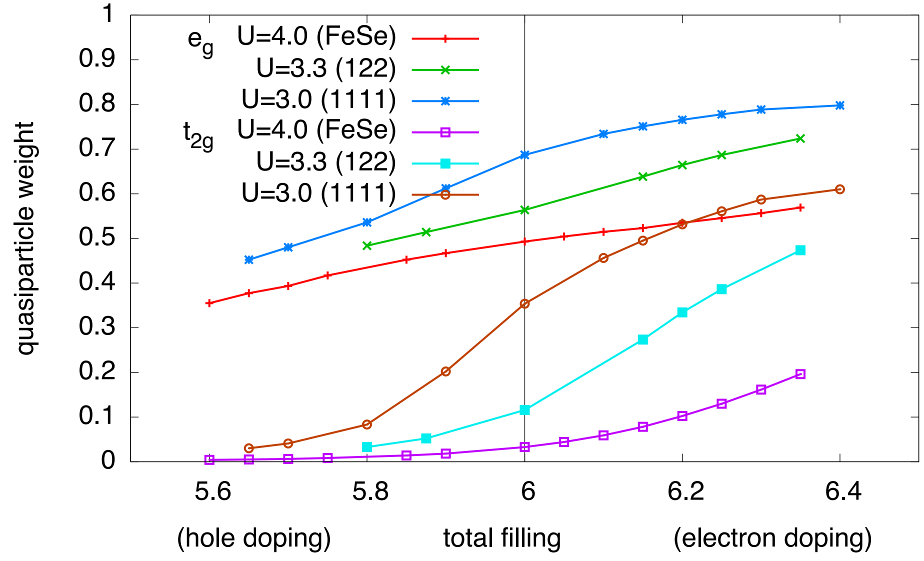


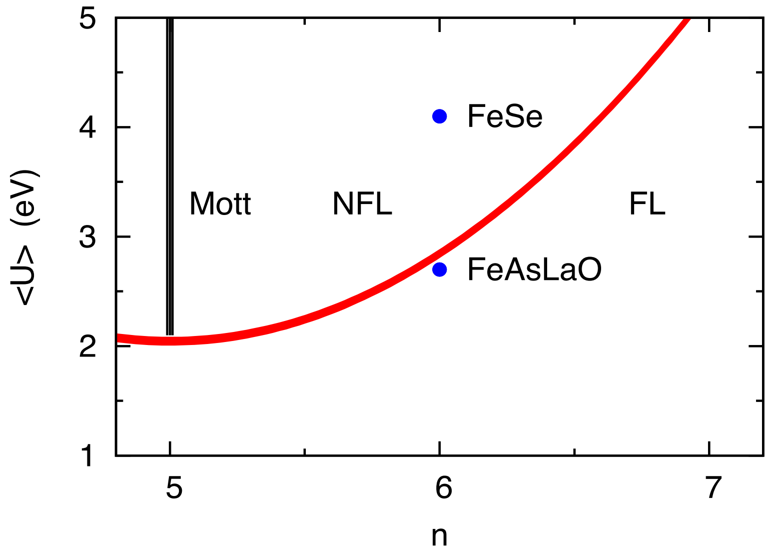
OSMT dependence on doping and U

FeSe

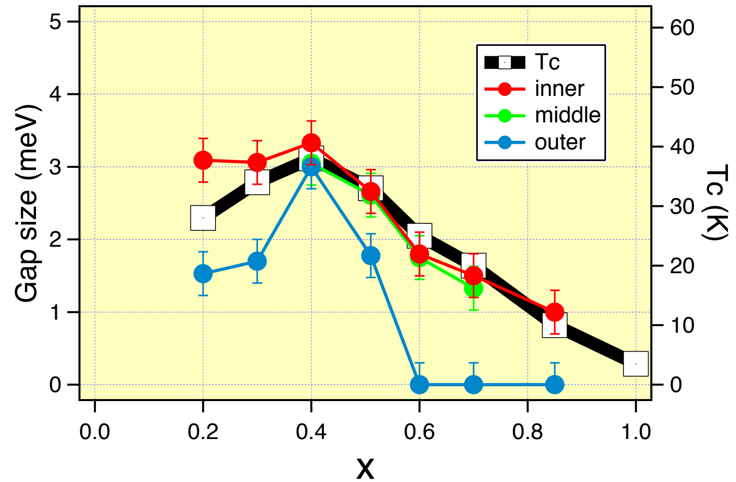


LdM, G. Giovannetti and M. Capone (unpublished)





