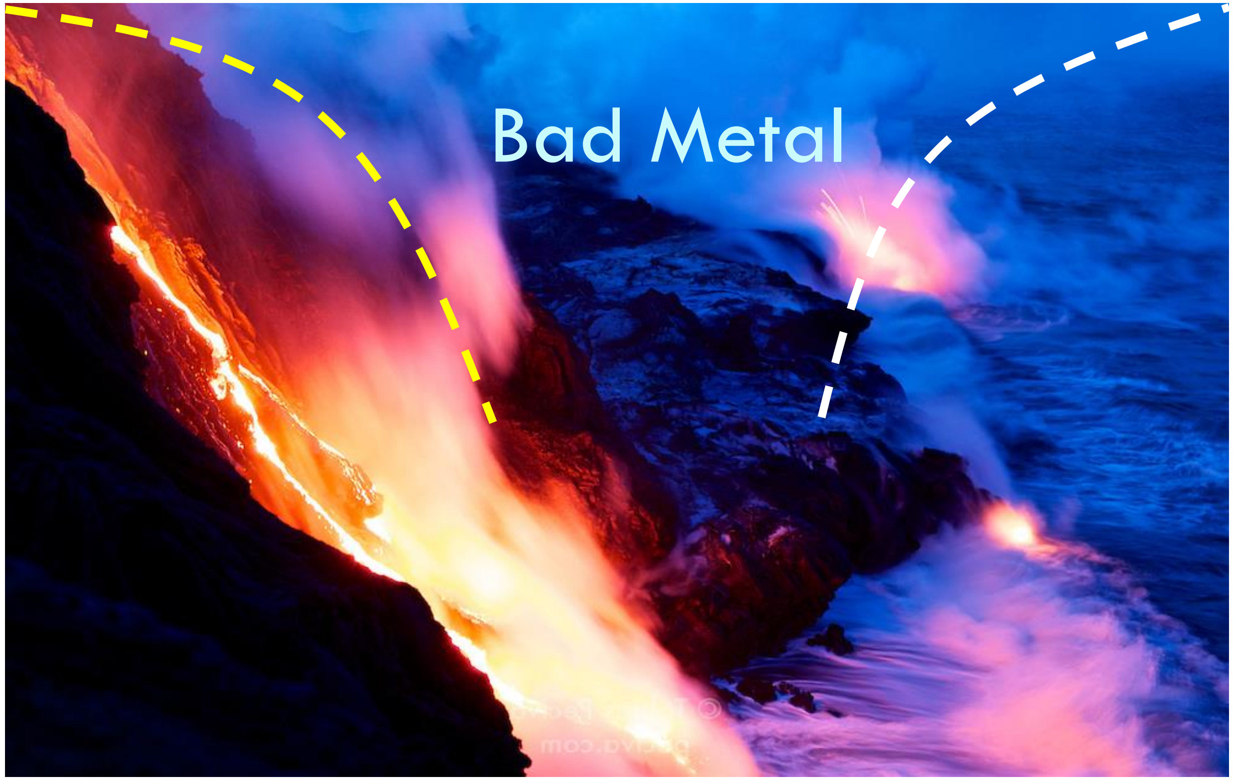
ORBITAL SELECTIVITY AND HUND'S PHYSICS IN IRON-BASED SC

Laura Fanfarillo

ma per seguir virtute e canoscenza
SISSA

FROM FERMI LIQUID TO NON-FERMI LIQUID

Strong Correlation



High Temperature

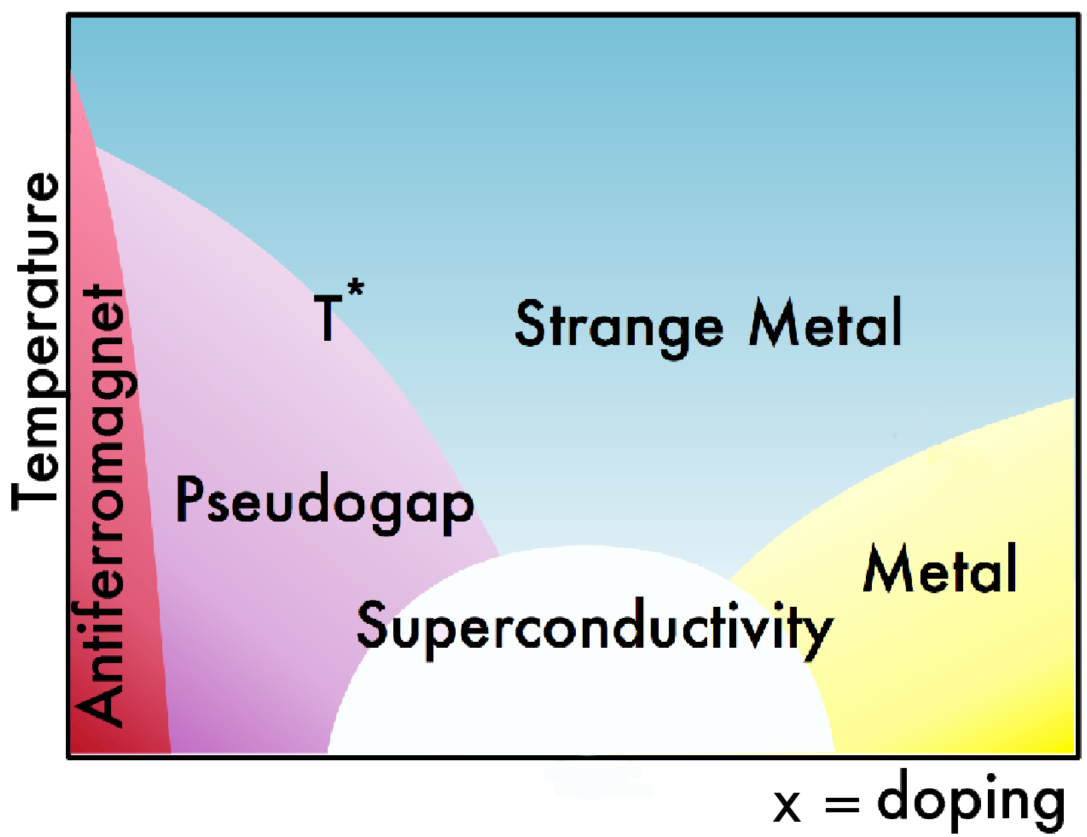
Fermi Liquid

Low Temperature

Tuning parameter

Unconventional SC emerges at low temperature from a state that is far from an ideal metal

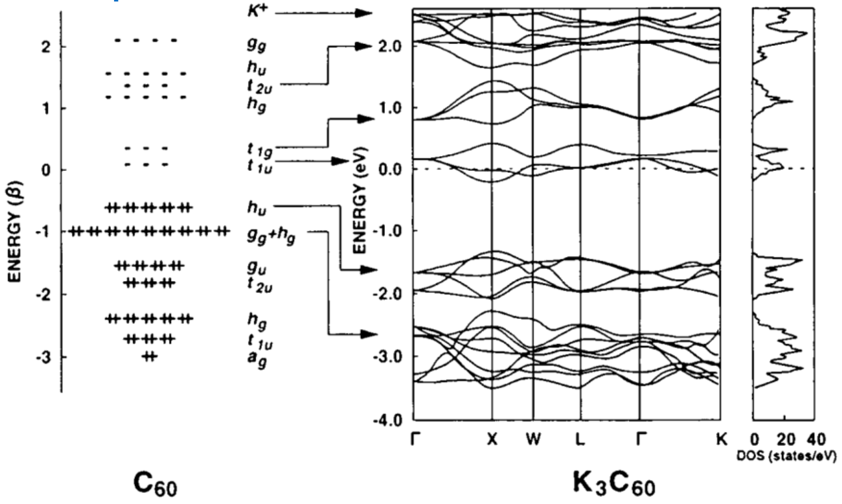
FROM FERMI LIQUID TO NON-FERMI LIQUID : CUPRATES



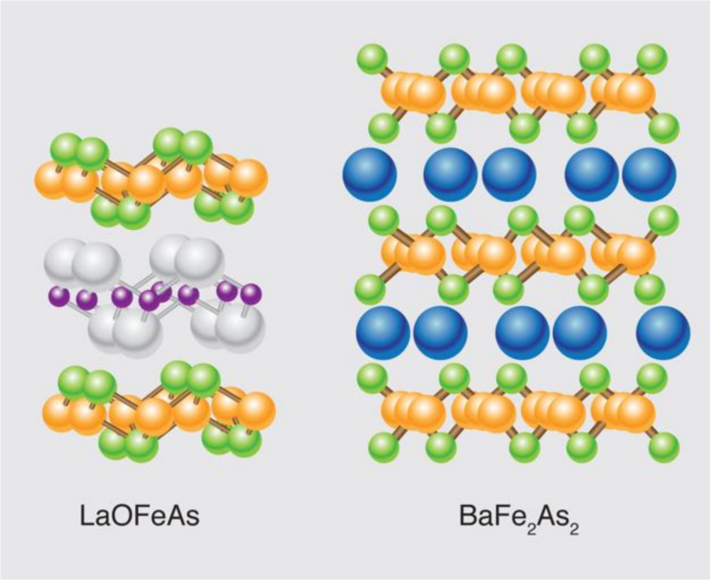
Physics of a doped Mott Insulator

Unconventional SC emerges at low temperature from a state that is far from an ideal metal

MULTIORBITAL PHYSICS IN CORRELATED SYSTEMS

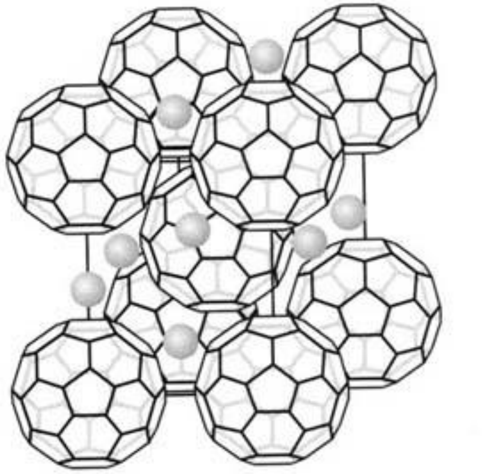


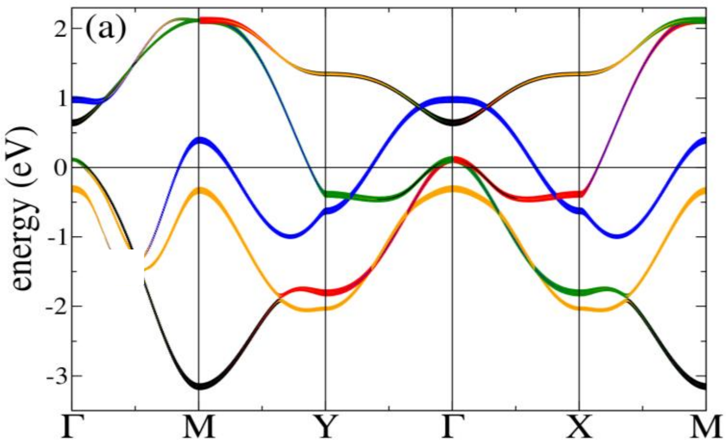
Ruthenates, Iridates …



… and
Iron based SC

A_3C_{60}





IRON-BASED MATERIALS: INTERMEDIATE CORRELATED MATERIAL?

