Electronic correlations in Hund metals

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Outline

- Introduction:

  * Mott physics and Quasiparticle weight: basic notions

  * Iron superconductors as Hund metals

  * The role of Hund's coupling in correlations. Hund vs Mott

- Correlations in Multi-orbital systems

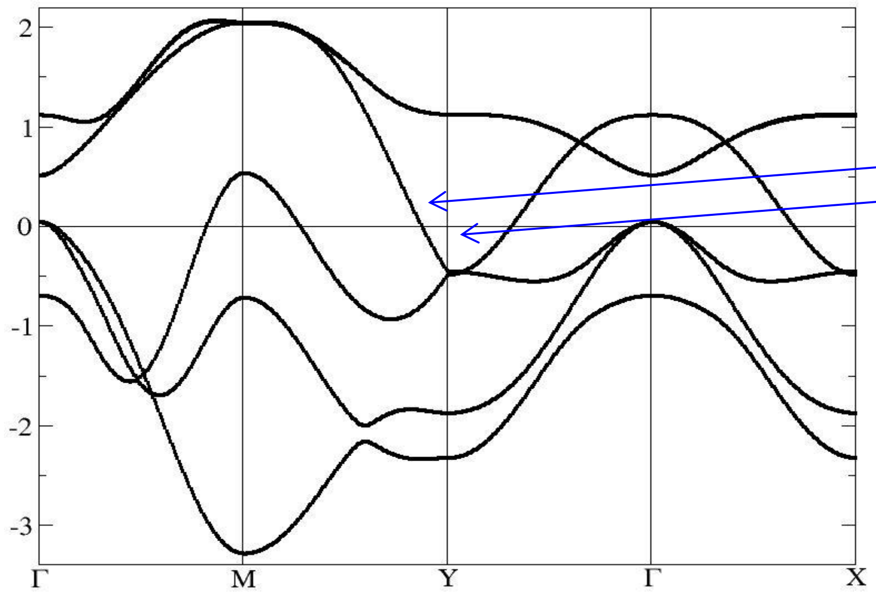
  * Quasiparticle weigth vs interactions, filling and number of orbitals

  * Charge and spin fluctuations

  * Simple understanding of correlations in Hund metals

- Summary

Metals and Insulators in band theory. Independent electrons



Metallicity
in clean systems
Bands crossing
the Fermi level
(finite DOS)

Fig: Calderón et al, PRB, 80, 094531 (2009)

Insulating behaviour
in clean systems
Bands below
Fermi level filled

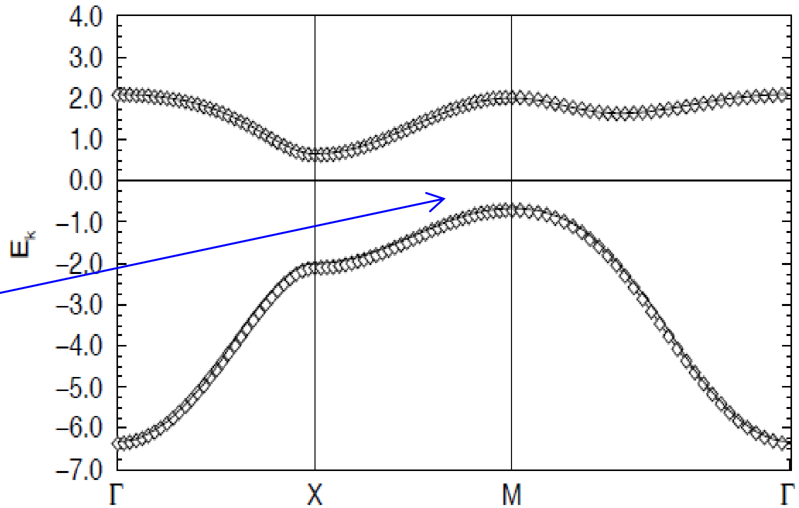


Fig: Hess & Serene, PRB 59, 15167 (1999)

Metals and Insulators in band theory. Independent electrons

Spin degeneracy:

Each band can hold 2 electrons per unit cell

Odd number of electrons per unit cell → Metallic

Even number of electrons per unit cell → Insulating

Even number of electrons per unit cell → Metallic (in case of band overlap)

Failure of independent electron picture. Mott insulators

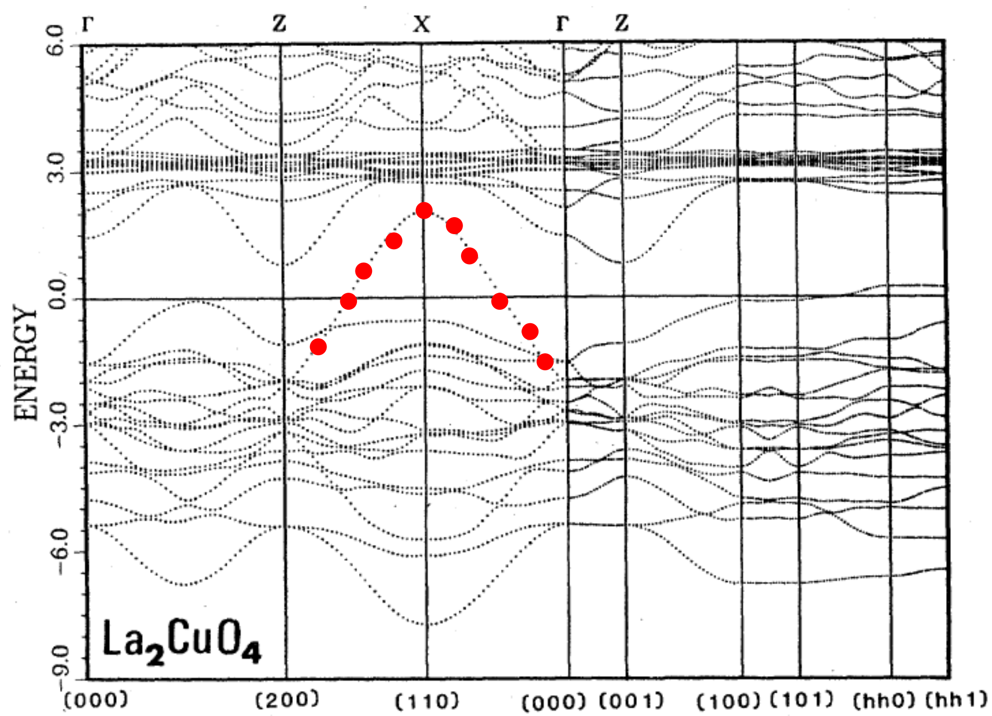


Fig: Pickett, RMP 61, 433 (1989)

Electron counting La_2CuO_4:

2 La (57x2)+Cu (29) + 4 O (4x8)

=175 electrons

Metallic behavior expected

Failure of independent electron picture. Mott insulators

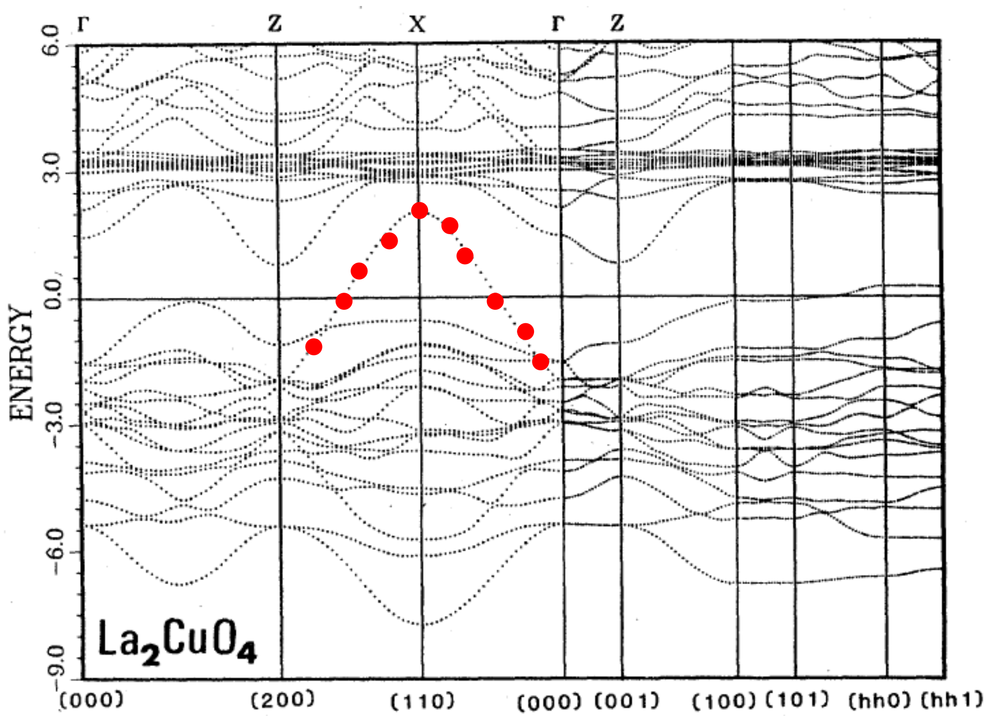


Fig: Pickett, RMP 61, 433 (1989)

Electron counting La_2CuO_4:

2 La (57x2)+Cu (29) + 4 O (4x8)

=175 electrons

Metallic behavior expected

but

Insulating behavior is found

Mott insulator:

Insulating behavior due to electron-electron interactions

Breakdown of independent electron picture

Mott insulators. The single-orbital Hubbard model at half-filling

$$H = \sum_{i,j,\sigma} t \, c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c. + U \sum_{j} n_{j,\uparrow} n_{j,\downarrow}$$

Kinetic energy

Intra-orbital repulsion

Atomic lattice with a single orbital per site and average occupancy 1 (half filling)

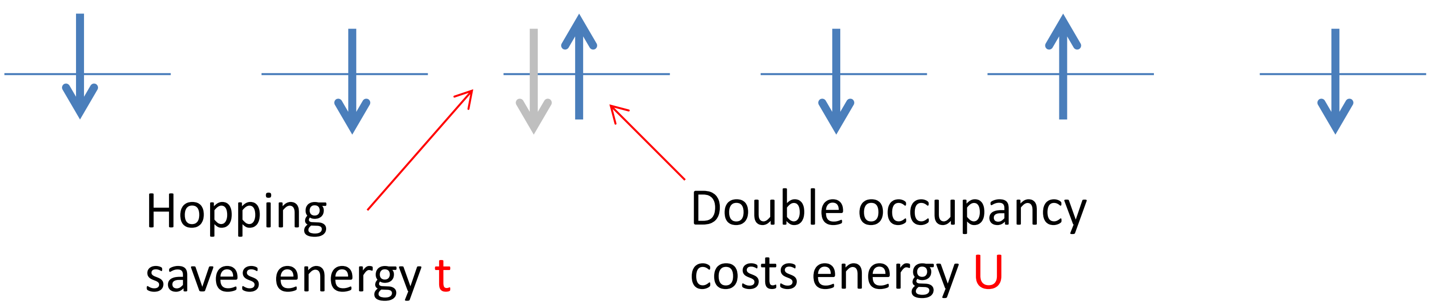
Mott insulators. The Hubbard model at half-filling

$$H = \sum_{i,j,\sigma} t\, c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c. + U \sum_{j} n_{j\uparrow} n_{j\downarrow}$$

Kinetic energy

Intra-orbital repulsion

Atomic lattice with a single orbital per site and average occupancy 1 (half filling)