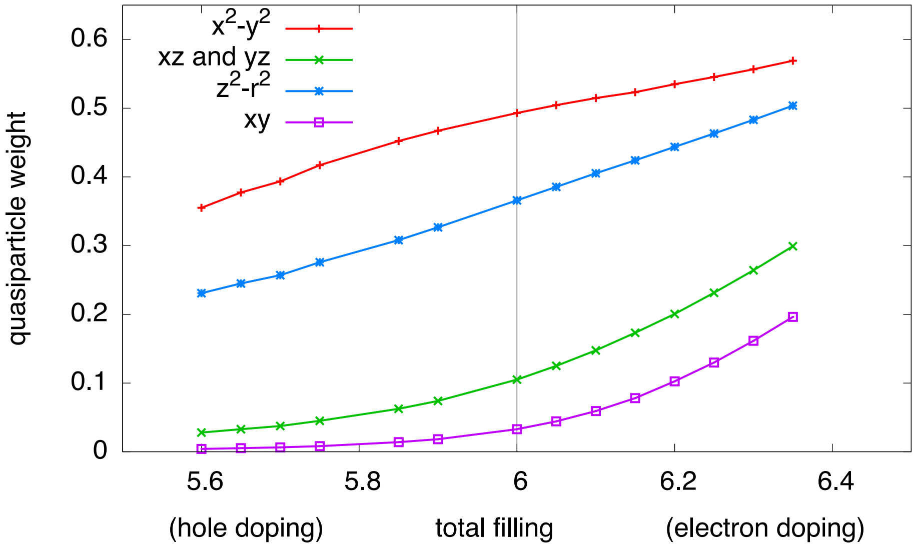
Liebsch and Ishida PRB 82,155106 (2010)



ARPES BaK-122: Malaeb et al. ArXiv:1204.0326

OSMT dependence on doping and U

FeSe



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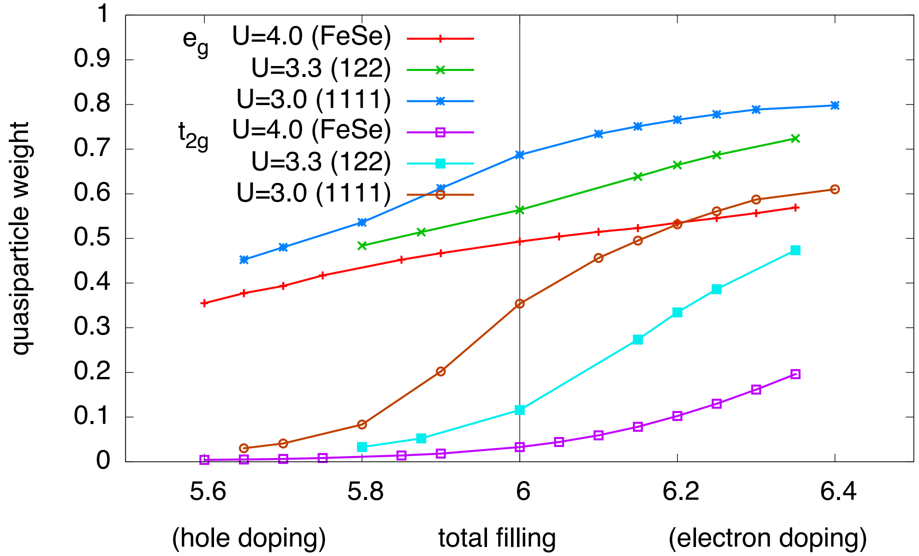
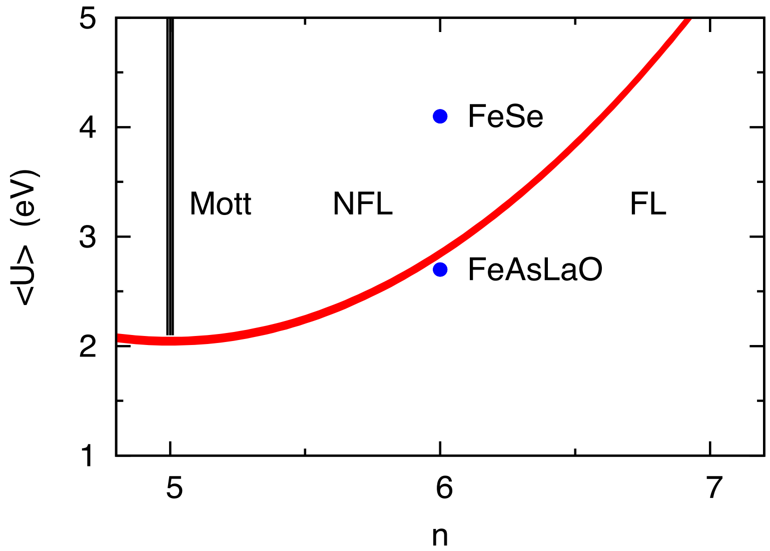
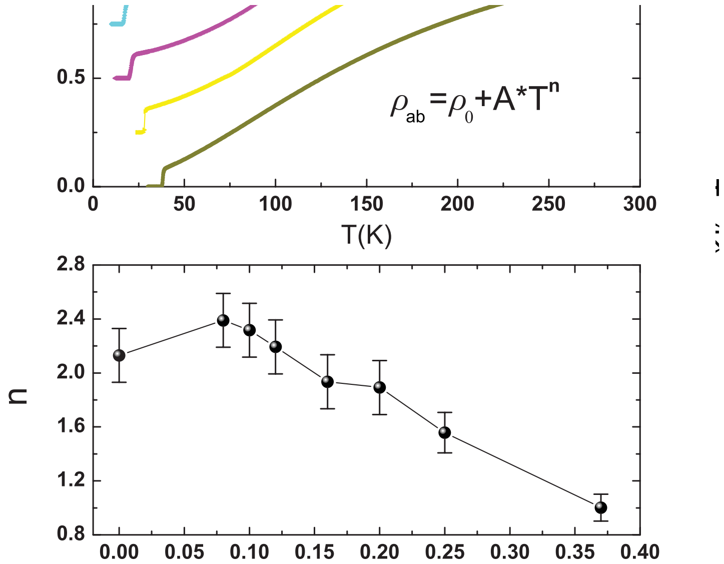