Strong Correlation

Hund's Physics

Fermi Liquid

Orbital Selective Mott Physics

Small Crystal Field Splitting + Hund's coupling

Localized Electrons Picture

Magnetic SuperExchange

Itinerant Electrons Picture

Fermi-Surface Instabilities (Nesting)

DeMedici et al PRL 107 2011,
DeMedici et al, PRL 112 2014,
Fanfarillo et al PRB 92 2015 …

HUND'S PHYSICS CONCEPTS

Itinerant but heavy quasiparticles

High spin atomic configuration

Bad Metal

Orbital Decoupling

Orbital Selective Mott physics

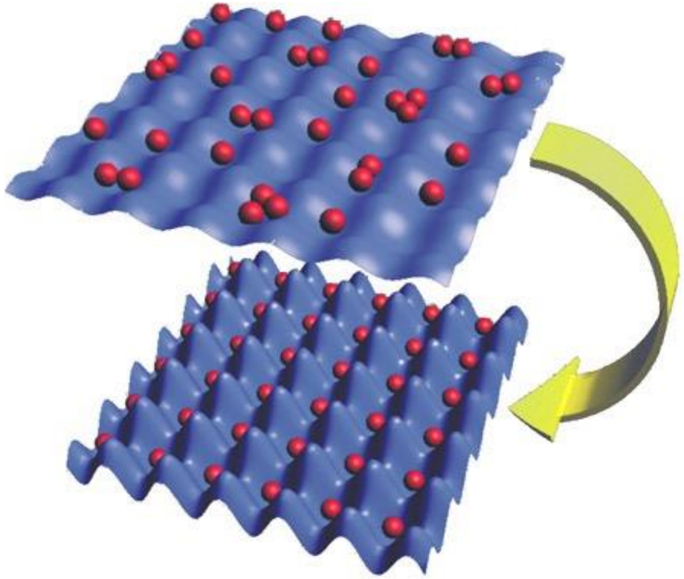
MOTT-HUBBARD INSULATOR: SINGLE ORBITAL CASE HALF FILLING

Despite the conduction band is half-filled the system is insulating because of the strong Coulomb repulsion

Quasiparticle Spectral Weight Suppressed
$Z \sim 1/m^*$ increasing of correlation

Charge Fluctuations Suppressed:
localization of the electrons

Spin Fluctuations Enhanced
atoms are locally spin polarized

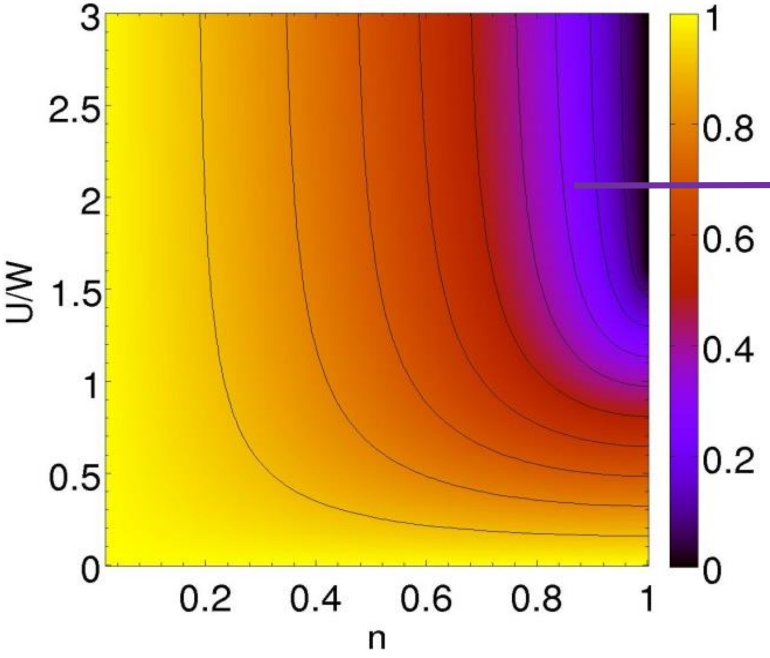


U >> t

Z=1 FL - Metal
Z=0 Correlated electrons - Insulator

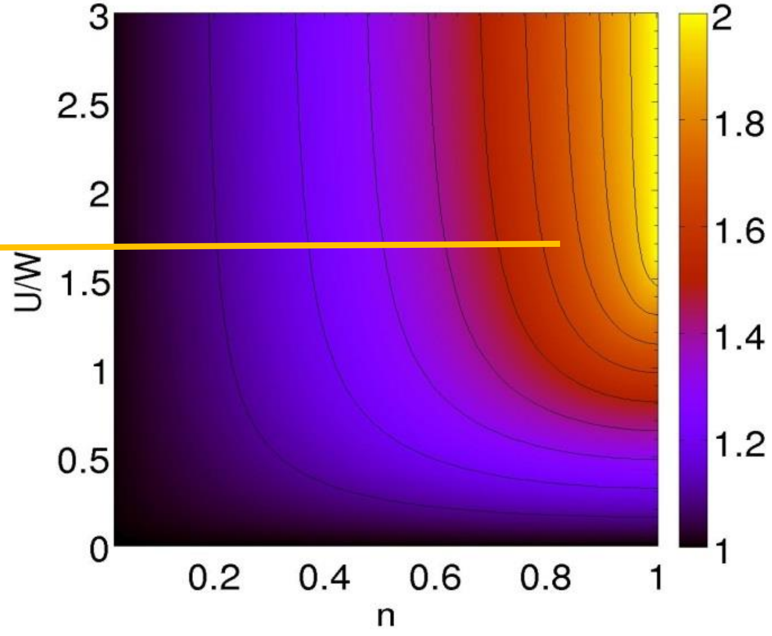
MOTT-HUBBARD INSULATOR: SINGLE ORBITAL CASE IN DOPING

Far from half-filling ($n \neq 1$) :



Correlated bad metal close to the Mott insulator

High Spin Phase



MULTIORBITAL MODEL: U, JH

tb (hopping term)

Intra-orbital repulsion

Inter-orbital repulsion

Hund's coupling

Pair hopping

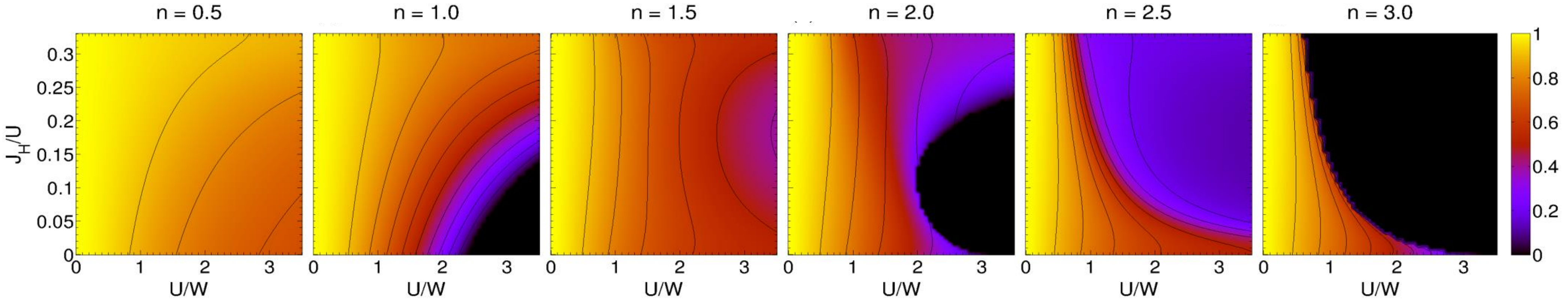
$$
\begin{aligned}
H \; = & \sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_{i,\gamma,\sigma}^{\dagger} c_{j,\beta,\sigma} + h.c. + U \sum_{j,\gamma} n_{j,\gamma,\uparrow} n_{j,\gamma,\downarrow} \\
+ & \left(U' - \frac{J_H}{2}\right) \sum_{j,\gamma>\beta,\sigma,\tilde{\sigma}} n_{j,\gamma,\sigma} n_{j,\beta,\tilde{\sigma}} - 2J_H \sum_{j,\gamma>\beta} \vec{S}_{j,\gamma} \vec{S}_{j,\beta} \\
+ & J' \sum_{j,\gamma\neq\beta} c_{j,\gamma,\uparrow}^{\dagger} c_{j,\gamma,\downarrow}^{\dagger} c_{j,\beta,\downarrow} c_{j,\beta,\uparrow} + \sum_{j,\gamma,\sigma} \epsilon_{\gamma} n_{j,\gamma,\sigma} \, .
\end{aligned}
$$

Interactions are local and satisfy rotational invariance: $U' = U - 2J_H$

U and J_H are free parameters

MORE IS DIFFERENT: 3 ORBITALS

Quasiparticle Spectral Weight $Z(U, J_H)$



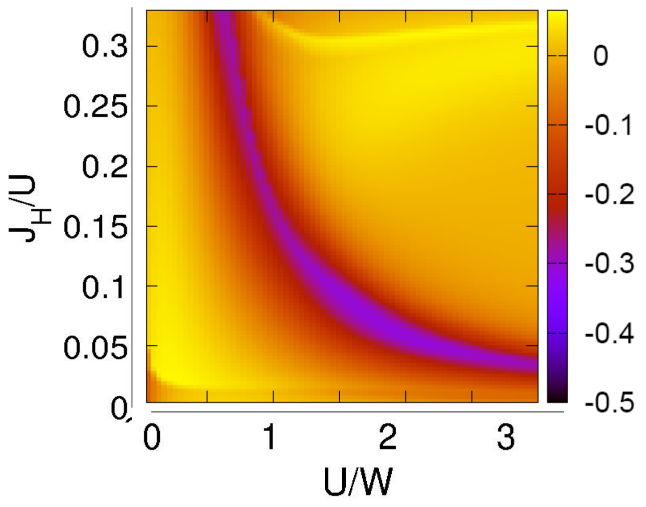
- Bad metals close to HF Mott Insulator

- Hund's metal boundary follows the MI transition line

- Strong doping dependence:

2(4) el/3orb Hund induces correlated metal state

$\frac{dZ}{dJ_H}$



Fanfarillo & Bascones, PRB 92(2015)

MORE IS DIFFERENT: 3 ORBITALS

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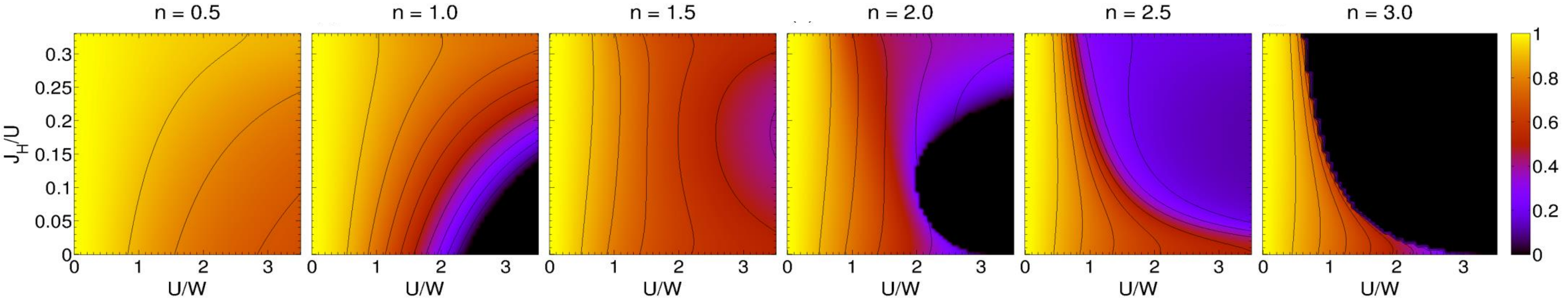
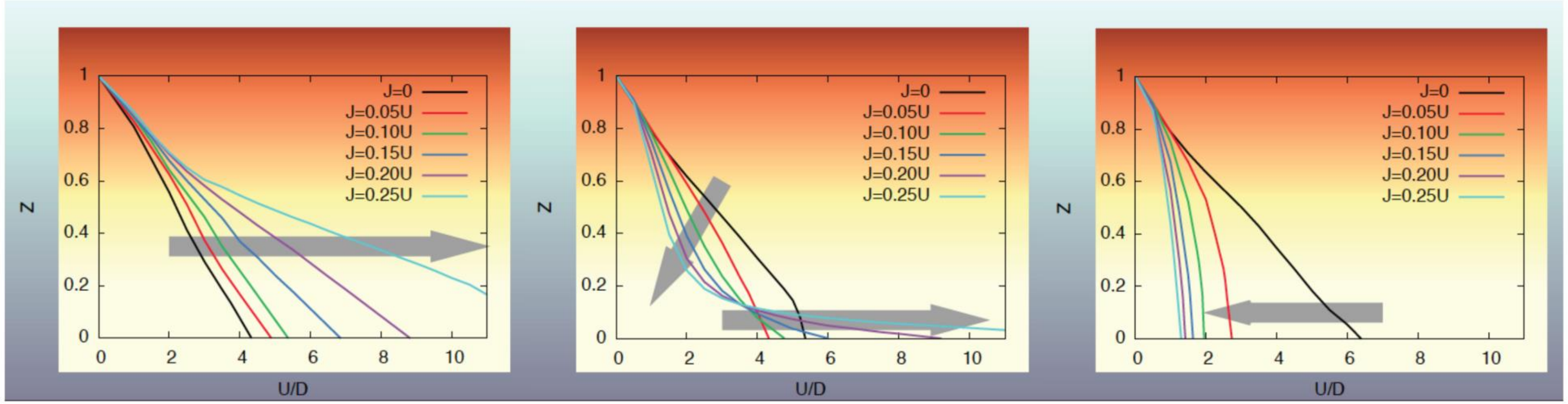