For U >> t electrons localize: Mott insulator
Mott transition at Uc

But away from half-filling the system is always metallic → Correlated metal

The quasiparticle weight in the single-orbital Hubbard model

Z: a way to quantify the correlations

$$0 \leq Z \leq 1$$

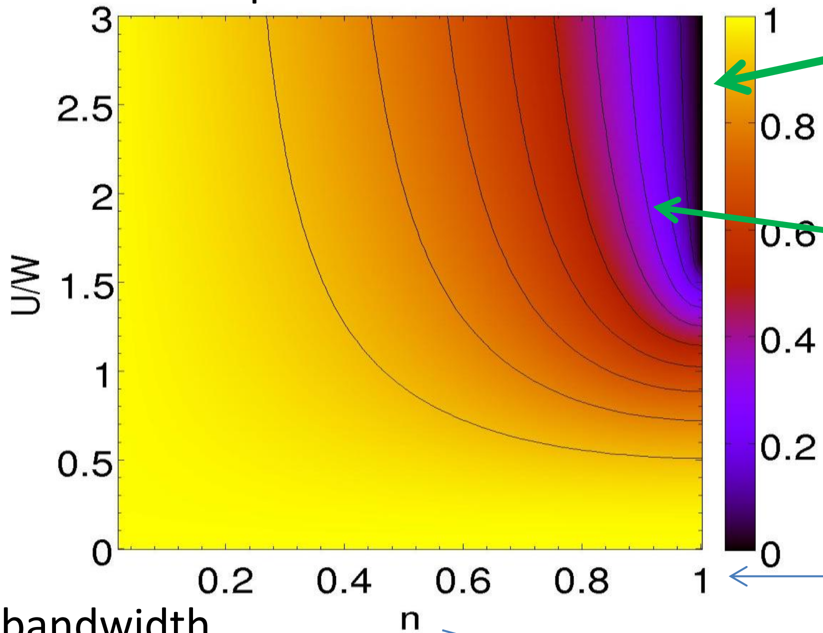
Z=1 Single-particle picture

Z=0 There are no quasiparticles
Breakdown of single-particle picture

Simple description: Heavy electron

$$Z^{-1} \propto m^*/m$$

Z colour plot for the Hubbard model



Z vanishes at the Mott transition

Correlated metal as U is increased
or half-filled is approached
(only close to the Mott transition)

Half-filling

W bandwidth
of non interacting system

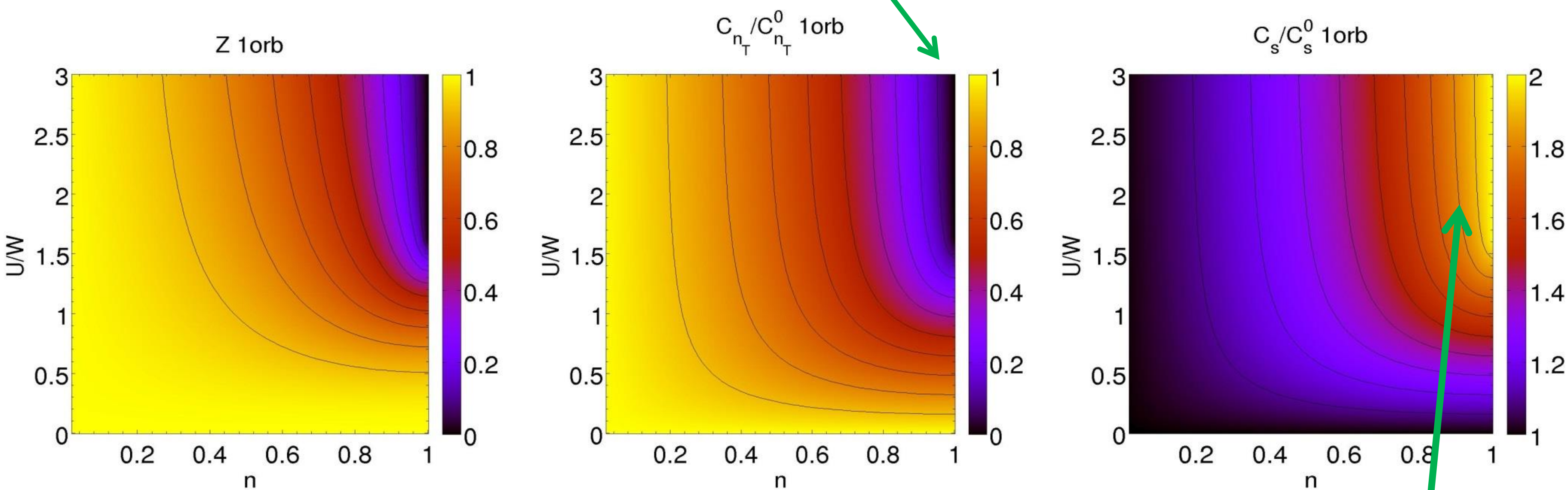
n: number of electrons per atom

Charge and spin fluctuations in the single-orbital Hubbard model

$n = \langle n \rangle + \delta n$ $\qquad C_T = \langle n^2 \rangle - \langle n \rangle^2 = \langle (\delta n)^2 \rangle$ $\qquad C_S = \langle S^2 \rangle - \langle S \rangle^2 = \langle S^2 \rangle$

C_s larger when atoms are spin polarized even if there is no long range order

Localization



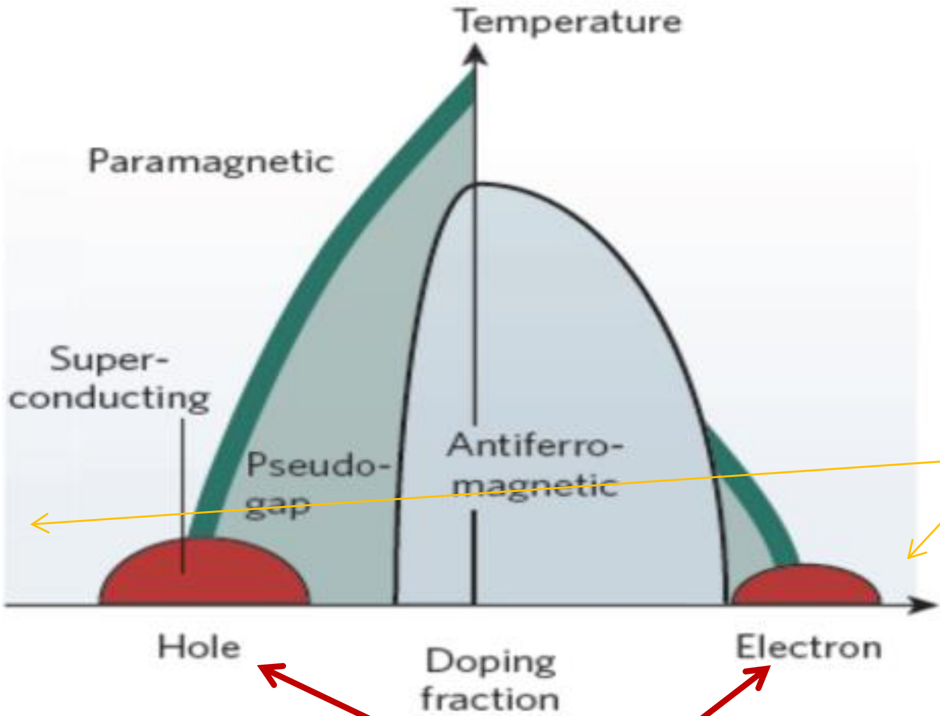
Enhancement of spin fluctuations

Mott insulator:

Suppression of charge fluctuations ⟹ **Localized spins**

$n = \langle n \rangle$

High-Tc superconductors cuprates are doped Mott insulators



Cuprates usually described with a single-orbital Hubbard model

Quasiparticles and Fermi liquid at high-doping

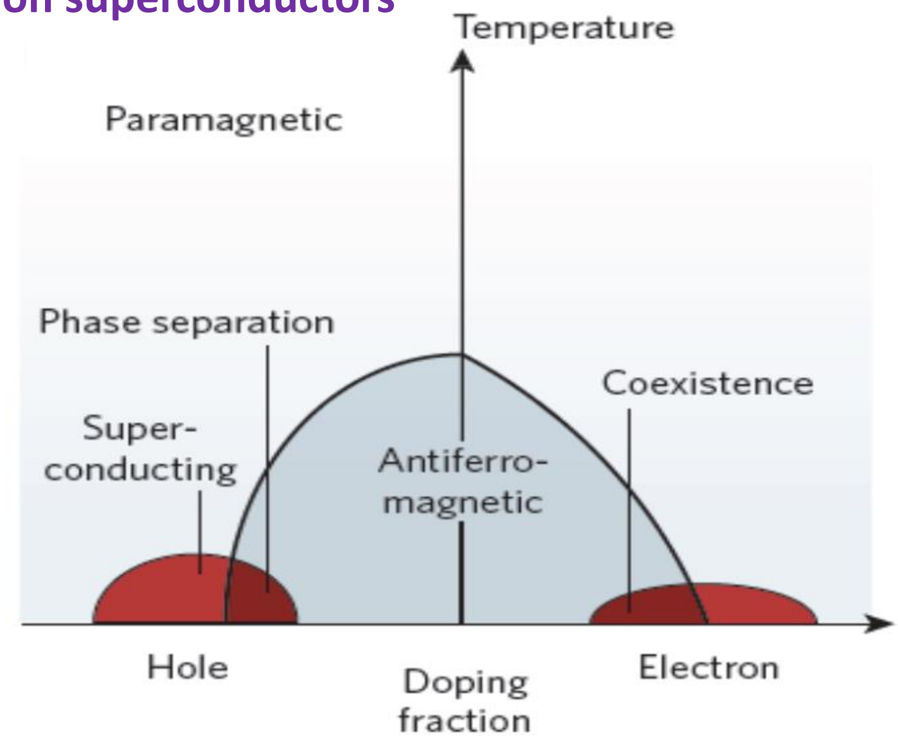
Mott insulator
at half filling (AF)

AF disappears with doping
Metallicity and superconductivity appear

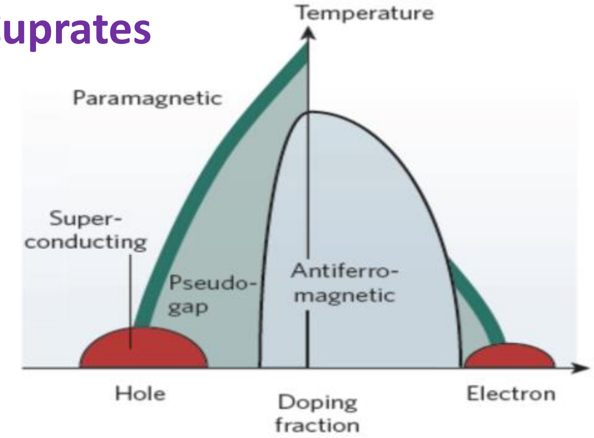
Fig: Nature 464,183 (2010)

Iron superconductors: metallic when "undoped"