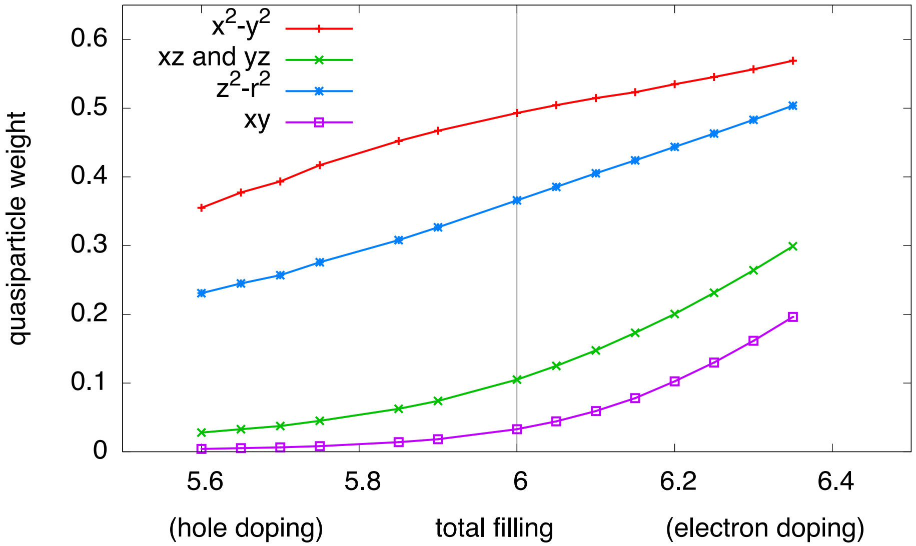


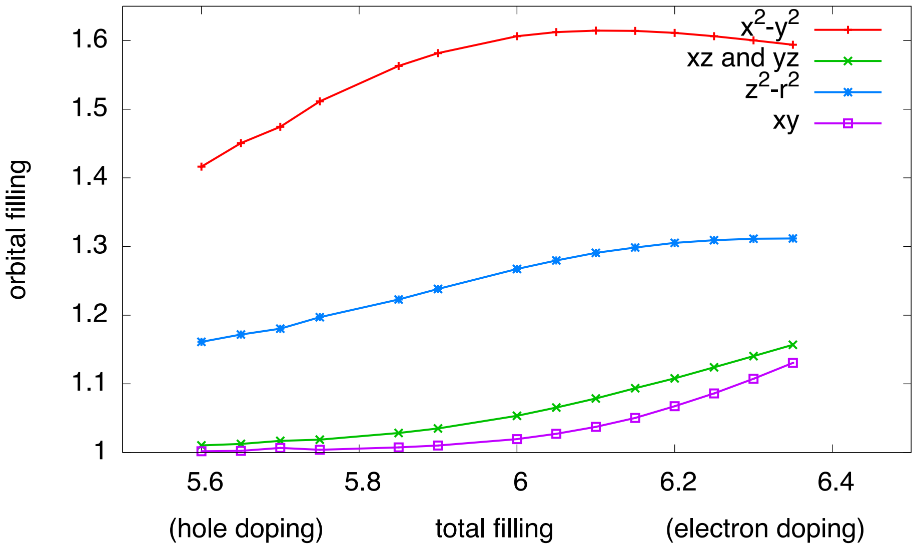
Liebsch and Ishida PRB 82,155106 (2010)