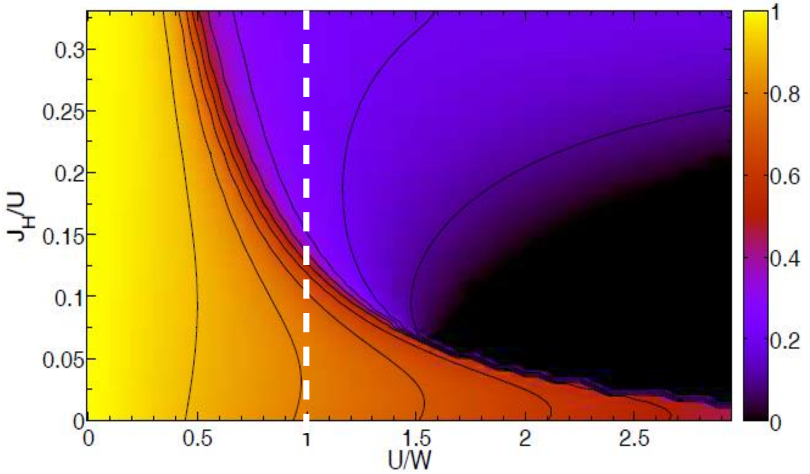
(a) $N = 1$ (b) $N = 2$ (c) $N = 3$

Strong doping dependence: 2(4) el/3orb Hund induces correlated metal state

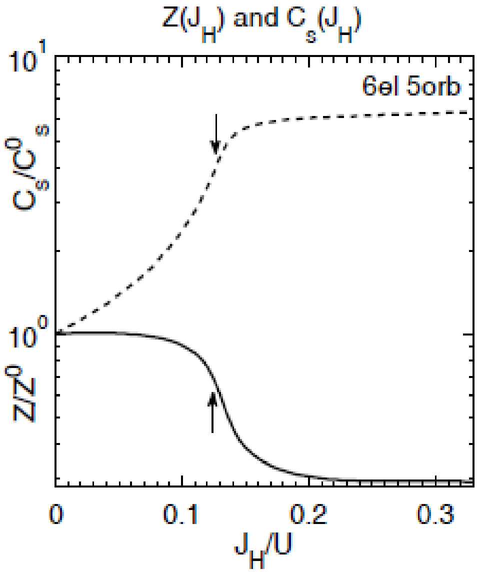
DeMedici et al PRL 107 (2011)

THE IBS CASE: 6 ELECTRONS IN 5 ORBITALS

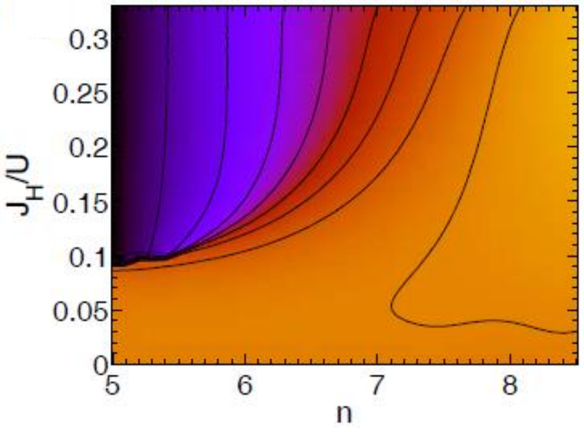
6 el in 5 orb



Hund's coupling induced high spin configuration



U = W



Hund'metal linked to the half-filled n=5 Mott insulator

doping asymmetry around n=6

Fanfarillo & Bascones, PRB 92(2015)

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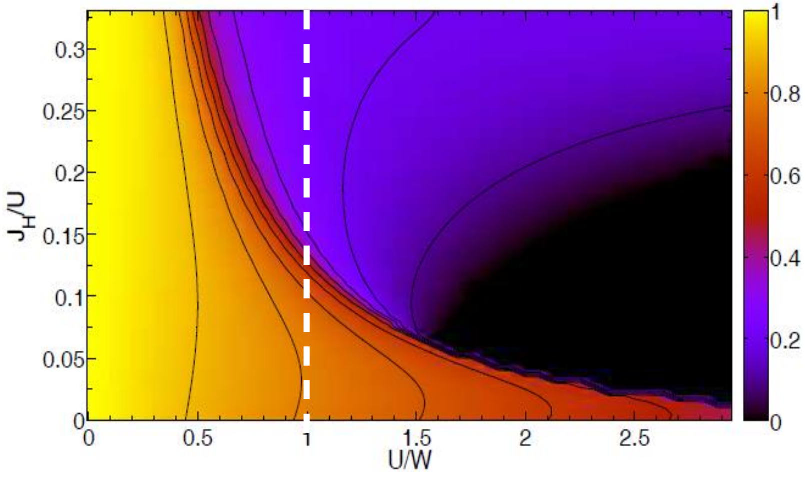

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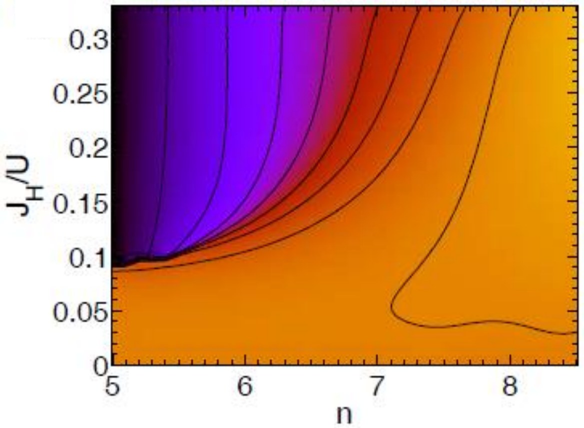

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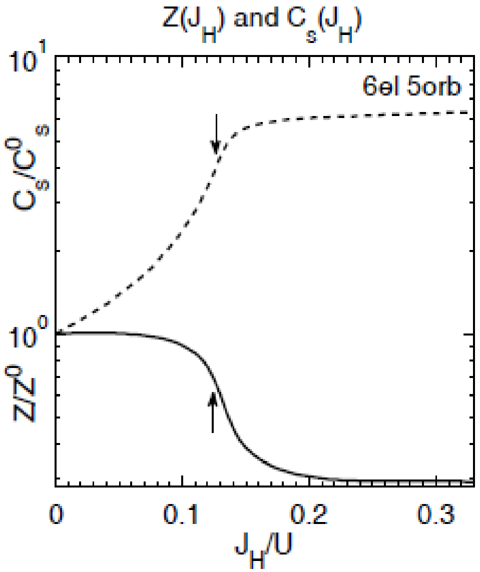
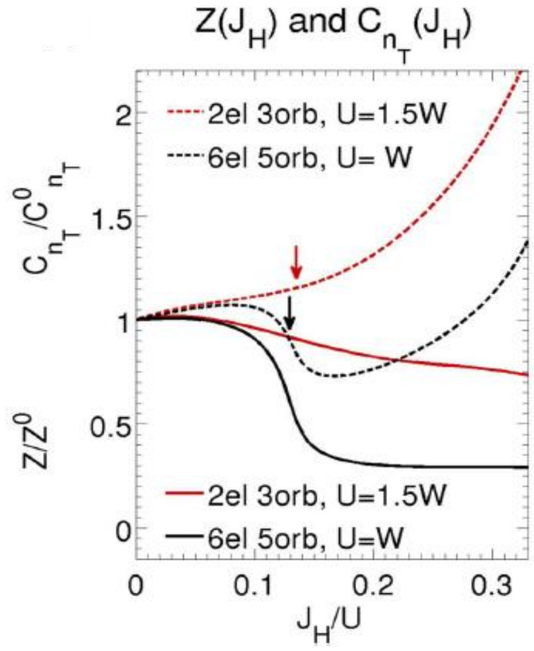




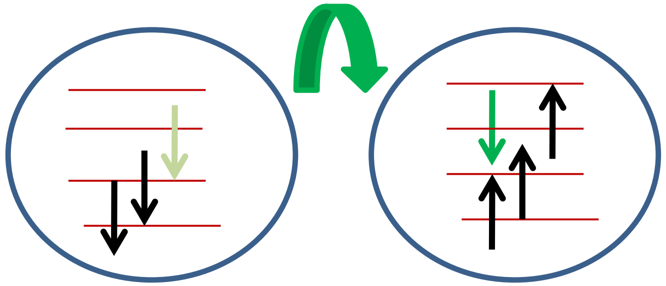
Quasiparticle weight and charge fluctuations:

Correlation vs Localization

Fanfarillo & Bascones, PRB 92(2015)

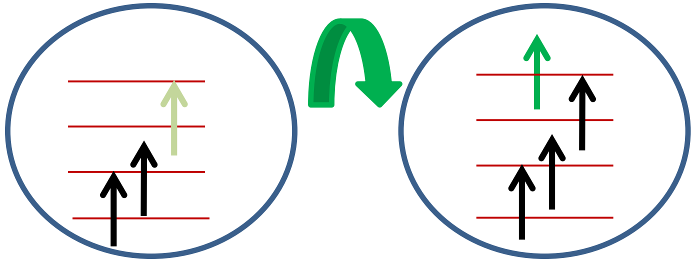
HUND'S METAL: LINK TO HF MOTT TRANSITION