Iron superconductors



Cuprates

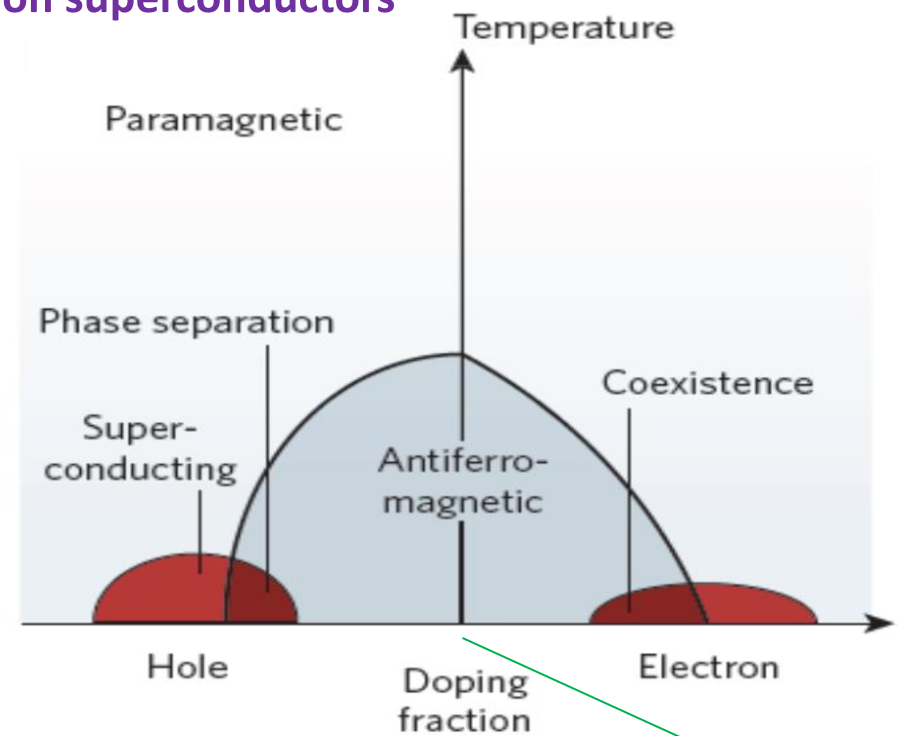


"Undoped" iron superconductors are antiferromagnetic but metallic

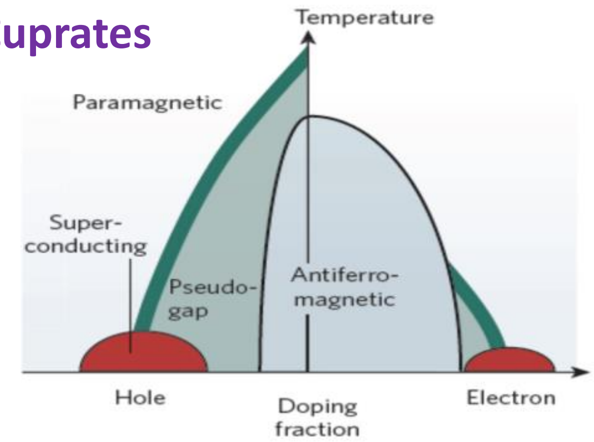
Fig: Nature 464,183 (2010)

Iron superconductors: metallic when "undoped"

Iron superconductors



Cuprates



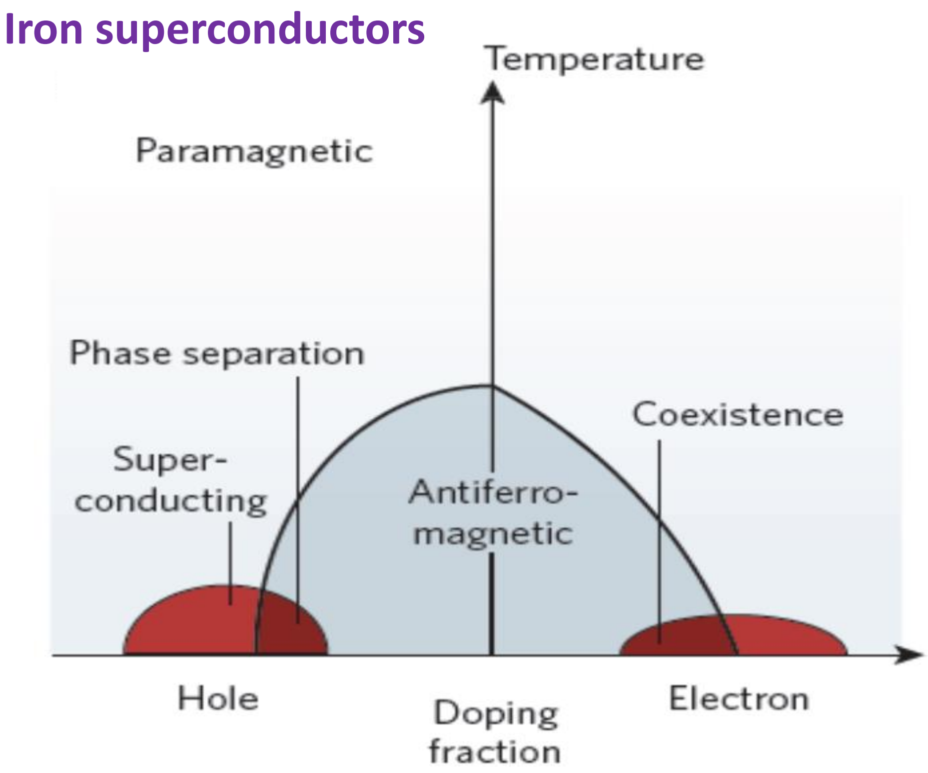
Single orbital system:
1 electron in 1 orbital
(half-filling)

"Undoped" iron superconductors
are antiferromagnetic but metallic

Multi-orbital system:
6 electrons in 5 orbitals

Fig: Nature 464,183 (2010)

Iron superconductors: metallic when “undoped”



“Undoped” iron superconductors are antiferromagnetic but metallic

Multi-orbital system:
6 electrons in 5 orbitals

- Correlated metal m*/m ~ 3 (Z ~0.33)
- Far from a Mott transition U/W < 1 (U interorbital repulsion, W bandwidth)
- Hund’s coupling plays a key role in the correlations

↓

Iron superconductors as Hund metals

Fig: Nature 464,183 (2010)

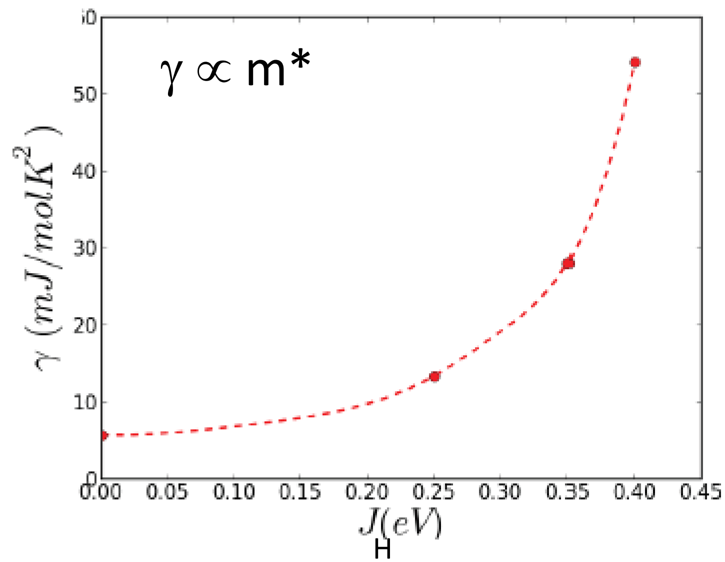
Correlations in Hund metals and iron superconductors: Hund vs Mott

Iron superconductors as Hund metals

- Correlations driven by Hund J_H weakly dependent on U,

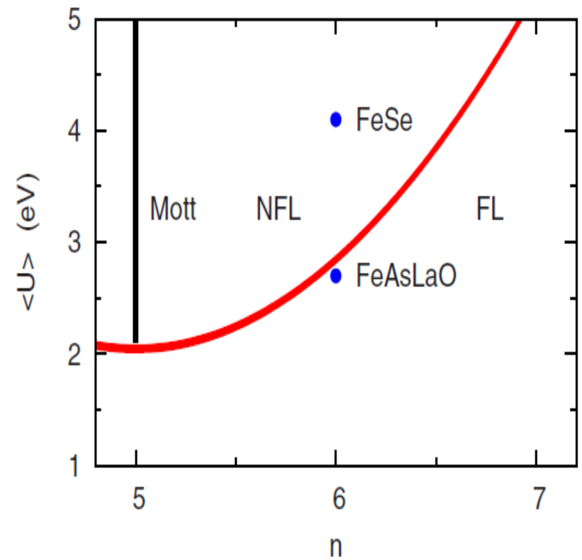
- Not in proximity to a Mott insulator

- Properties essentially different to a doped Mott insulator



Haule & Kotliar NJP 11,025021 (2009)

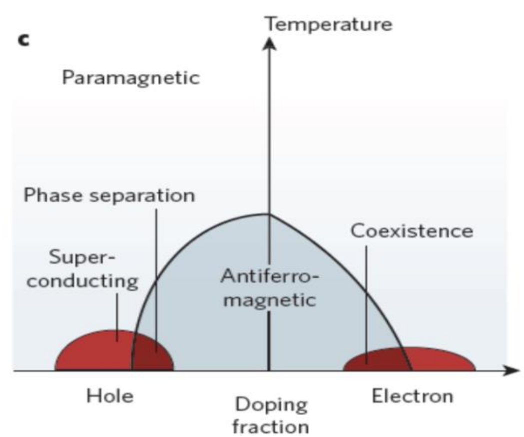
Iron superconductors as doped Mott insulators



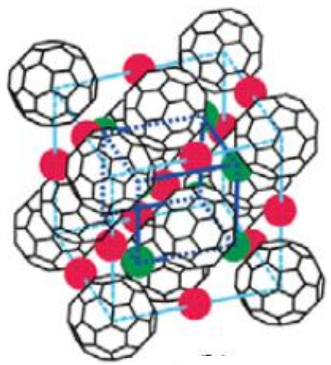
J_H/U=0.25

Ishida & Liebsch, PRB 81, 054513 (2010)
Liebsch & Ishida, PRB 82, 155106 (2010)

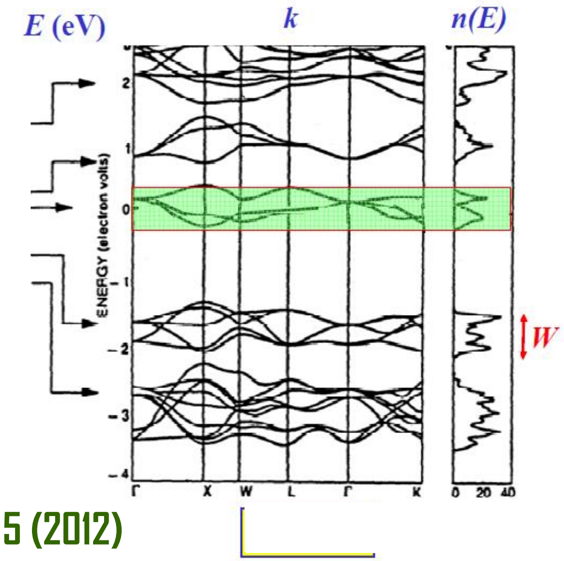
Correlations controlled by the **proximity in doping** to a Mott insulating state



Multi-orbital systems



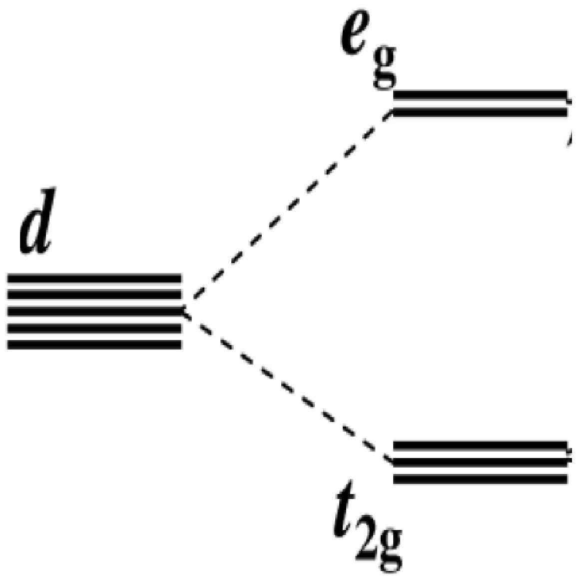
A_3C_{60}

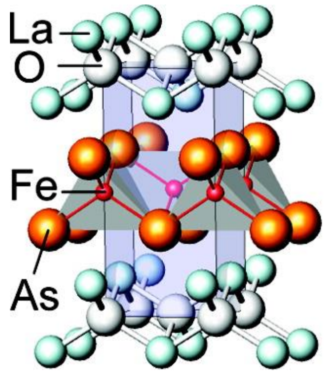


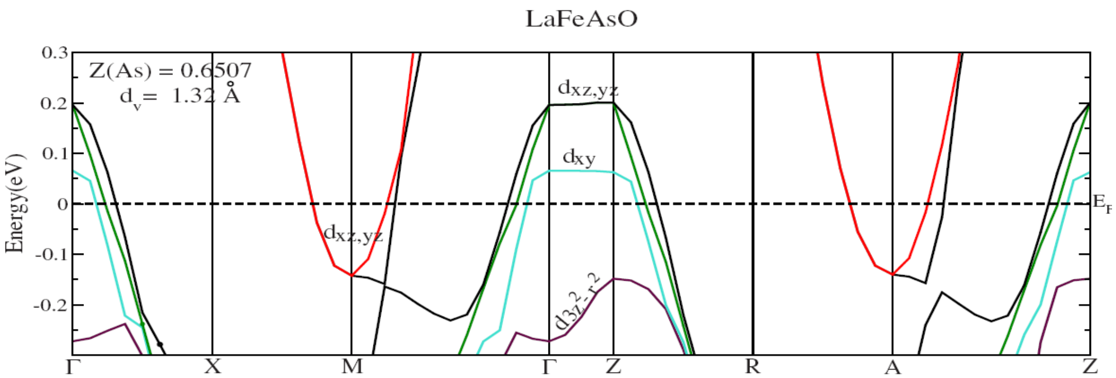
Alloul, EPJ Web of Conf. 23, 15 (2012)

Erwin & Pickett, Science 254, 842 (1991)

Oxides with cubic symmetry







Kamihara et al, JACS, 130, 3296 (2008).