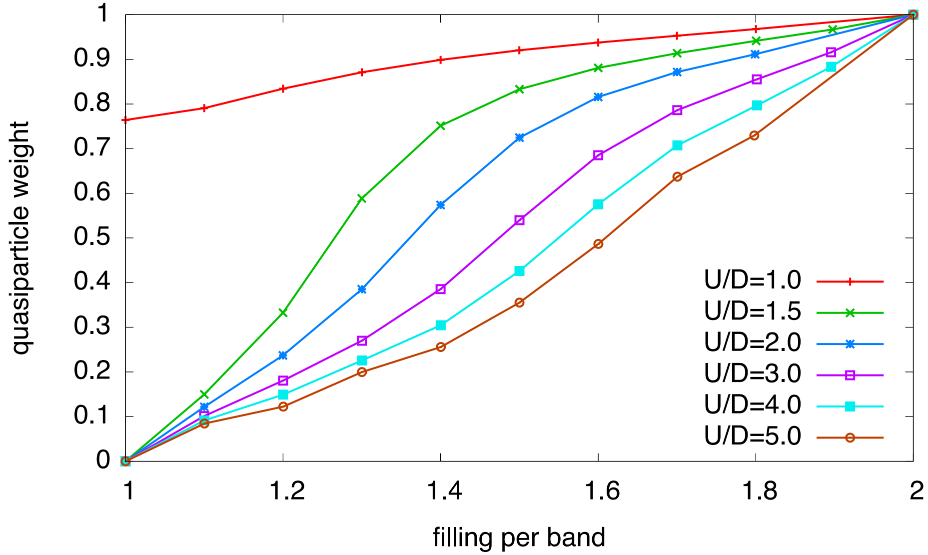
Resistivity BaK-122: Bing Shen et al. PRB 84, 184512 (2011)