- ❑ Suppression of coherence due to suppression of hopping processes which involve
  intraorbital double occupancy



$$E^{intra\uparrow\downarrow} = U + (n-1)J_H$$

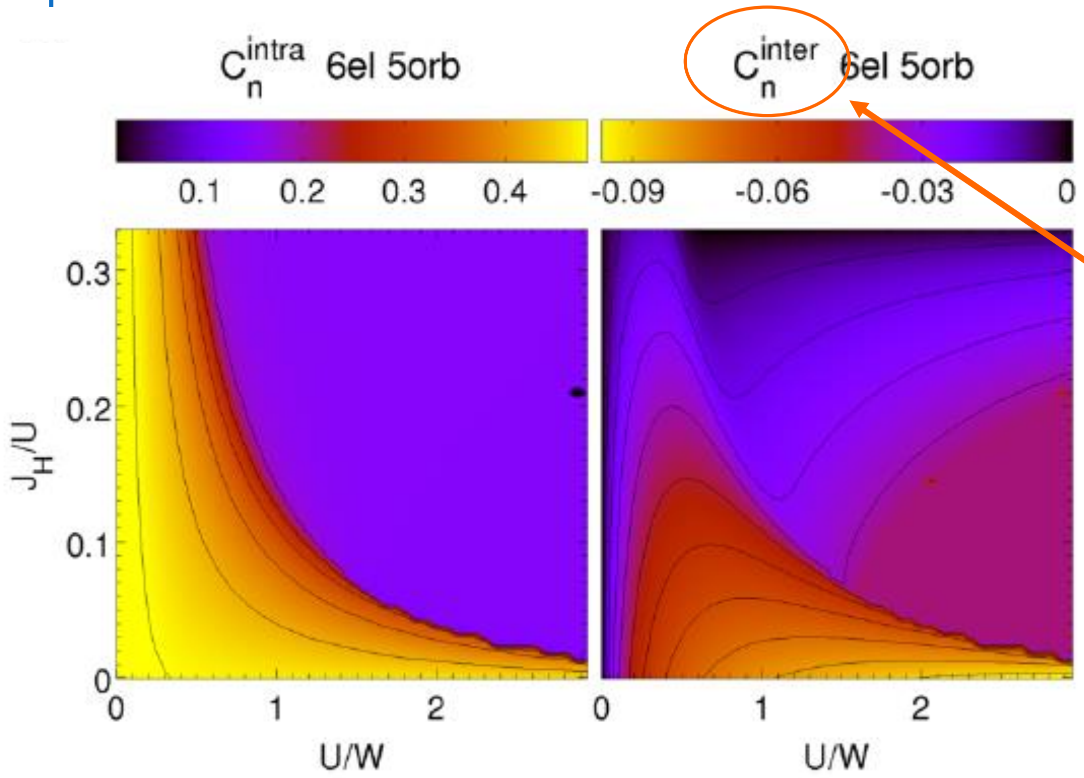
- ❑ Enhancement of charge fluctuations due to hopping processes which involve parallel spins to an empty orbital



$$E^{\uparrow\uparrow} = U - 3J_H$$

Fanfarillo & Bascones, PRB 92 (2015)

HUND'S METAL: LINK TO HF MOTT TRANSITION



As the double occupancies are suppressed:

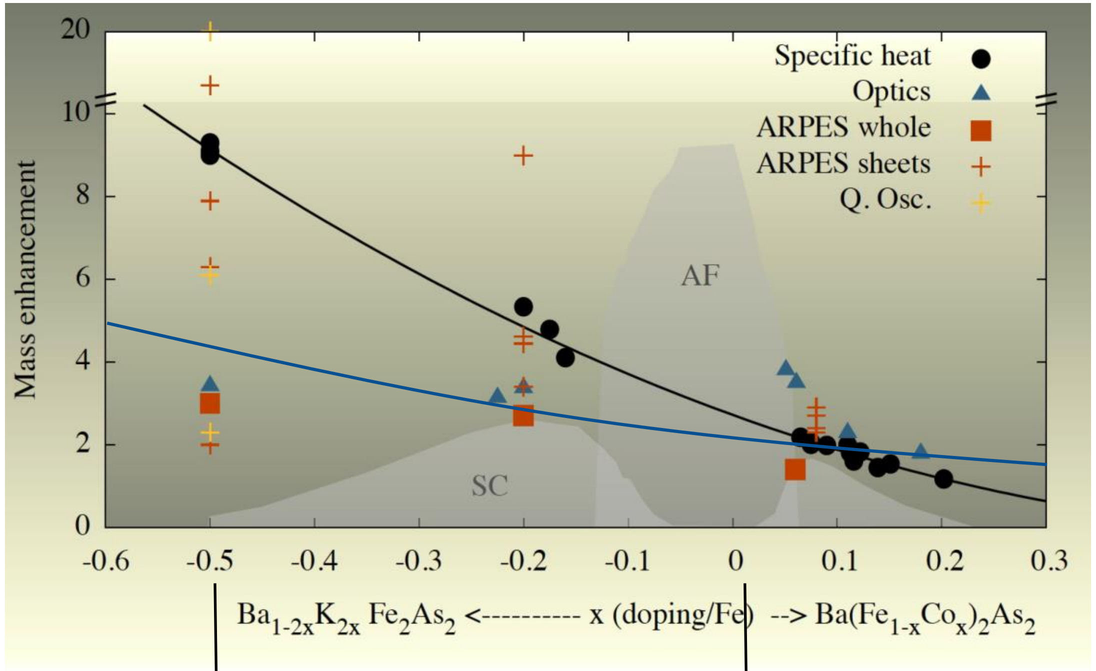
- atoms becomes spin polarized

- *orbitals decoupled*

In the polarized state the effective interorbital interaction between the electrons decreases. It vanishes at $J_H = U/3$.

Fanfarillo & Bascones, PRB 92(2015)

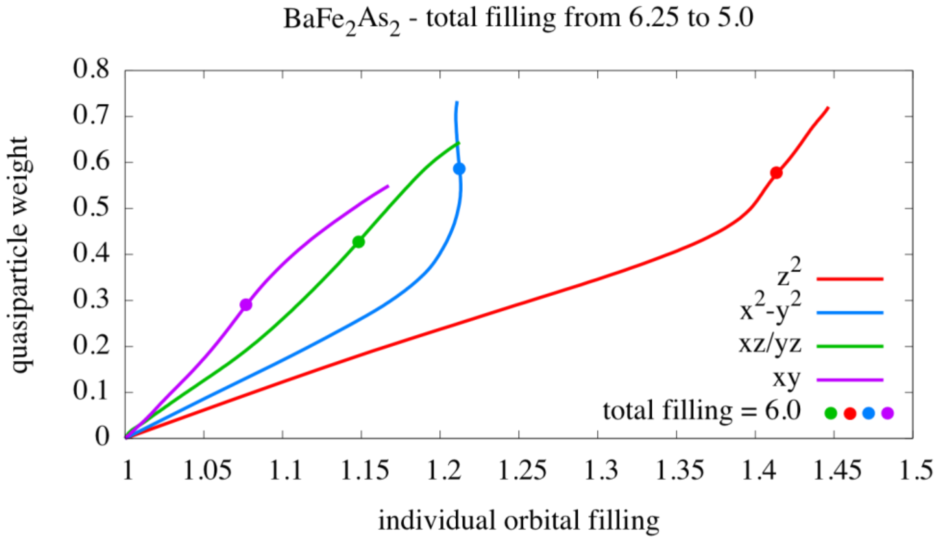
HUND'S PHYSICS IN IBS:
EFFECTIVE MASS



- m*increases reducing the # of electrons
- m* strongly orbital selective

KFe2As2
5.5el-5orb

BaFe2As2
6el-5orb



- Each orbital has a different $Z_a \sim 1/m_a^*$ proportional to the orbital filling

Each orbital behaves as a doped Mott insulator

De Medici *et al* PRL 112 (2014)

CONCLUSIONS: HUND'S PHYSICS IN IBS

- More is different:
  - The degree of correlation is **complicated by the multiorbital physics**
  - The entrance at the Hund's metal is due to the **suppression of the double occupancies**

    Consequences: local spin polarization and orbital decoupling
  - Correlation **is not** a good measure of localization

- IBS (parent compound 6 el/5 orb)

  IBS collection of five decoupled single-band doped Mott insulator

  Correlations increase reducing the number of electrons in d-bands:

  KFe_2As_2 is much more correlated than $BaFe_2As_2$

CAN WE GO FURTHER?

ORBITAL SELECTIVITY AND HUND'S PHYSICS IN THE PHASE DIAGRAM OF IBS

- *From the strong correlated side*

Try to figure out if local correlations can explain the phase diagram of IBS

Orbital selective SC …

DeMedici et al arXiv 1609.01303
Fanfarillo et al arXiv 1609.06672 …

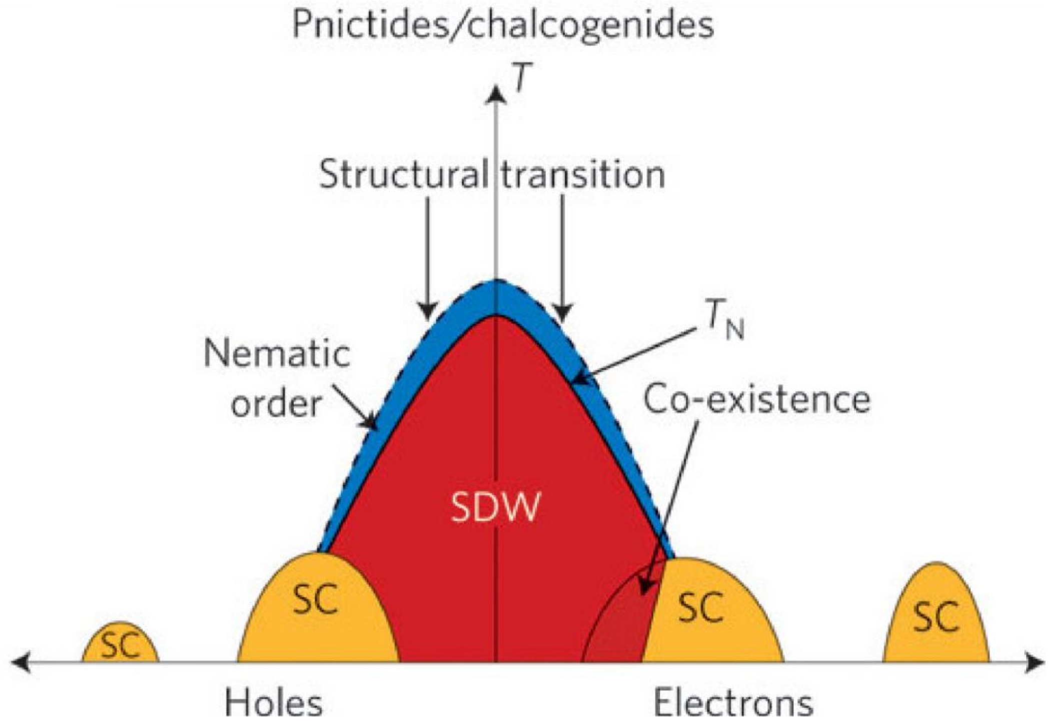
- *From the FL side*

Project interacting multiorbital Hamilonian into low-energy model for IBS

Orbital selective character of spin fluctuations

Fanfarillo et al. PRB 91 (2015),
Christenses et al. PRB 93 (2016)
Fanfarillo et al arXiv 1605.02482 …