Vildosola et al, PRB 78, 064518 (2008)

Hubbard-Kanamori Hamiltonian for multi-orbital systems

$$H = \sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c^\dagger_{i,\gamma,\sigma} c_{j,\beta,\sigma} + h.c. + U \sum_{j,\gamma} n_{j,\gamma,\uparrow} n_{j,\gamma,\downarrow}$$

Tight-binding (hopping) — Intra-orbital repulsion

$$+ \left(U' - \frac{J_H}{2}\right) \sum_{j,\gamma>\beta,\sigma,\tilde{\sigma}} n_{j,\gamma,\sigma} n_{j,\beta,\tilde{\sigma}} - 2J_H \sum_{j,\gamma>\beta} \vec{S}_{j,\gamma} \vec{S}_{j,\beta}$$

Inter-orbital repulsion — Hund's coupling

$$+ J' \sum_{j,\gamma\neq\beta} c^\dagger_{j,\gamma,\uparrow} c^\dagger_{j,\gamma,\downarrow} c_{j,\beta,\downarrow} c_{j,\beta,\uparrow} + \sum_{j,\gamma,\sigma} \epsilon_\gamma n_{j,\gamma,\sigma} .$$

Pair hopping — Crystal-field

In the presence of rotational symmetry $U' = U - 2J_H$ $J' = J_H$

Two interaction parameters: U, J_H

Hubbard-Kanamori Hamiltonian: Interaction terms

Intra-orbital repulsion — Inter-orbital Repulsion (different spin) — Inter-orbital Repulsion (same spin)

$$U\sum_{m}\hat{n}_{m\uparrow}\hat{n}_{m\downarrow}+U'\sum_{m\neq m'}\hat{n}_{m\uparrow}\hat{n}_{m'\downarrow}+(U'-J_H)\sum_{m<m',\sigma}\hat{n}_{m\sigma}\hat{n}_{m'\sigma}+$$

$$-J_H\sum_{m\neq m'}d^{+}_{m\uparrow}d_{m\downarrow}d^{+}_{m'\downarrow}d_{m'\uparrow}+J'\sum_{m\neq m'}d^{+}_{m\uparrow}d^{+}_{m\downarrow}d_{m'\downarrow}d_{m'\uparrow}$$

Spin flip — Pair hopping

$U'=U-2J_H$

Hubbard-Kanamori Hamiltonian: Interaction terms

Intra-orbital repulsion | Inter-orbital Repulsion (different spin) | Inter-orbital Repulsion (same spin)

$$U\sum_{m}\hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U'\sum_{m\neq m'}\hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U'-J_H)\sum_{m<m',\sigma}\hat{n}_{m\sigma}\hat{n}_{m'\sigma} +$$

$$-J_H\sum_{m\neq m'}d^{+}_{m\uparrow}d_{m\downarrow}d^{+}_{m'\downarrow}d_{m'\uparrow} + J'\sum_{m\neq m'}d^{+}_{m\uparrow}d^{+}_{m\downarrow}d_{m'\downarrow}d_{m'\uparrow}$$

Spin flip | Pair hopping

$U' = U - 2J_H$

Hubbard-Kanamori Hamiltonian: Interaction terms

Intra-orbital repulsion

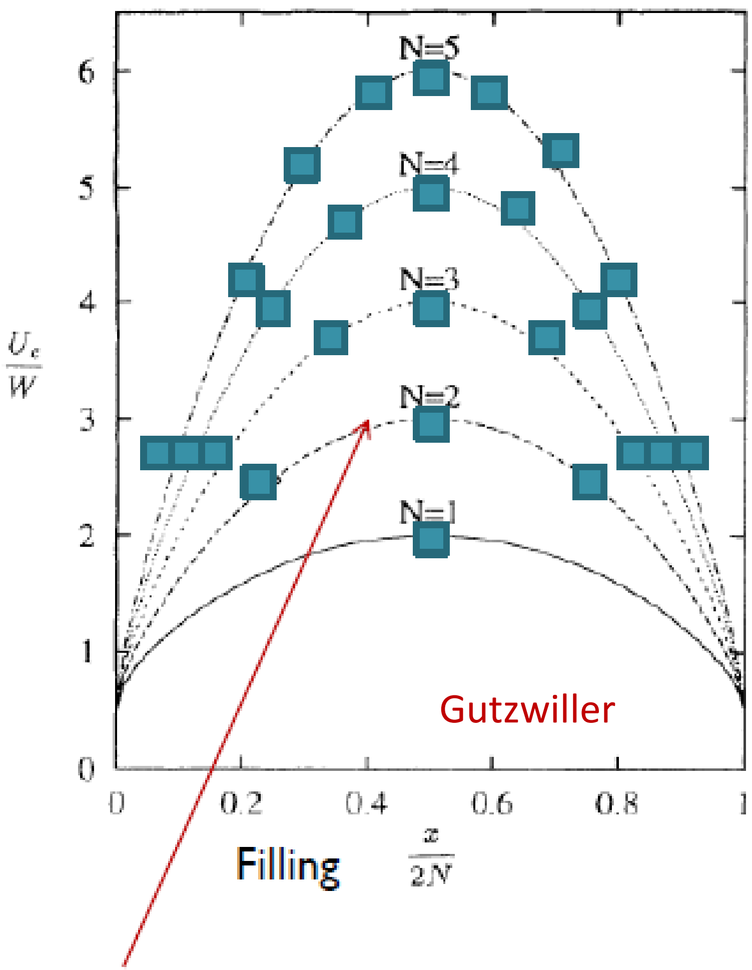
Inter-orbital Repulsion (different spin)

Inter-orbital Repulsion (same spin)

$$U \sum_{m} \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U' \sum_{m \neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U' - J_H) \sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma} +$$

$U' = U - 2J_H$

Mott transition in multi-orbital systems at Zero Hund

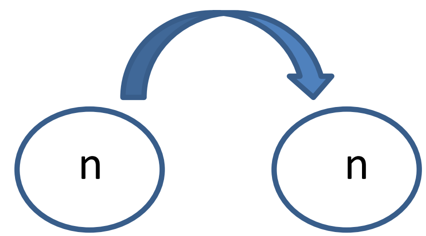


Zero Hund. Uc larger at half filling

N-orbital system with n electrons/atom:

- It can hold up to 2N electrons
- Half-filling n=N (1 electron/orbital)
- Mott transition not only at half-filling but for all integer n

Lu PRB 49, 5687 (1994)



Atomic gap: E(n+1)+E(n-1)- 2E(n)=U
vs
Kinetic Energy

Effective kinetic energy larger due to orbital degeneracy

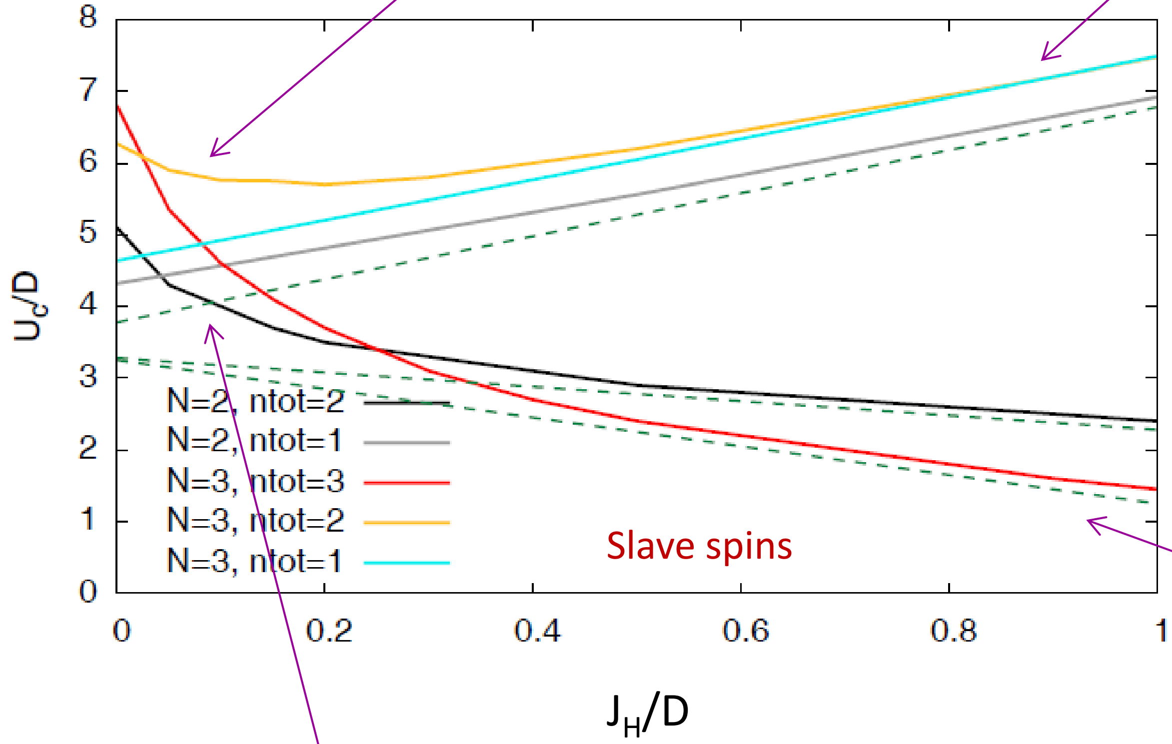
Mott transition in multi-orbital systems at Finite Hund

Degeneracy
reduced by Hund's coupling

Away fom half filling:
With J_H the atomic gap decreases.