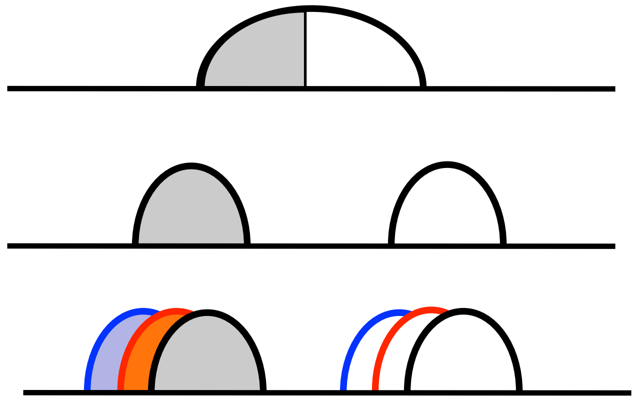
Decoupled band picture



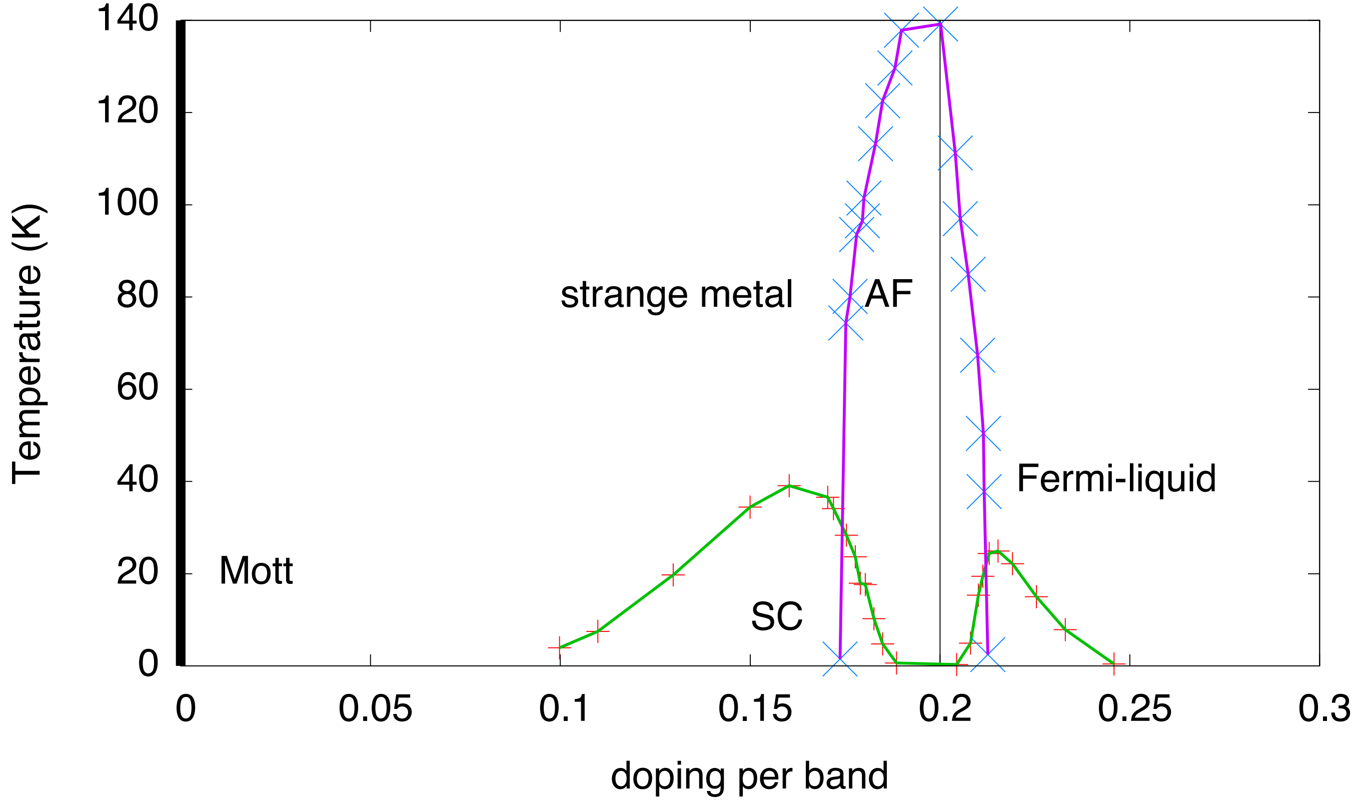


5 orbital degenerate Hubbard model



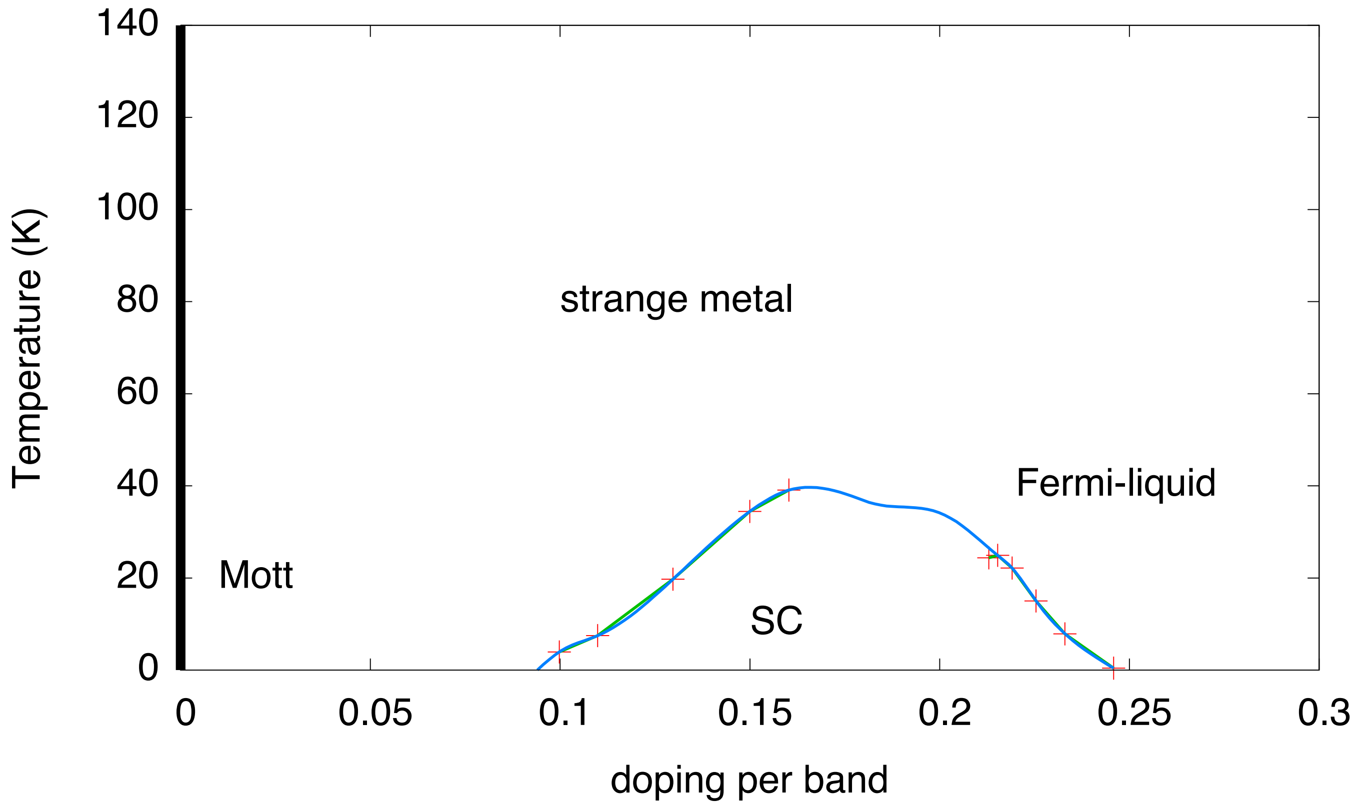