NEMATIC PHASE OF IBS

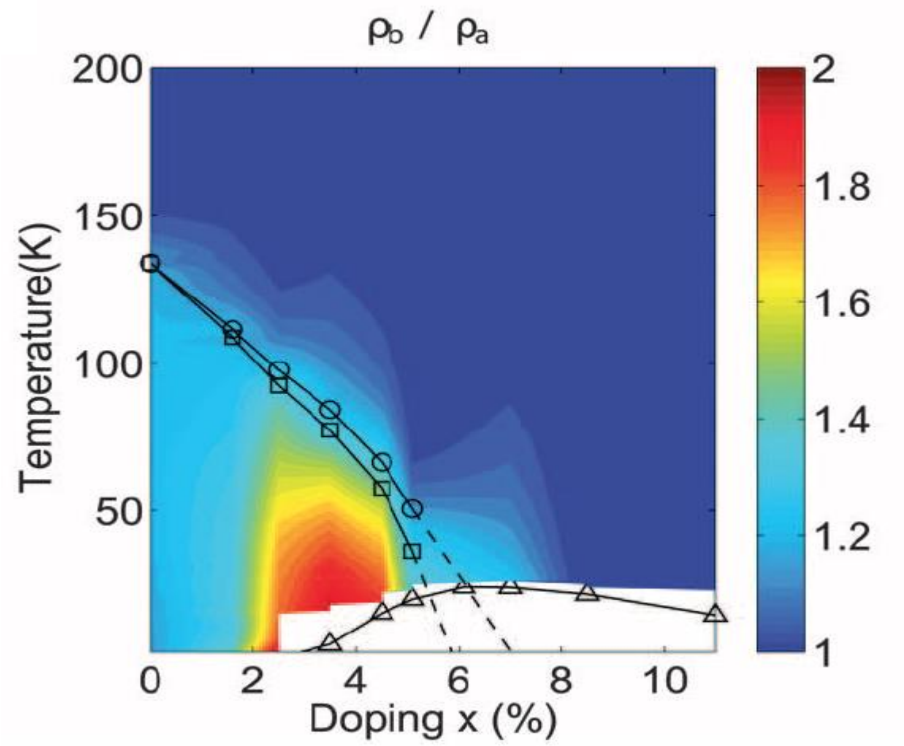


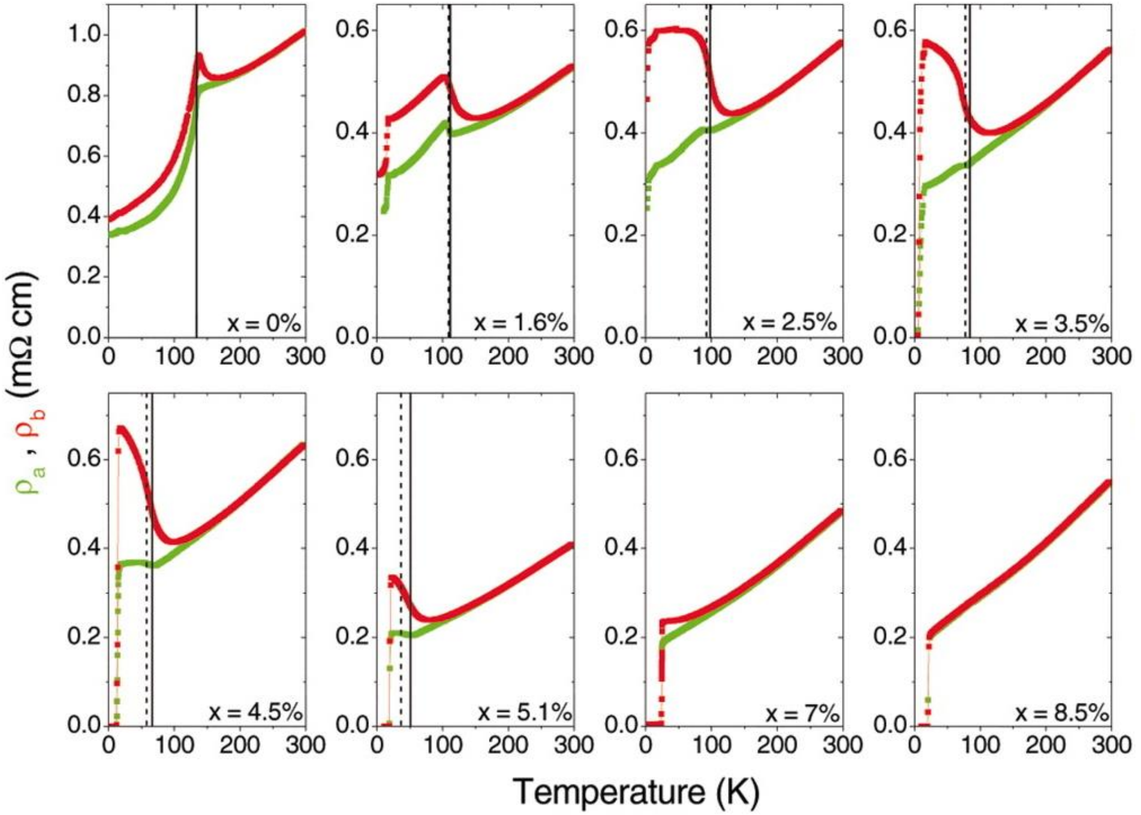
Structural transition takes place before/simultaneously to the magnetic one:

Several experimental probes revealed x,y anisotropy above the magnetic transition not only in the lattice parameter but also in the electronic properties: **NEMATIC PHASE**

Resistivity anisotropy measurements

NEMATIC PHASE OF IBS





J-H Chu at al. Science 329 (2010)

Structural transition takes place before/simultaneously to the magnetic one:

Several experimental probes revealed x,y anisotropy above the magnetic transition not only in the lattice parameter but also in the electronic properties: **NEMATIC PHASE**

MATTER OF ANISOTROPY

Possible origin of "nematic phase":

- Structural distortion → Anisotropy from the lattice parameters (odd!)
- Orbital/Charge order → Anisotropy from the orbital filling
- Spin order → Anisotropy from spin fluctuations along x,y

Classical *"chicken and egg problem"*

All three types of order (structural, orbital and spin-driven nematic) are very entangled

no matter which drives the nematic instability.

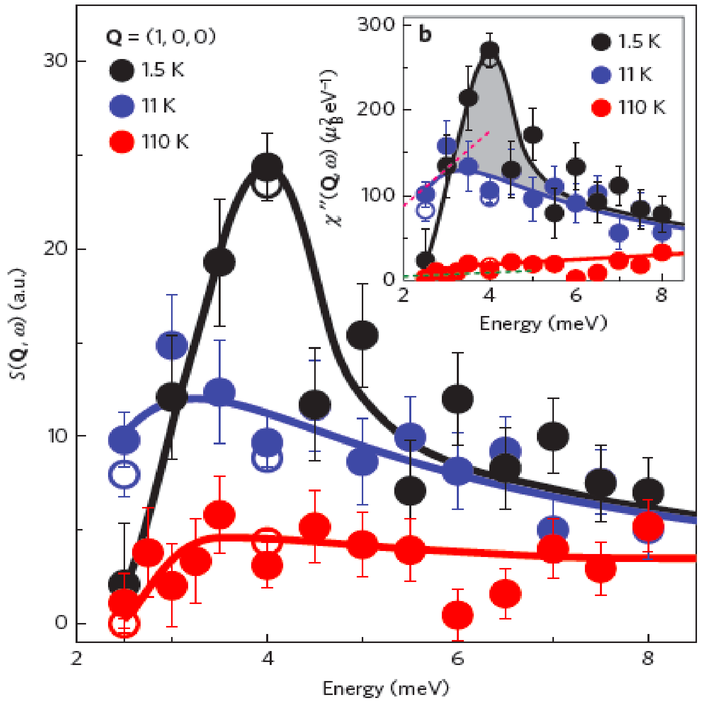
What drives nematic order in iron-based superconductors?

R.M. Fernandes et al. NATURE PHYSICS | VOL 10 | FEBRUARY 2014

Enigmatic nematic

J. C. Davis and P. J. Hirschfeld NATURE PHYSICS | ADVANCE ONLINE PUBLICATION 2014

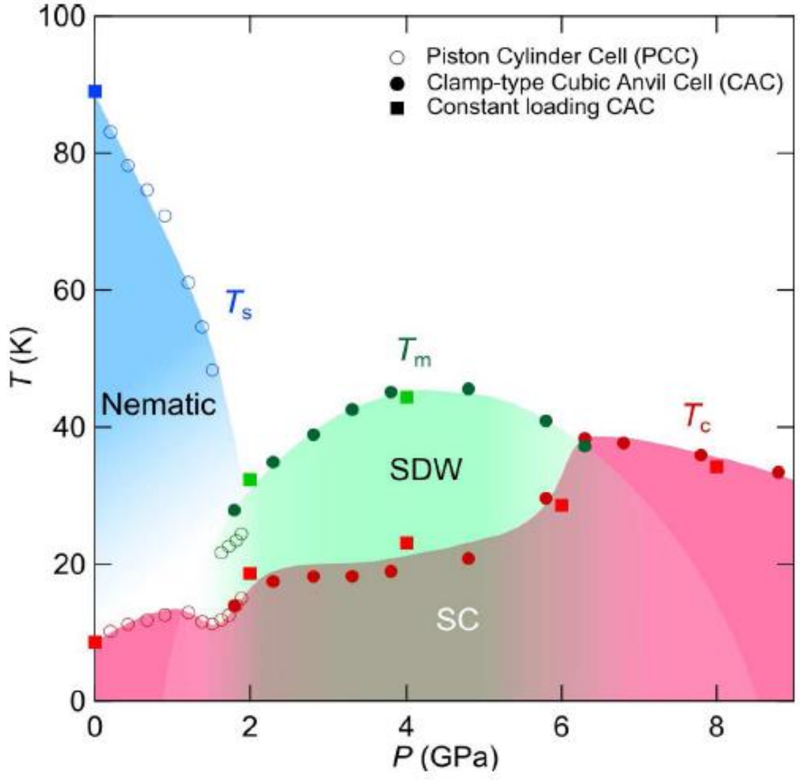
THE CASE OF FESE: NEMATIC PHASE NOT FOLLOWED BY THE MAGNETIC ONE



Q. Wang et al. Nat. Mat. (2015)

Sizeble SDW fluctuations
but NO magnetic long range ordered phase

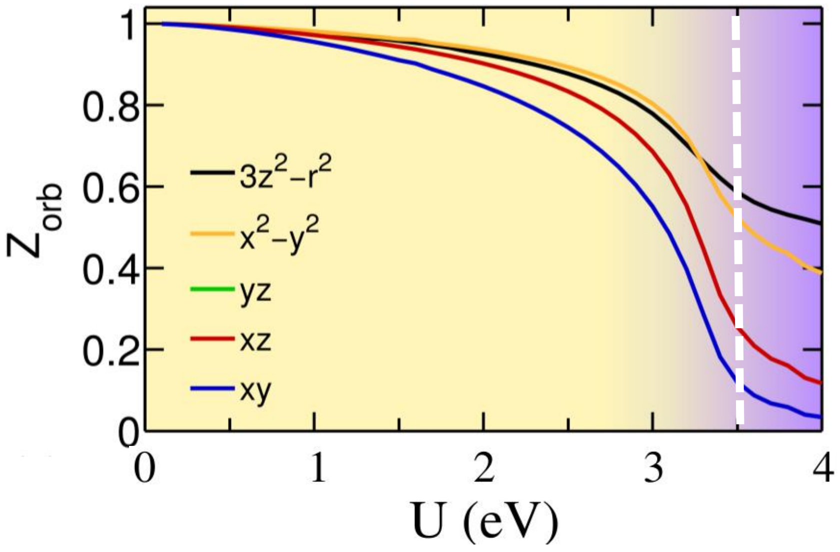
Sun et al Nat. Commun. 7 (2016)



Is the charge degree of freedom the driver?

Can local correlations induce a nematic phase transition?