$U-3J_H$

Uc increases



Half filling : with J_H
Atomic gap increases

$U+(N-1)J_H$

Uc decreases with J_H

Degeneracy (effective kinetic energy)
strongly reduced by Hund's coupling

De'Medici PRB 83, 205112 (2011)

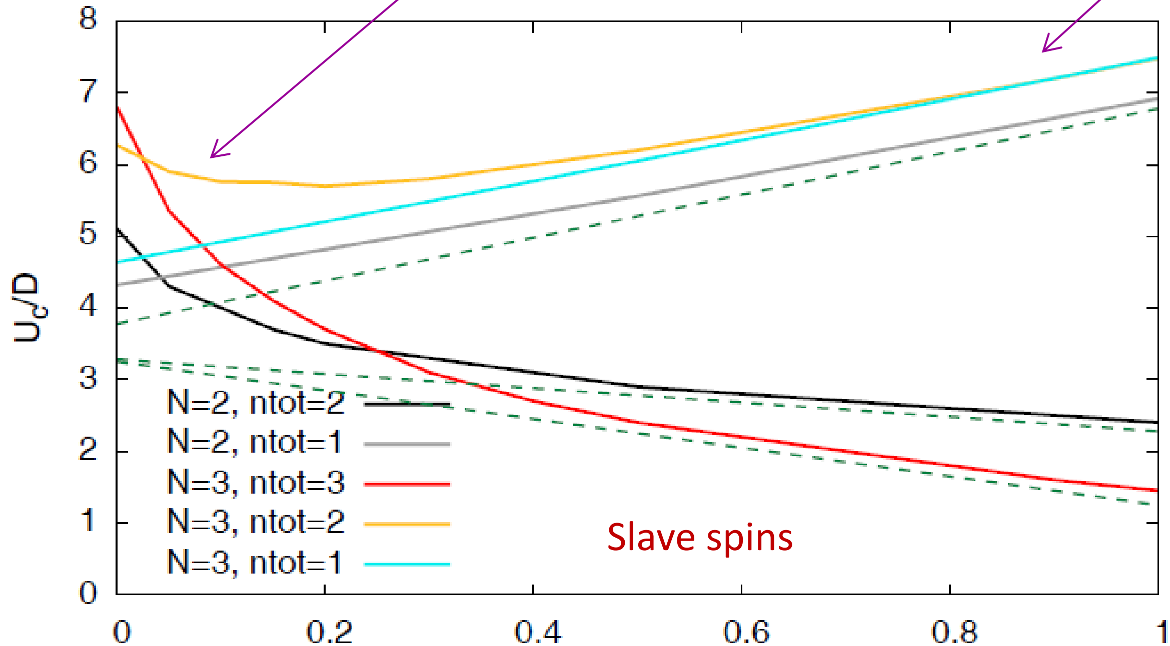
Mott transition in multi-orbital systems at Finite Hund

Effective kinetic energy reduced by Hund's coupling

Away fom half filling:
With J_H the atomic gap decreases.

$U-3J_H$

Uc increases and promotes metallicity



J_H/D

De'Medici PRB 83, 205112 (2011)

n ≠ 1, N, N-1
Conflicting behavior of Hund's coupling

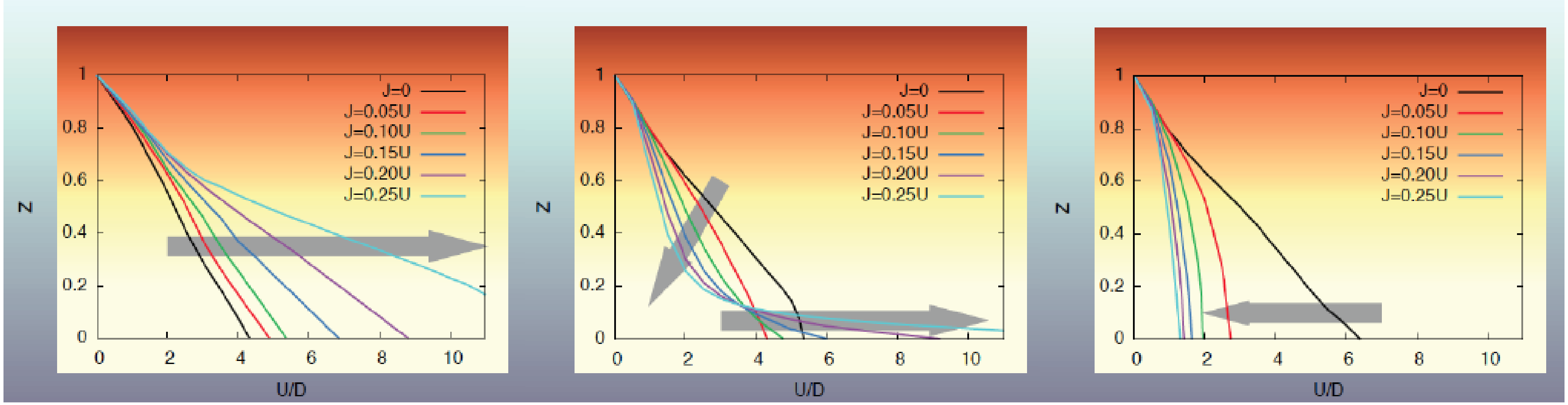
Examples:

* iron superconductors 6 electrons in 5 orbitals
* ruthenates 4 electrons in 3 orbitals
* $SrCrO_3$ 2 electrons in 3 orbitals

Hund's coupling and bad metallicity

3 orbital system

DMFT



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

n=1 electron or 1 hole

J_H promotes metallicity

Uc increases

Quasiparticle weight increases

n=half-filling

J_H promotes insulating behavior

Uc increases

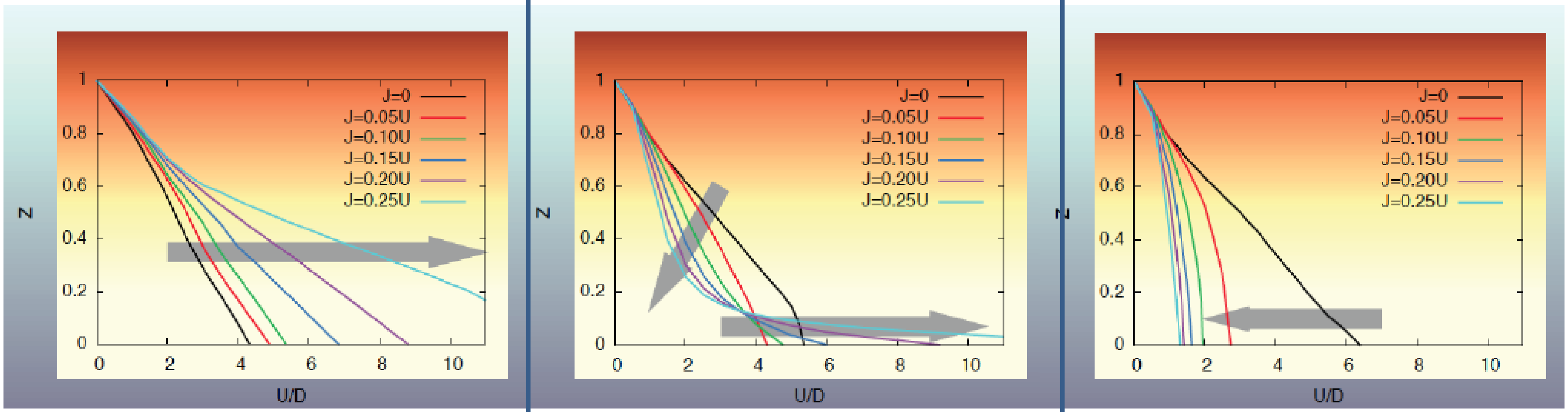
Z decreases

De'Medici et al PRL 107, 255701 (2011)

Hund's coupling and bad metallicity

3 orbital system

DMFT



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

n=1 electron or 1 hole

J_H promotes metallicity

Uc increases

Qp weight Z increases

n ≠ 1 electron ,1 hole, half-filling

J_H promotes bad metallic Behavior (correlated metal)

Large Uc but small Z

n=half-filling

J_H promotes insulating behavior

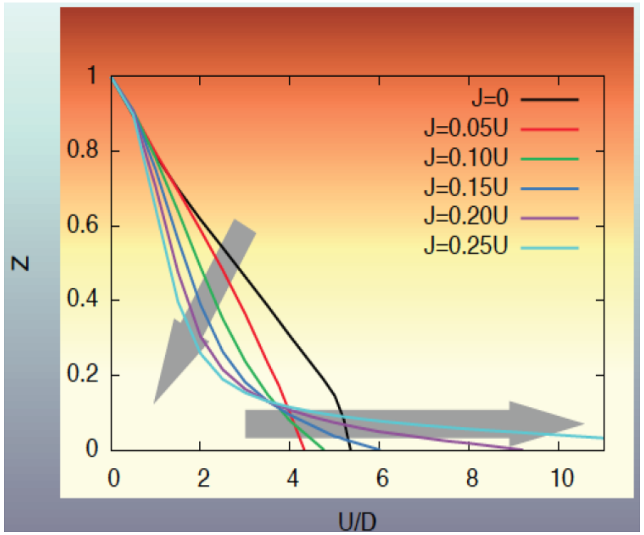
Uc increases

Z decreases

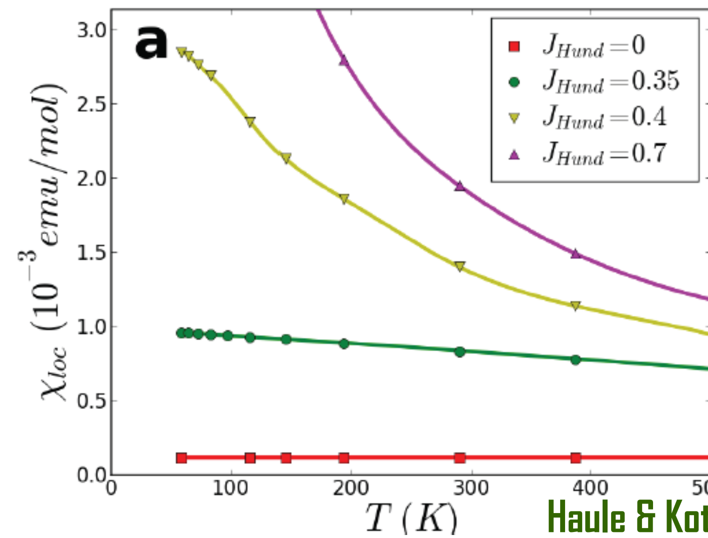
De'Medici et al PRL 107, 255701 (2011)

Hund metals and spin freezing

3 orbital system DMFT



Iron superconductors DMFT



Haule & Kotliar
NJP 11,025021 (2009)

n ≠ 1 electron ,1 hole,
half-filling

J_H promotes bad metallic

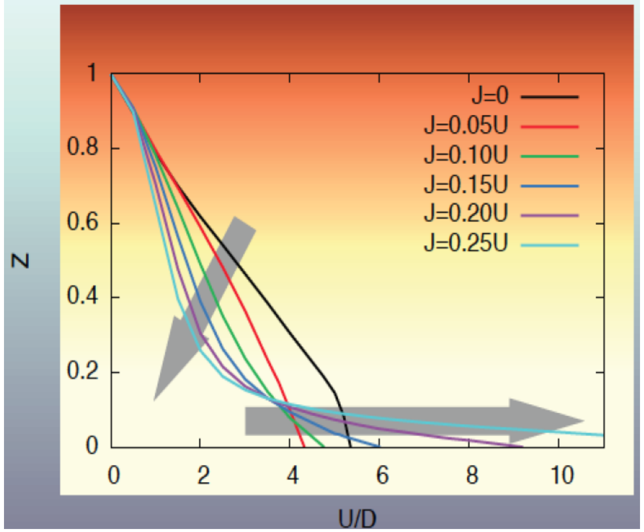
Behavior (correlated metal)

Large Uc but small Z

De'Medici et al PRL 107, 255701 (2011)

Hund metals and spin freezing

3 orbital system DMFT



n ≠ 1 electron ,1 hole, half-filling

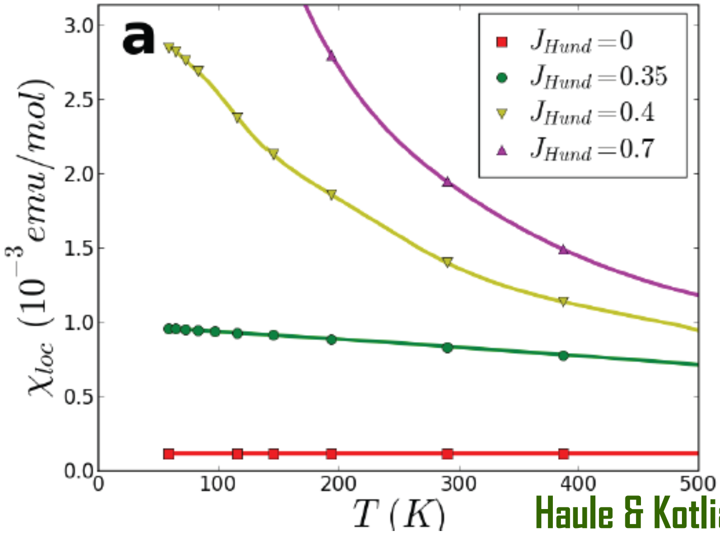
J_H promotes bad metallic

Behavior (correlated metal)