Analogies



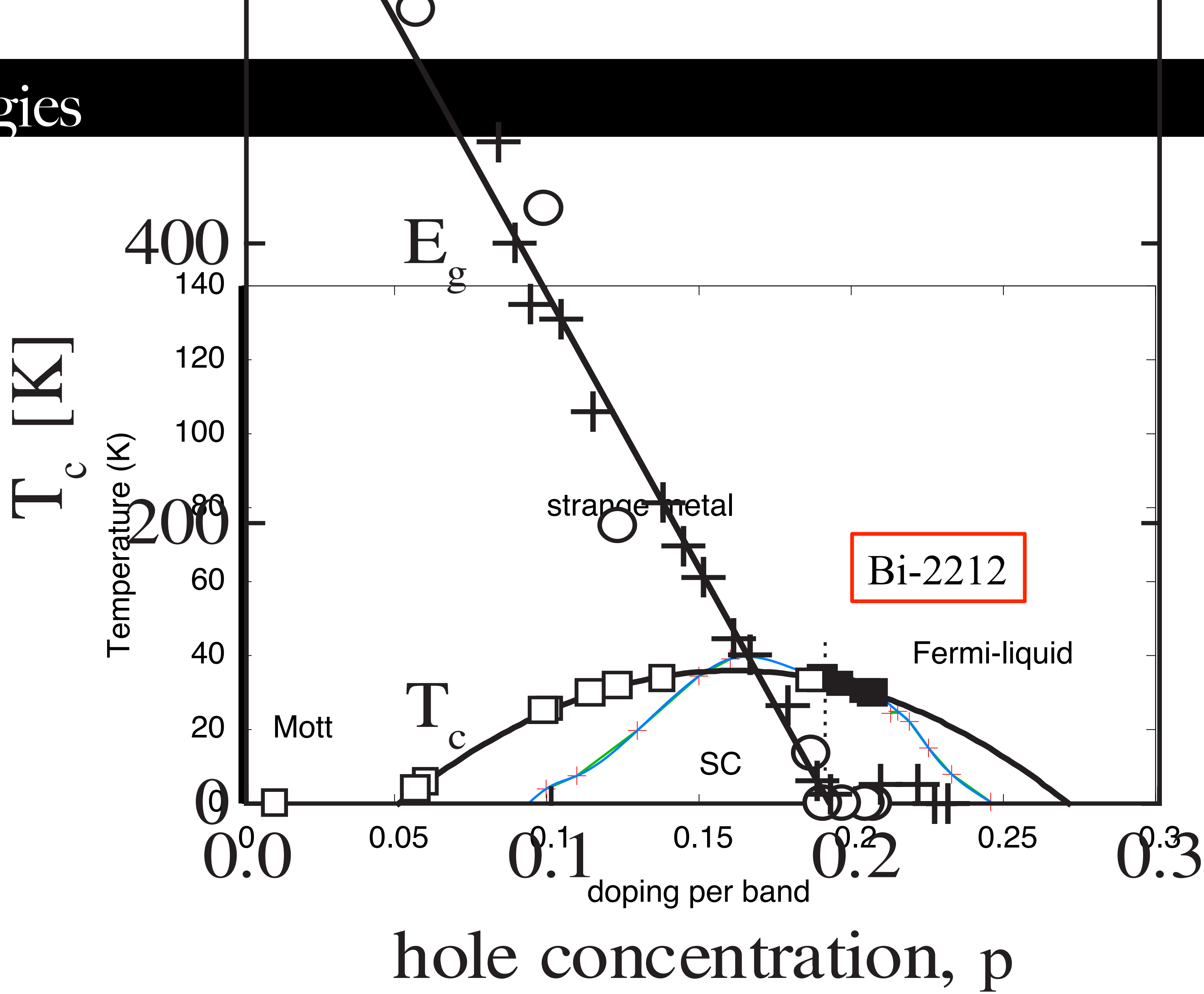
140
120
100
80
60
40
20
0
Temperature (K)
0
0.05
0.1
0.15
0.2
0.25
0.3
doping per band
strange metal
AF
Fermi-liquid
Mott
SC