ORBITAL NEMATIC PERTURBATION



Compute the Response of the system to orbital perturbations modulated in k-space:

$$\delta H^m_{A_{1g}/B_{1g}} = \sum_{\mathbf{k}} (n_{xz}(\mathbf{k}) \pm n_{yz}(\mathbf{k})) f_m(\mathbf{k}) h_m$$

Orbital Nematic Parameter:

$$\Delta_m = -\langle \sum_{\mathbf{k}} (n_{xz}(\mathbf{k}) \pm n_{yz}(\mathbf{k})) f_m(\mathbf{k}) \rangle$$

From ARPES, Quantum oscillations, X ray

FeSe ~ $U = 3.5$ eV and $J_H/U = 0.20$

Linear response:

$$\chi_m = \frac{\delta \Delta_m}{\delta h_m}$$

ORBITAL NEMATIC PERTURBATION

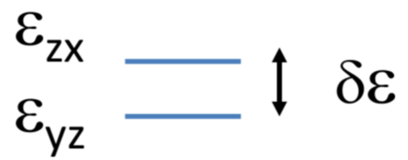
$$\delta H^m_{A_{1g}/B_{1g}} = \sum_{\mathbf{k}} (n_{xz}(\mathbf{k}) \pm n_{yz}(\mathbf{k})) f_m(\mathbf{k}) h_m$$

$$\Delta_m = -\langle \textstyle\sum_{\mathbf{k}} (n_{xz}(\mathbf{k}) \pm n_{yz}(\mathbf{k})) f_m(\mathbf{k}) \rangle$$

3 Orbital Orders considered in literature:

Onsite ferro-orbital

$$h_{OFO} = \delta\epsilon \qquad f_{OFO}(\mathbf{k}) = 1$$



Sign-change orbital order

$$h_{SCO} = \delta t' \qquad f_{SCO}(\mathbf{k}) = \cos k_x \cos k_y$$

Lift the degeneracy of the second neighbor hopping

d-wave bond order

$$h_{DBO} = \delta t \qquad f_{DBO}(\mathbf{k}) = (\cos kx - \cos ky)/2.$$

Lift the degeneracy of the nn hopping

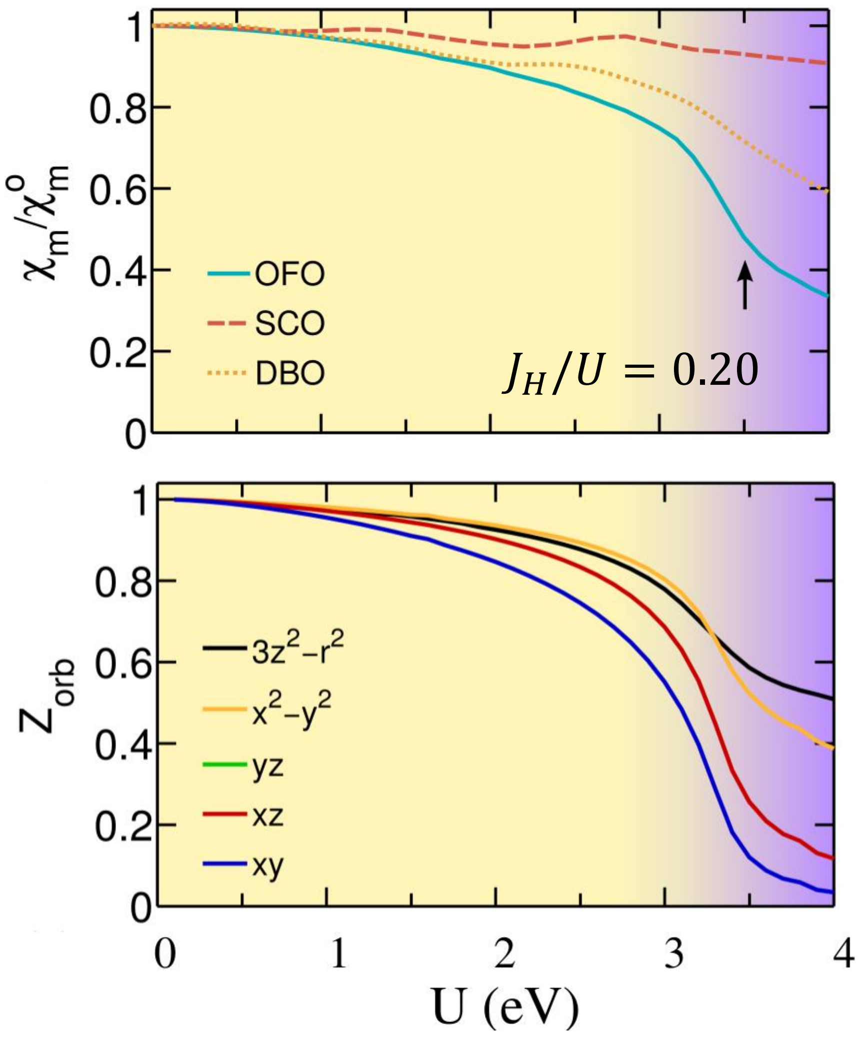
Chubukov et al. arxiv 1602.05503

ORBITAL RESPONSE FUNCTIONS

No divergence = no phase transition

Interactions strongly suppress OFO order:
Suppression in correspondence of the entrance in the Hund Metal region.

SCO order independent by U

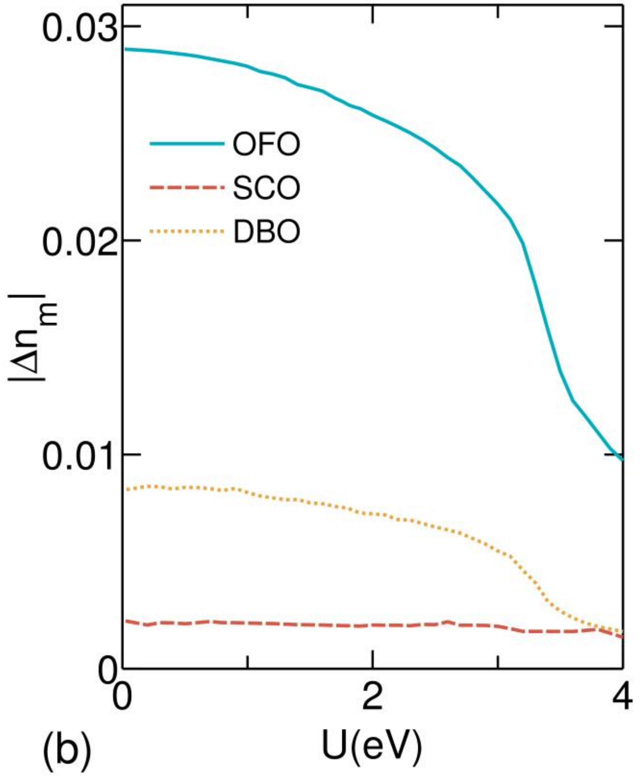


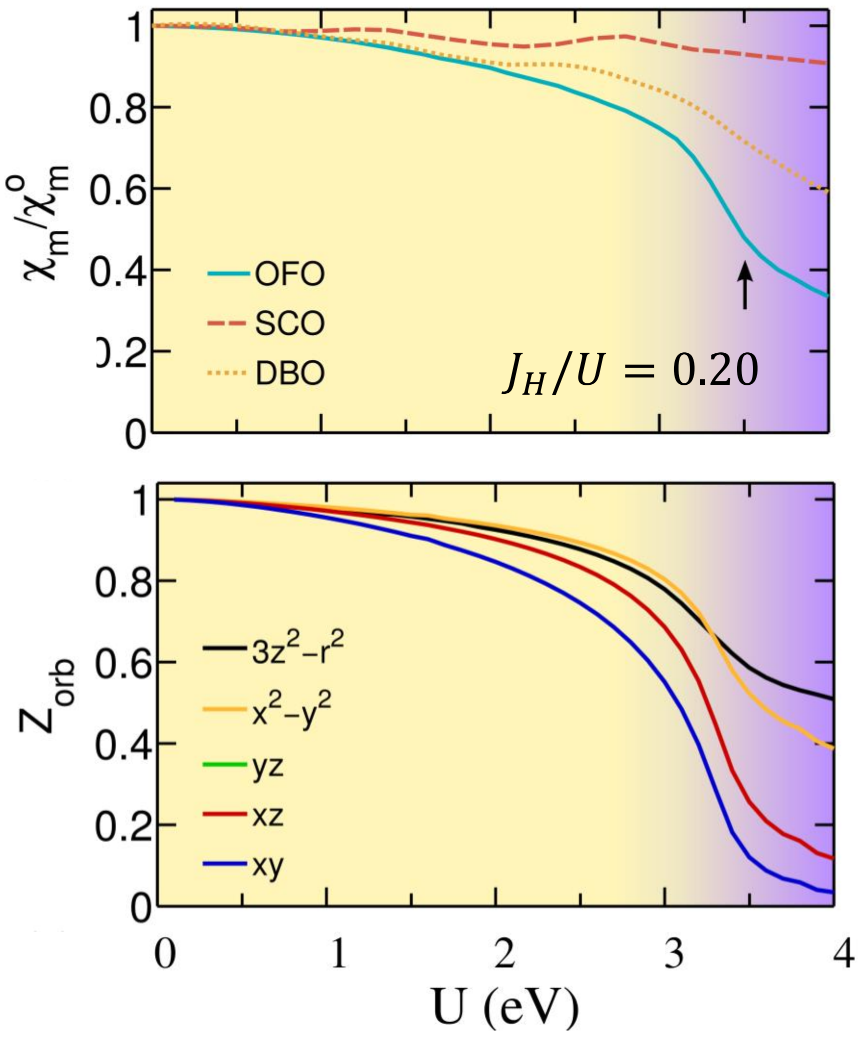
ORBITAL RESPONSE FUNCTIONS

Sign-changing orbital order

small occupation imbalance between *zx* and *yz* orbitals

not suppressed by interactions!





Fanfarillo et al. arxiv 1609.06672

ORBITAL RESPONSE FUNCTIONS

✓ Local correlations cannot drive alone nematic transition

✓ Correlations constrain possible orbital orders

Onsite ferro-orbital ordering strongly suppressed by interactions

Sign-changing orbital order = small occupation imbalance between *zx* and *yz* orbitals = not suppressed by Hund's coupling.

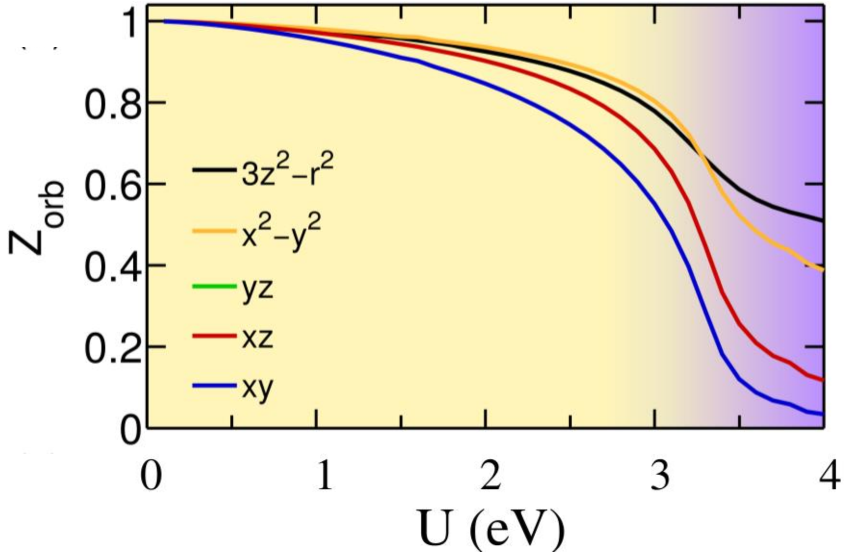
From RG Analysis:
Nematicity in the Pomeranchuk d-wave assisted by spin fluctuations