Large Uc but small Z

De'Medici et al PRL 107, 255701 (2011)

Iron superconductors DMFT



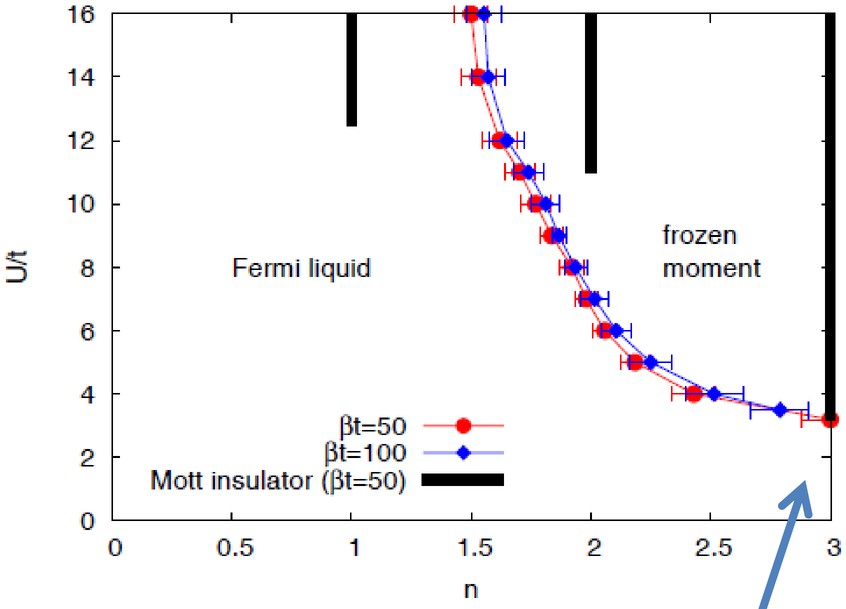
Haule & Kotliar NJP 11,025021 (2009)

Hund metals

- Correlations driven by Hund J_H weakly dependent on U,
- Not in proximity to a Mott insulator
- Properties essentially different to a doped Mott insulator (wide Hubbard bands)

Doping dependence in Hund metals

DMFT 3 orbitals $J_H/U=1/6=0.167$

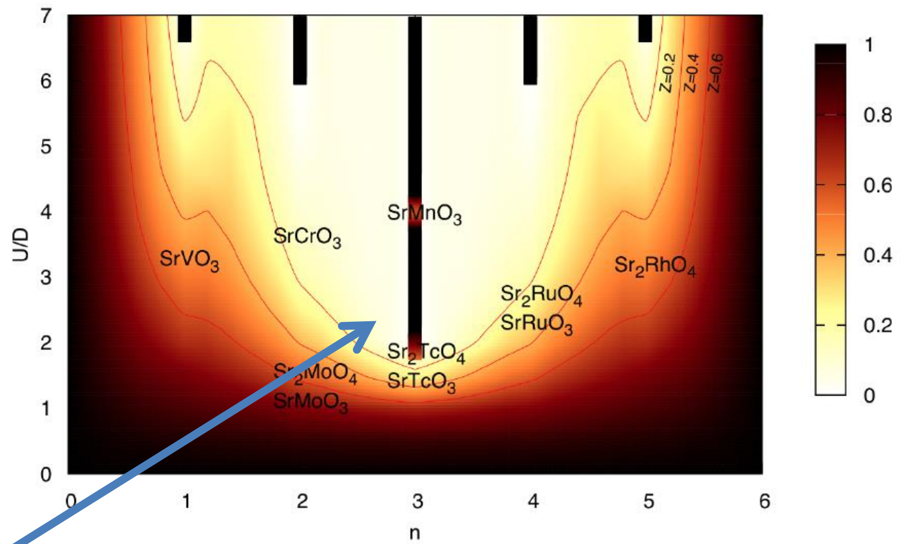


Werner et al PRL 101, 166405 (2008)

Fermi liquid behavior with very small Z

DMFT N=3 orbitals and J/U=0.15

Z colour plot



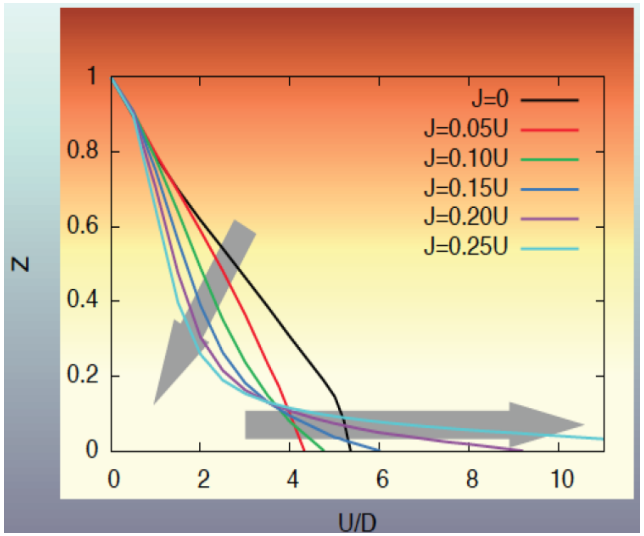
De'Medici et al PRL 107, 255701 (2011),
Georges et al, Ann. Rev. Cond. Matt. Phys. 4,137 (2013)

The Mott transition at half-filling seems to play a special role in setting the value of Z

Correlations in Hund metals: Hund vs Mott

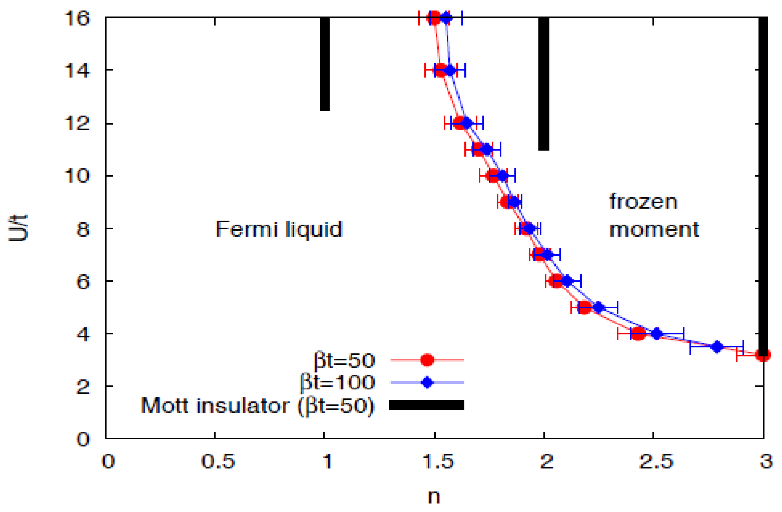
Hundness as oppossed to Mottness

- Correlations driven by Hund J_H weakly dependent on U,
- Not in proximity to a Mott insulator
- Properties essentially different to a doped Mott insulator



Haule & Kotliar NJP 11,025021 (2009)
Georges et al, Ann. Rev. Cond. Matt. Phys. 4,137 (2013)

Hund metals as doped Mott insulators



Correlations controlled by the **proximity in doping** to a Mott insulating state

Werner et al PRL 101, 166405 (2008)
Ishida & Liebsch, PRB 81, 054513 (2010)

Summary

- Single-orbital Hubbard model:

  * Mott transition at half-filling U>>t (U/W ~1.5)

  * Away from half-filling or for $U<U_c$: correlated metal. Suppression of Quasiparticle weight Z and Charge fluctuations & enhancement of spin fluctuations

- Multi-orbital Hubbard-Kanamori Hamiltonian:

  * Mott transition at all integer filling. U_c depends on J_H and filling n

  * J_H promotes metallic behavior for n=1 electron or 1 hole. Z and U_c increase.

  * J_H promotes insulating behavior at half-filling. Z and U_c decrease.

  * J_H promotes bad metallic behavior for n≠1 electron, 1 hole, half-filling. **Hund metal**

    U_c non-monotonic, but increases at large J_H

    Z small. Coherent-incoherent crossover with temperature. Spin freezing

    Dependence on doping. **Hund vs Mott ?**

The model: Degenerate orbitals with density-density interactions

- Multi-orbital systems with N orbitals (N=2-5) and n electrons (half-filling n=N)
- **Equivalent orbitals**: No crystal field splitting or hybridization between orbitals

  Hopping to 1st nearest neighbors equal for all the orbitals

  Non-interacting bandwidth W (2D but generic results)

Intra-orbital repulsion — Inter-orbital Repulsion (different spin) — Inter-orbital Repulsion (same spin)

$$U\sum_{m}\hat{n}_{m\uparrow}\hat{n}_{m\downarrow}+U'\sum_{m\neq m'}\hat{n}_{m\uparrow}\hat{n}_{m'\downarrow}+(U'-J_H)\sum_{m<m',\sigma}\hat{n}_{m\sigma}\hat{n}_{m'\sigma}$$

$U'=U-2J_H$ → U, J_H two interaction parameters **max $J_H/U=1/3$**

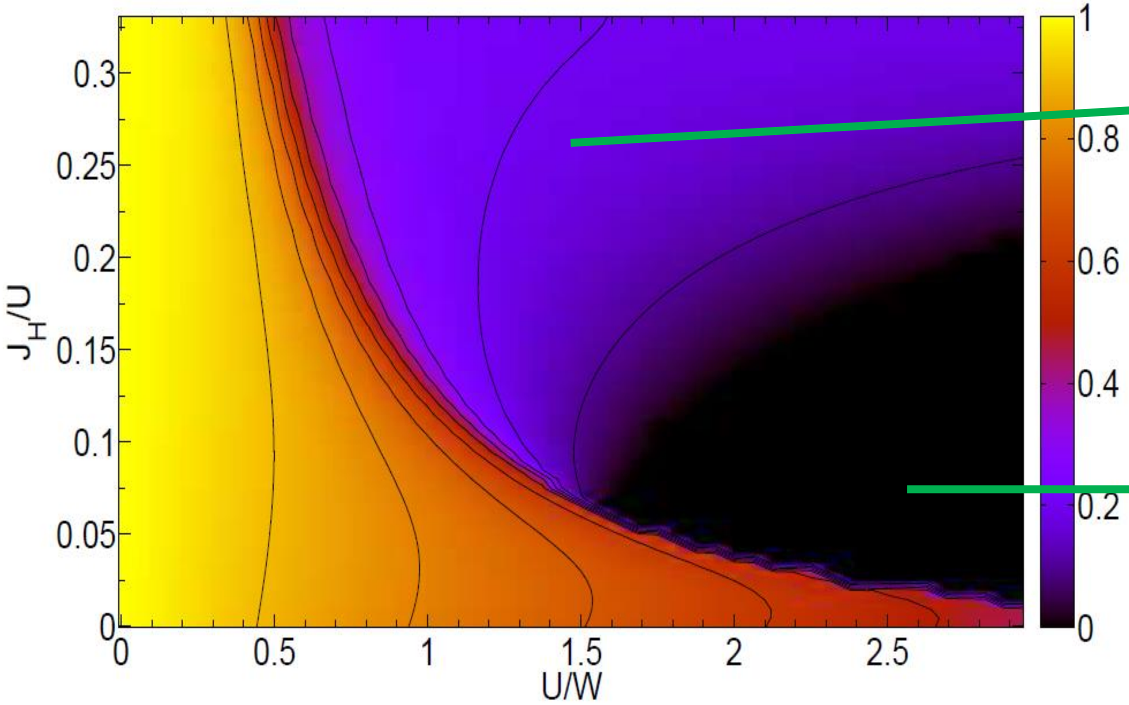
- Hamilonian solved with Slave Spin Technique: Z, Charge & Spin fluctuations