Analogies



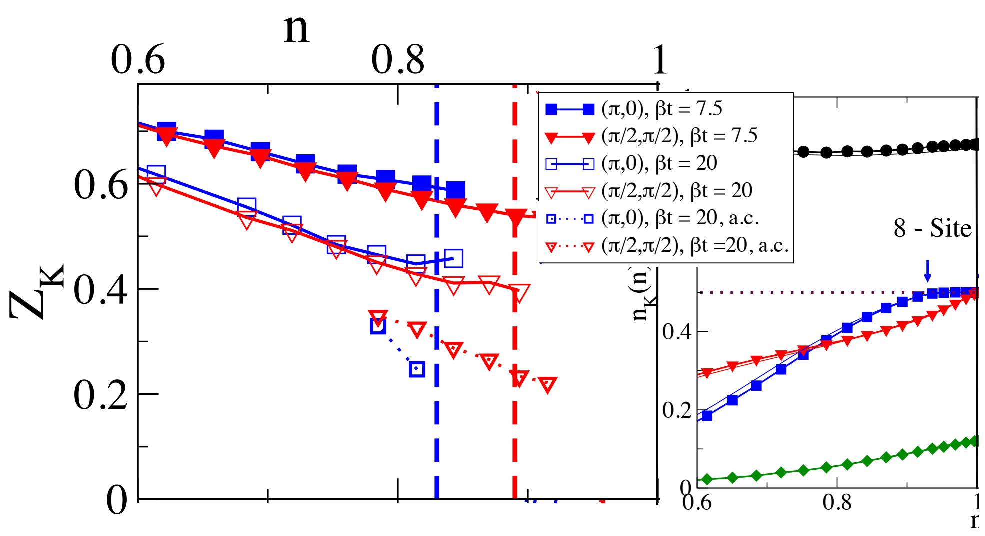
140
120
100
80
60
40
20
0
Temperature (K)
0
0.05
0.1
0.15
0.2
0.25
0.3
doping per band
strange metal
Fermi-liquid
Mott
SC