Chubukov et al. arxiv 1602.05503

ENHANCED NEMATICITY & HUND METAL PHASE

New route to nematicity:
anisotropy in the orbital effective mass

$$\chi_Z^m(U) = \frac{\delta(Z_{zx} - Z_{yz})}{\delta h_m}$$



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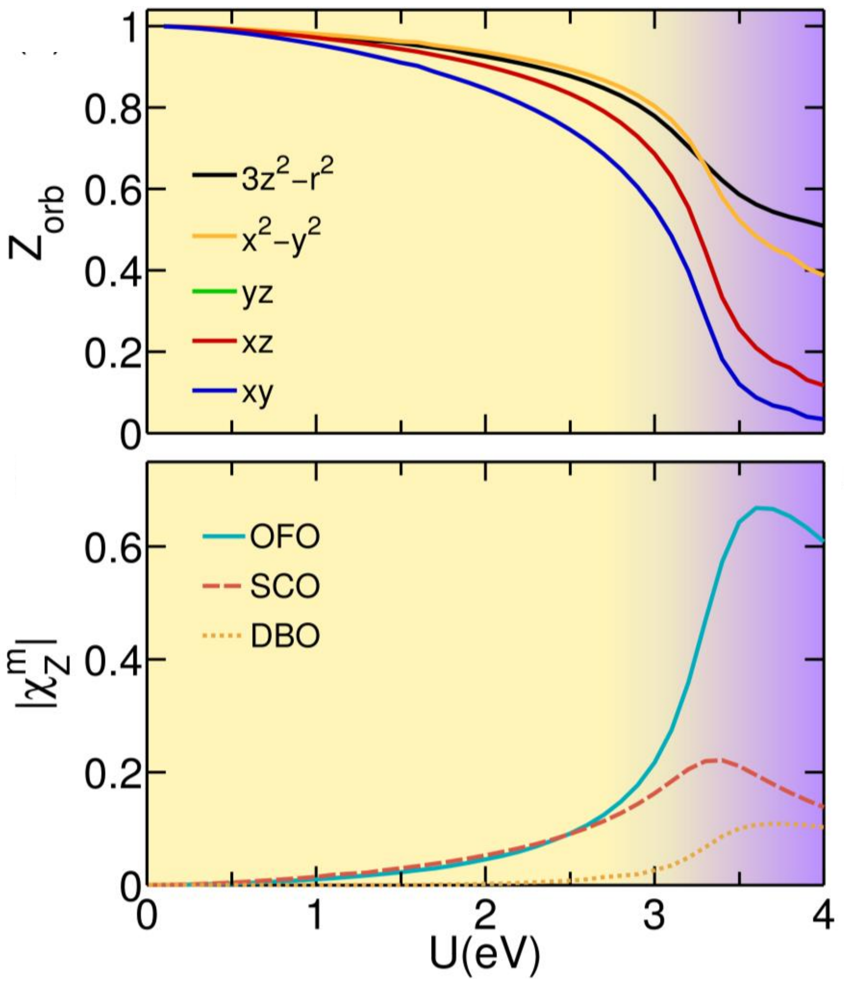
$$\chi_Z^m(U) = \frac{\delta(Z_{zx} - Z_{yz})}{\delta h_m}$$

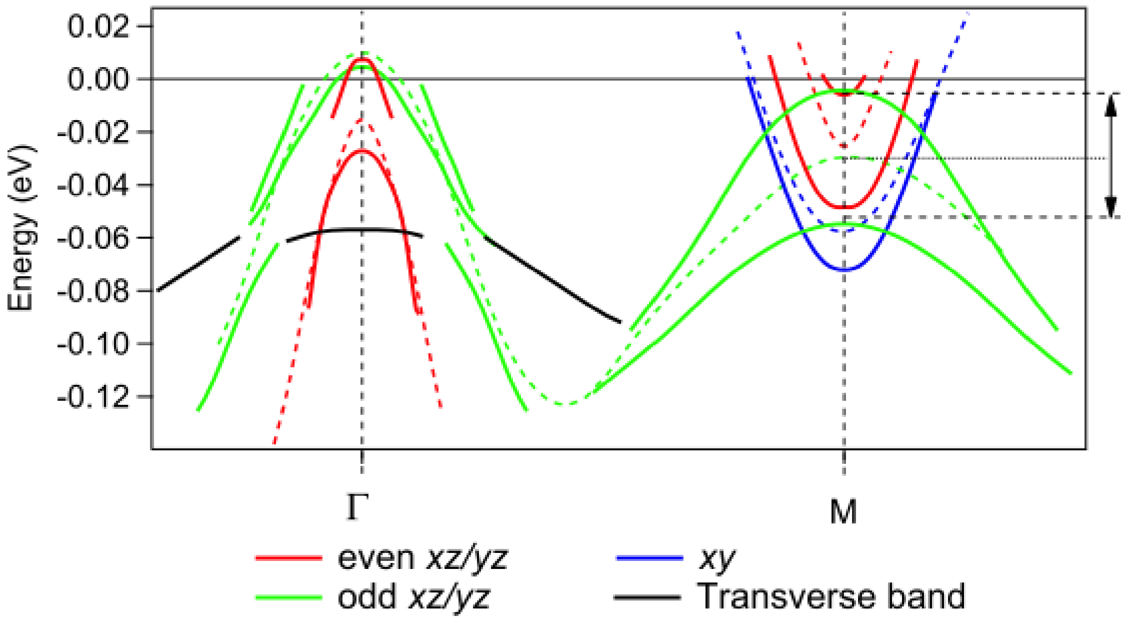
Anisotropy in the orbital mass is induced by the orbital order perturbation.
Enhanced response at the entrance of the Hund Metal.

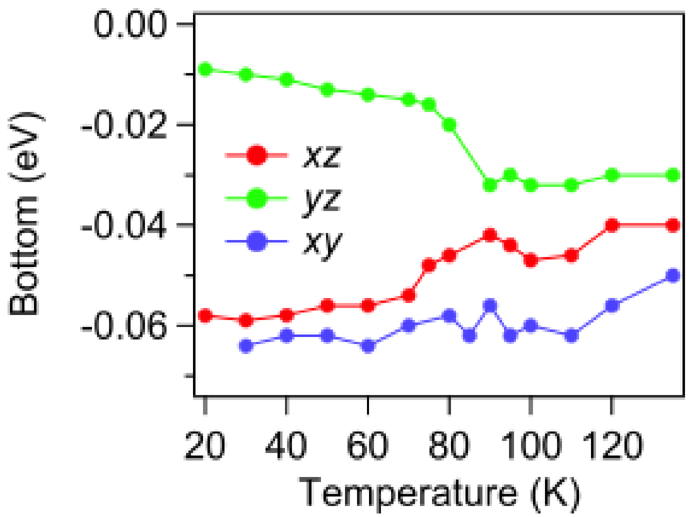


EFFECT ON THE BAND STRUCTURE

In the PARAMAGNETIC state zx and yz are degenerate = <u>NO splitting at the symmetry points</u>

In the NEMATIC state finite <u>splitting appears between zx and yz</u> bands at the symmetry points.





Fanfarillo et al. arxiv 1605.02482

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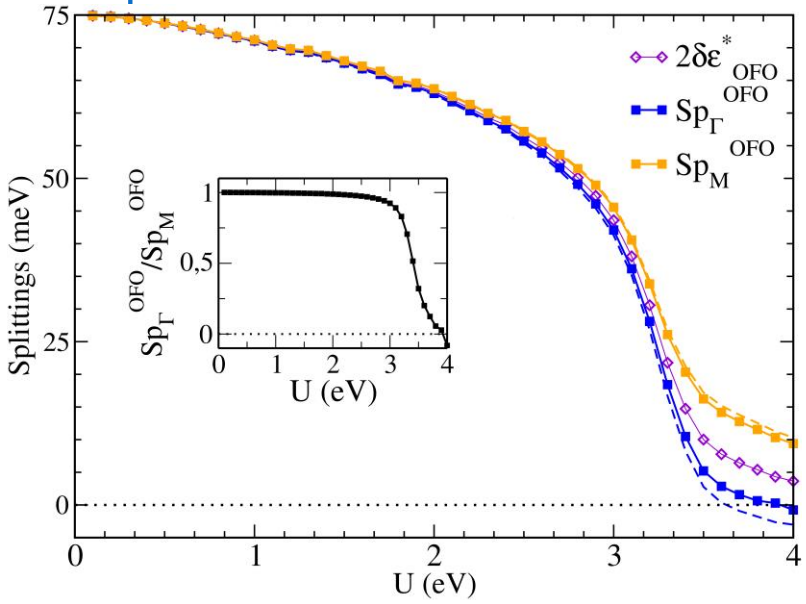
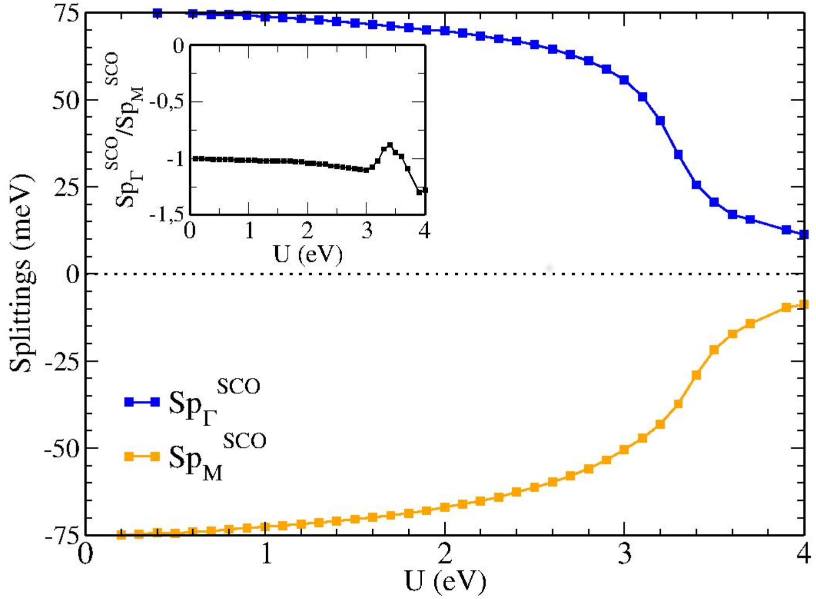
Given an orbital perturbation the naive splitting expected at the Γ and M point are:

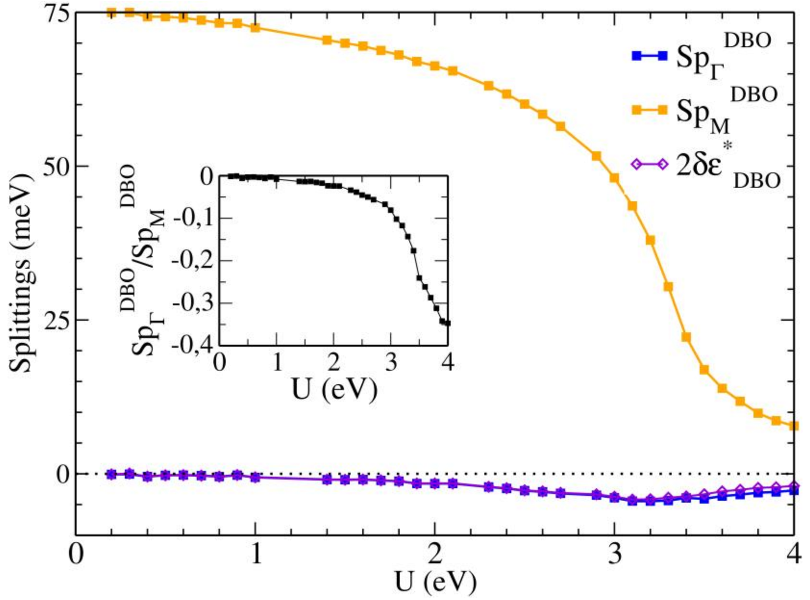
$$Sp_{\Gamma}^{OFO}(U=0) = 2\delta\epsilon \qquad Sp_{M}^{OFO}(U=0) = 2\delta\epsilon$$
$$Sp_{\Gamma}^{SCO}(U=0) = 2\delta t' \qquad Sp_{M}^{SCO}(U=0) = -2\delta t'$$
$$Sp_{\Gamma}^{DBO}(U=0) = 0 \qquad Sp_{M}^{DBO}(U=0) = 2\delta t \quad (\!$$

Interactions renormalize the band structure (via Z xz/yz anisotropy) and can modify the bare splitting

EFFECT ON THE BAND STRUCTURE







Local Correlations modify the orbital splitting:

Induce k-dependence, drive sign change …

Fanfarillo et al. arxiv 1609.06672

MASS ANISOTROPY AND ORBITAL SPLITTING

- ✓ Hund's coupling induces anisotropy in the correlation strength of *zx* and *yz* orbitals

- ✓ Hund's physics modifies the magnitude of these splittings, their relative value and even their sign.