The quasiparticle weight as a function of interactions

6 electrons in 5 orbitals, as in "undoped" iron superconductors (or 4 electrons in 5 orbitals)

Particle-hole symmetry with respect to half-filling

Quasiparticle weight, colour plot



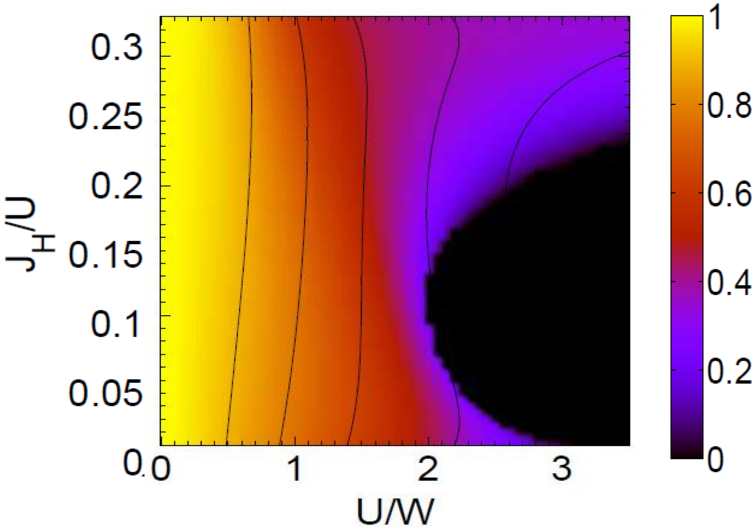
Hund metal

Mott insulator

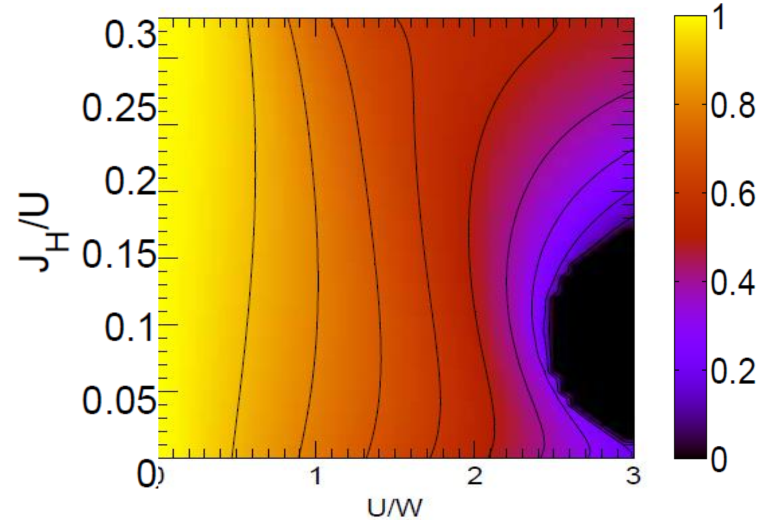
L. Fanfarillo, EB arXiv:1501.04607

The quasiparticle weight as a function of interactions

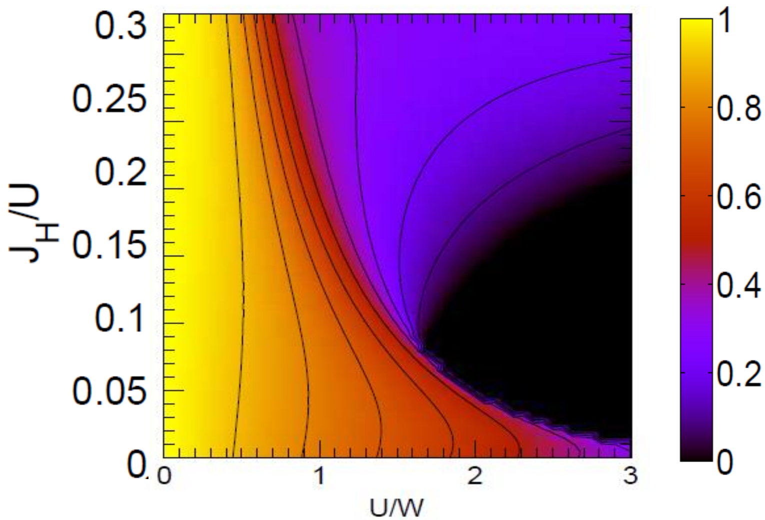
2 electrones en 3 orbitales, x=0.66



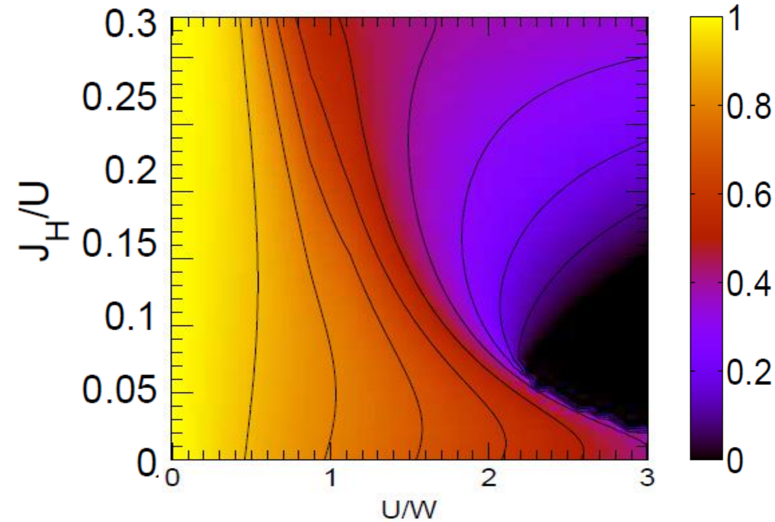
2 electrones en 4 orbitales, x=0.50



3 electrones en 4 orbitales, x=0.75

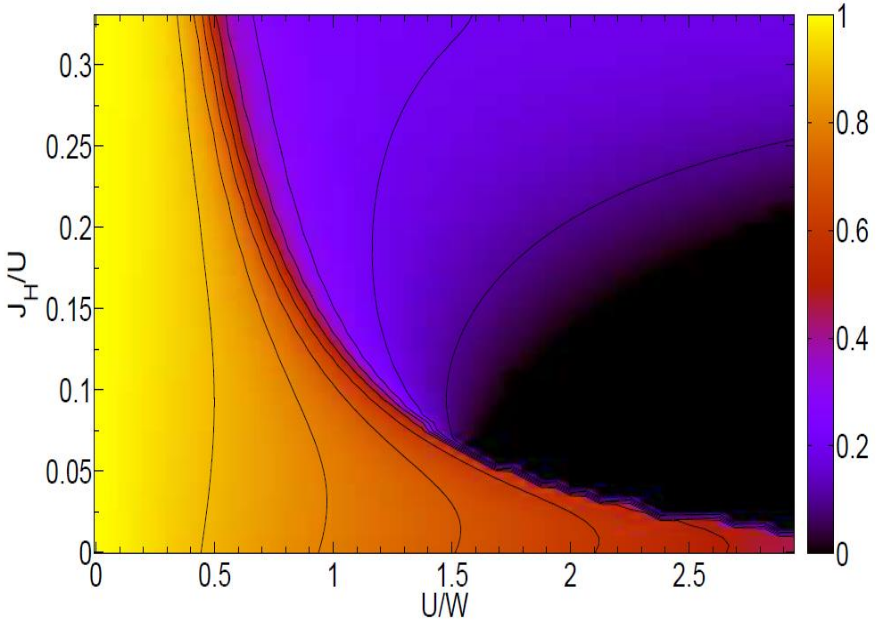


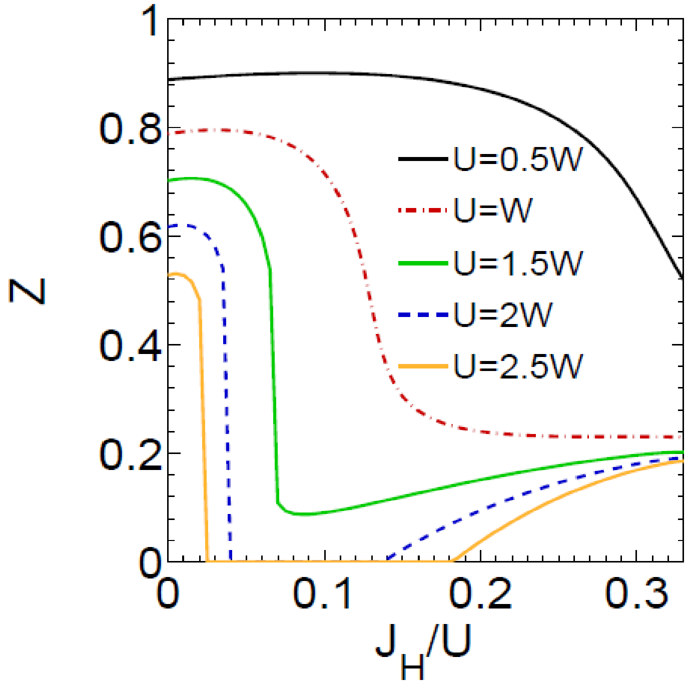
3 electrones en 5 orbitales, x=0.60



The quasiparticle weight as a function of interactions

6 electrons in 5 orbitals,

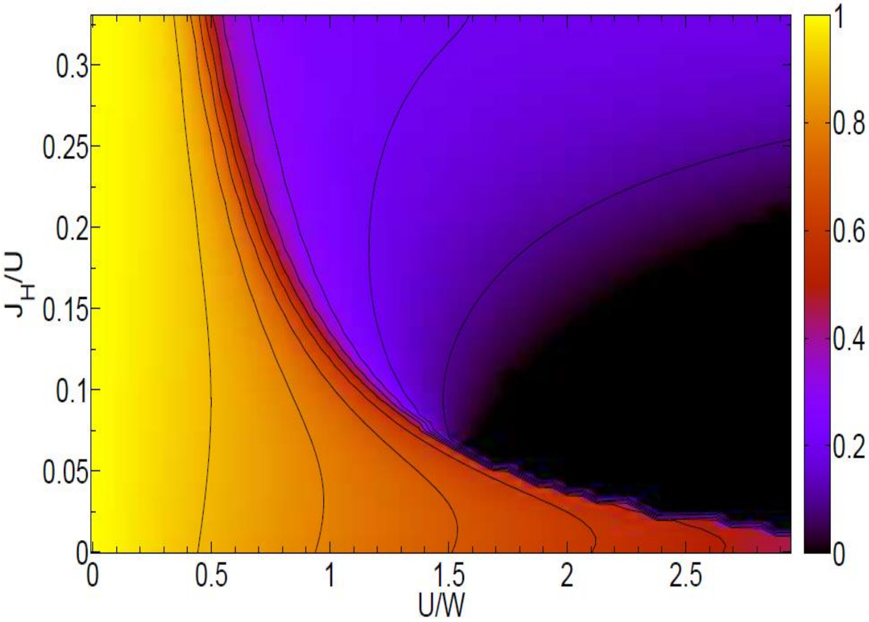