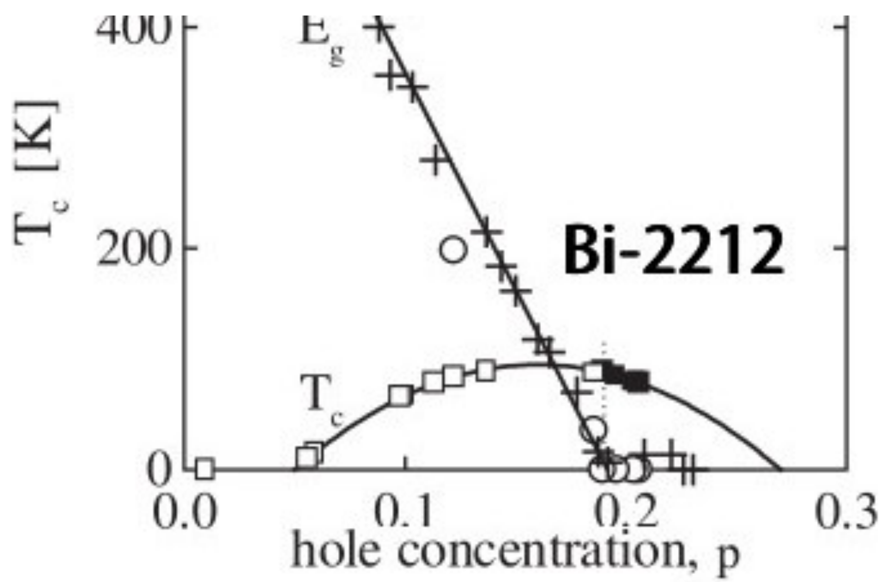
Analogies

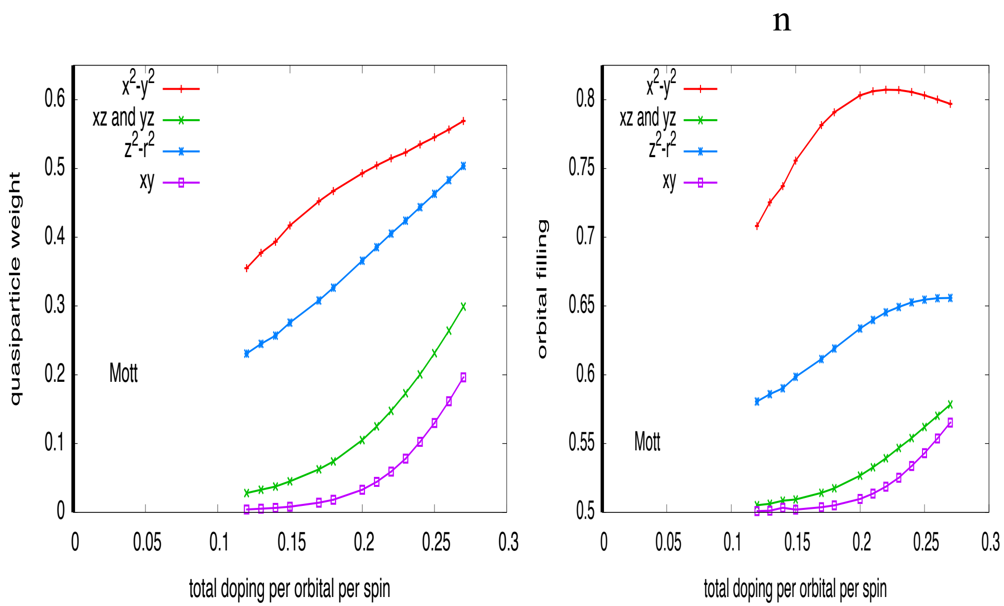


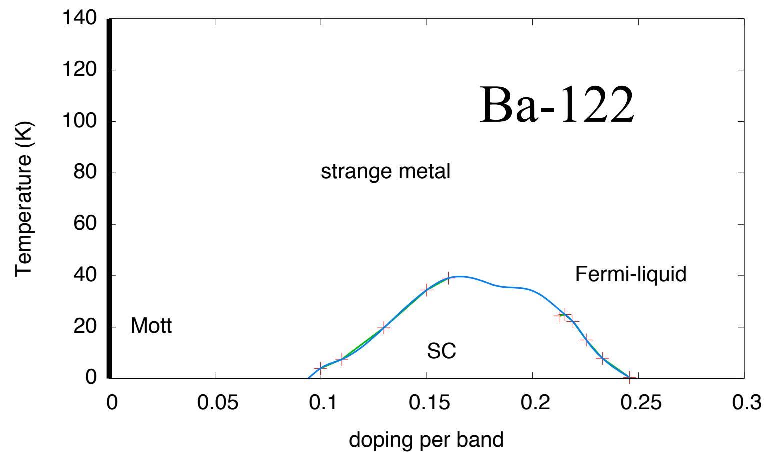
400
200
0
T_c [K]
E_g
T_c
0.0
0.1
0.2
0.3
hole concentration, p
140
120
100
80
60
40
20
0
Temperature (K)
strange metal
Bi-2212
Fermi-liquid
Mott
SC
0
0.05
0.1
0.15
0.2
0.25
0.3
doping per band

Analogies


n
0.6
0.8
1
Z_K
(π,0), βt = 7.5
(π/2,π/2), βt = 7.5
(π,0), βt = 20
(π/2,π/2), βt = 20
(π,0), βt = 20, a.c.
(π/2,π/2), βt =20, a.c.
8 - Site
$n_K(n)$
r


T_c [K]
E_g
T_c
Bi-2212
hole concentration, p


quasiparticle weight
x^2-y^2
xz and yz
z^2-r^2
xy
Mott
total doping per orbital per spin
orbital filling
total doping per orbital per spin


Ba-122
Temperature (K)
strange metal
Fermi-liquid
Mott
SC
doping per band

Conclusions:

Hund's coupling crucial influence makes Iron Superconductors:

- Correlated, but away from the n=6 Mott insulating state (Janus effect)
- Acting as a "**band-decoupler**" through the suppression of orbital fluctuations favors **orbital selectivity:**

  Fe-SC are in proximity of an Orbital-Selective Mott Phase
- **OSMT scenario as a proximity to the n=5 Mott insulator?**

  FeSC are like cuprates?

Experimental support for OSMT physics in Fe-SC

EPR-NMR: Arçon et al., Phys. Rev. B 82, 140508 (2010)

Neutrons: Xu et al, Phys. Rev. B 84, 052506 (2011),

Magnetoresistance: Yuan H-Q et al. ArXiv:1102.5476

ARPES BaK-122: Malaeb et al. ArXiv:1204.0326 ARPES $A_xFe_{2-y}Se_2$: Ming Yi et al (unpublished, 2012)

Scenarios for magnetism and superconductivity in Fe-SC based on OSMT

A. Hackl and M. Vojta, New J. Phys.11, 055064 (2009),

Kou et al. Europhys. Lett. 88 17010 (2009), You Y-Z et al., Phys. Rev. Lett.107, 167001 (2011)

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)