From ARPES:
Hole/electron sign change orbital polarization observed in FeSe interpreted as a self-energy effect of a low energy orbital selective model

Fanfarillo et al. arxiv 1605.02482

Fanfarillo et al. arxiv 1609.06672

CONCLUSIONS: HUND PHYSICS IN THE NEMATIC PHASE

✓ Only orbital orders that do NOT create large occupation unbalance survive to the correlations

✓ Hund's induce anisotropy in the effective masses of *zx* and *yz* orbitals.

This anisotropy affects the renormalization of the band structure,
leading to distinctive signatures in different experimental probes including ARPES.

Important insights for low-energy modeling of IBS

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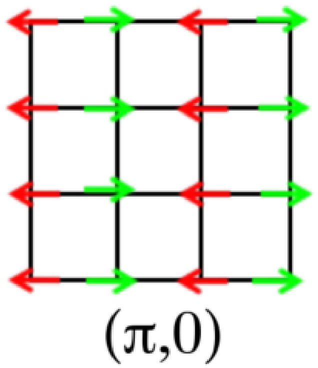
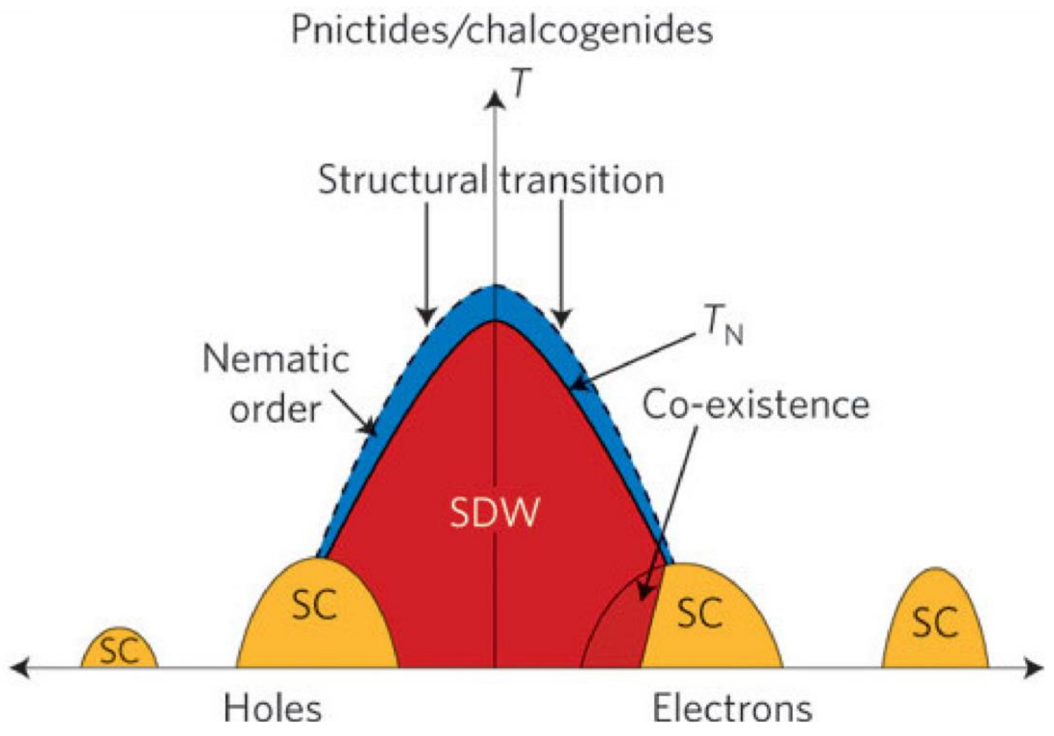
THE IRON AGE OF SC

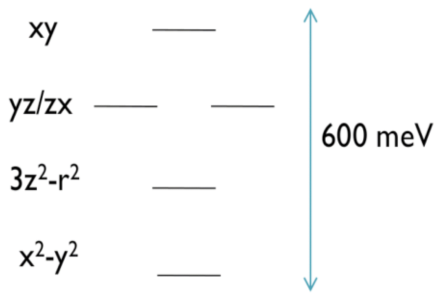
Parent Compound:

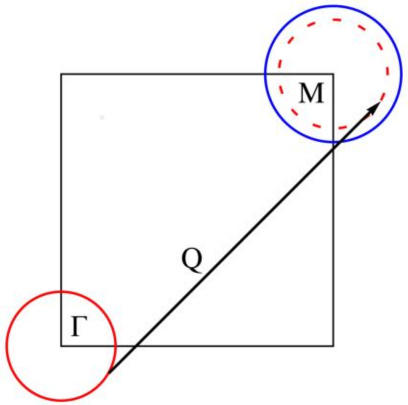
SDW bad metal

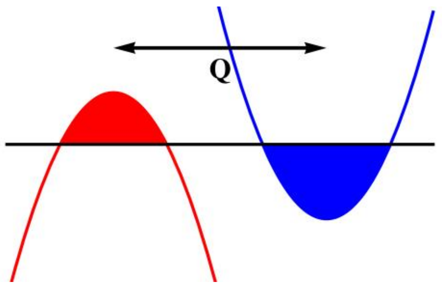




Multiband SC System:
3d Iron orbitals







Q - SDW vector

Nodless gap: s±
symmetry

IRON-BASED MATERIALS: CORRELATED OR NOT?

Contrasting evidences for correlation strength

weak

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

strong

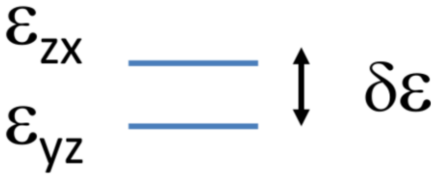
- Strong mass renormalization from ARPES, Q. Osc. with respect DFT
- bad metallicity
- strong sensitivity to doping

Itinerant electron vs Localized electrons picture

OFO PERTURBATION: JH ANALISYS

→ ***Onsite perturbation***

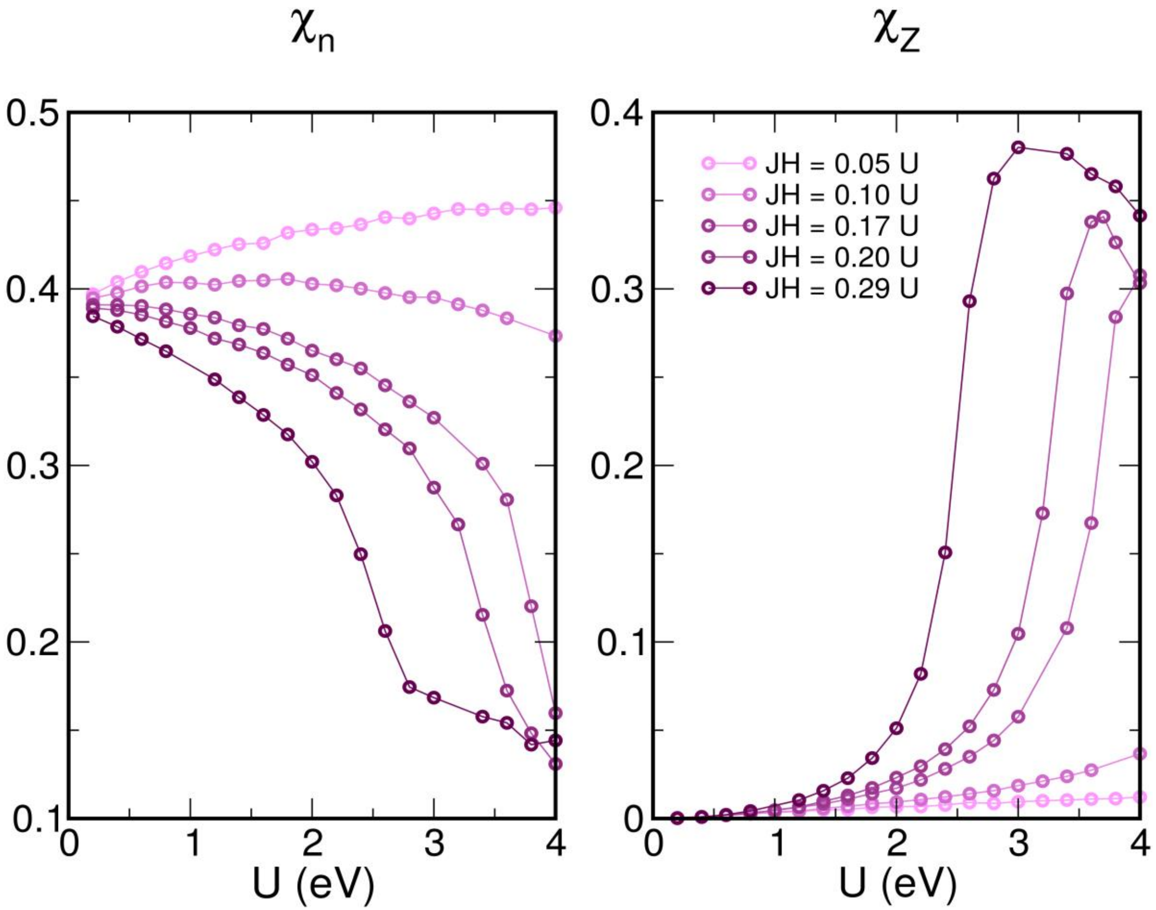
Onsite splitting $\delta\epsilon = \epsilon_{xz} - \epsilon_{yz}$



→ ***Susceptibility***

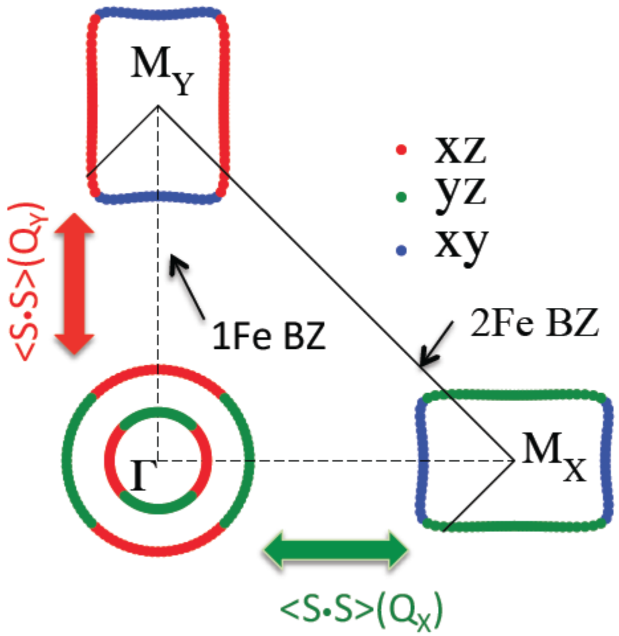
$$\chi_n = \frac{n_{yz} - n_{xz}}{\delta\epsilon}$$

$$\chi_Z = \frac{Z_{yz} - Z_{xz}}{\delta\epsilon}$$



ORBITAL SELECTIVITY IN LOW ENERGY MODEL

Project interacting multiorbital Hamilonian into low-energy model for IBS



- Nematicity follows from the yz/xz orbital
- Spin fluctuations are orbital selective
- Self-energy corrections orbital dependent shrinking of the Fermi Surfaces

Fanfarillo et al PRB 91 2015, Fanfarillo et al. arXiv: 1605.02428