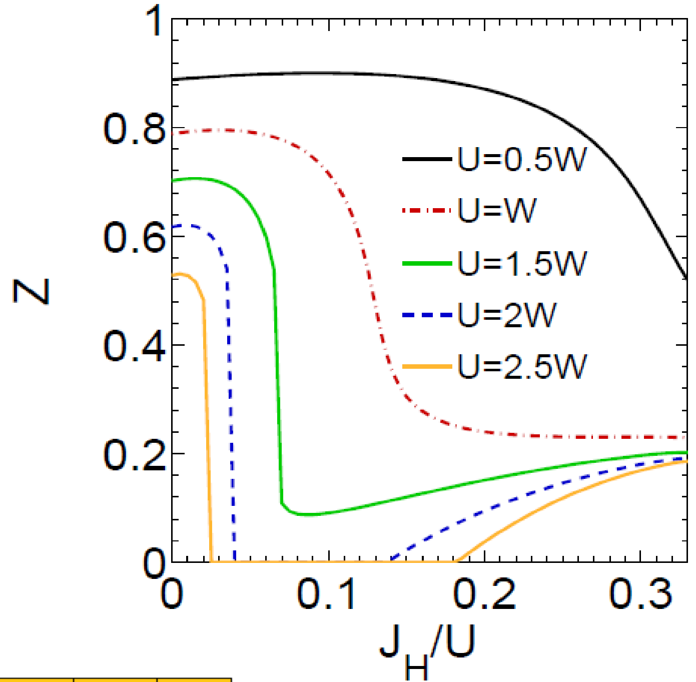


L. Fanfarillo, EB arXiv:1501.04607

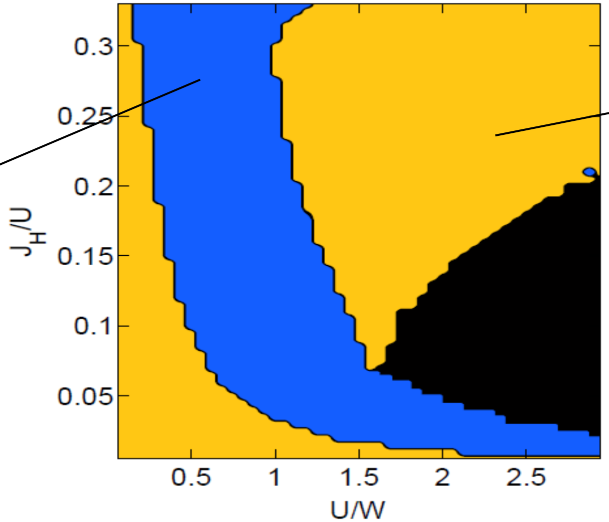
The quasiparticle weight as a function of interactions

6 electrons in 5 orbitals,





Z decreases with J_H

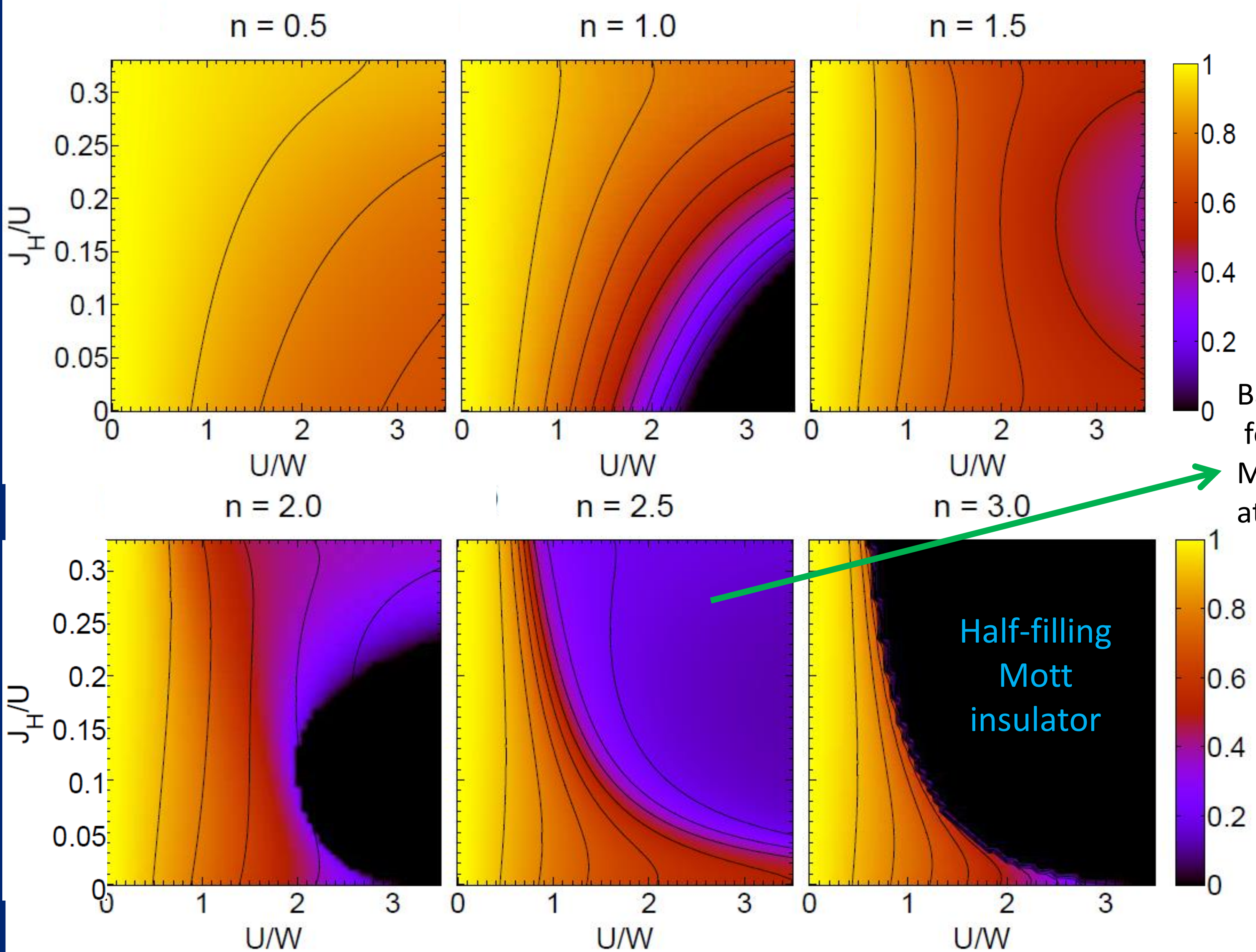


Z increases with J_H

L. Fanfarillo, EB arXiv:1501.04607

The quasiparticle weight as a function of doping

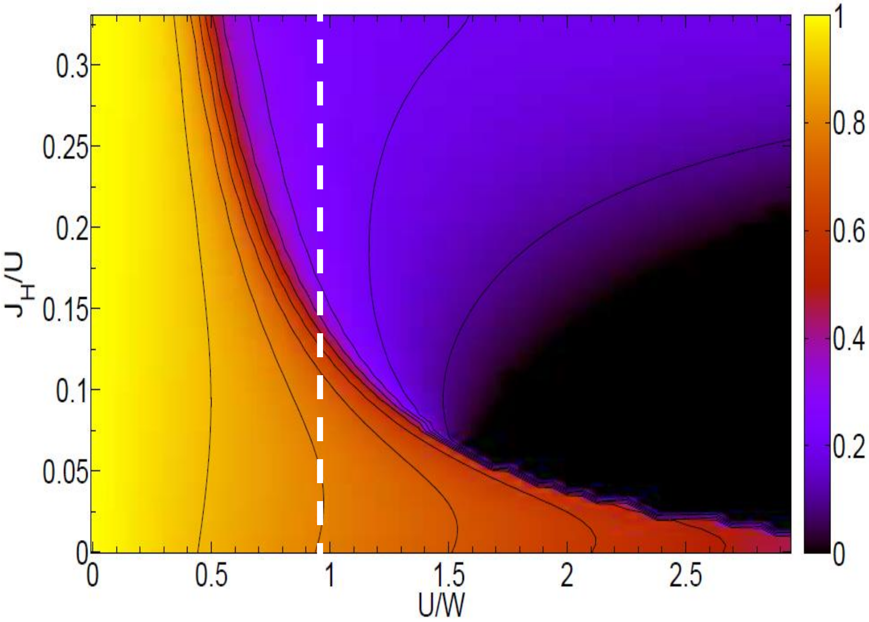
3 orbitals

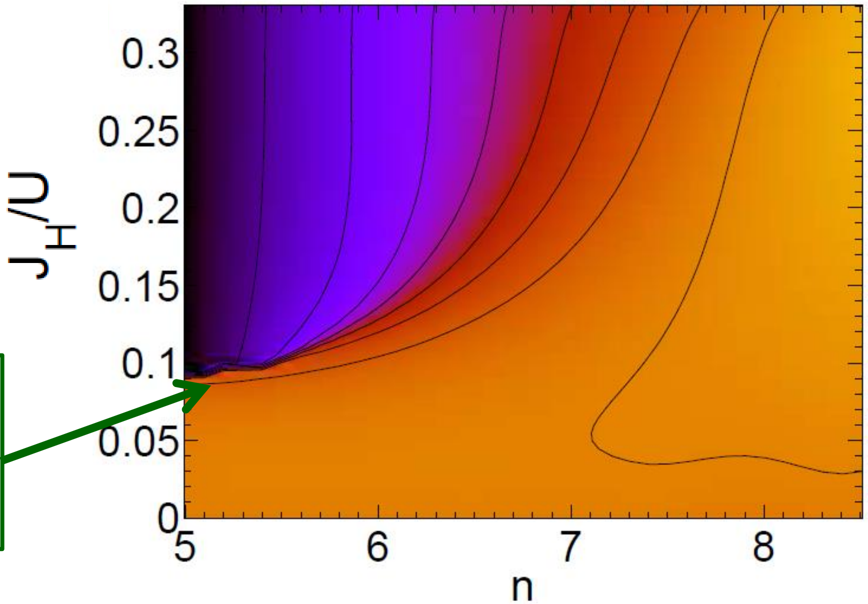


Bad metallicity follows the Mott transition at half-filling

The quasiparticle weight as a function of doping

6 electrons in 5 orbitals,





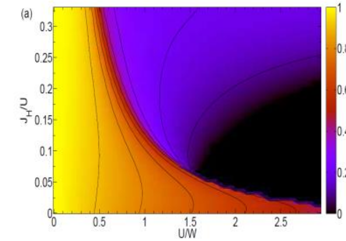
The suppression of the quasiparticle weight Z in the Hund metal is clearly connected with the half-filling Mott transition

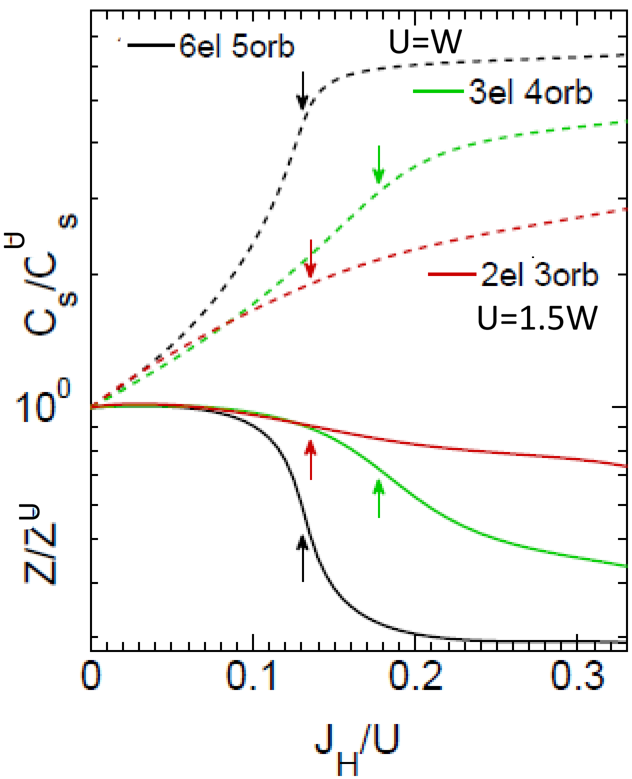
L. Fanfarillo, EB arXiv:1501.04607

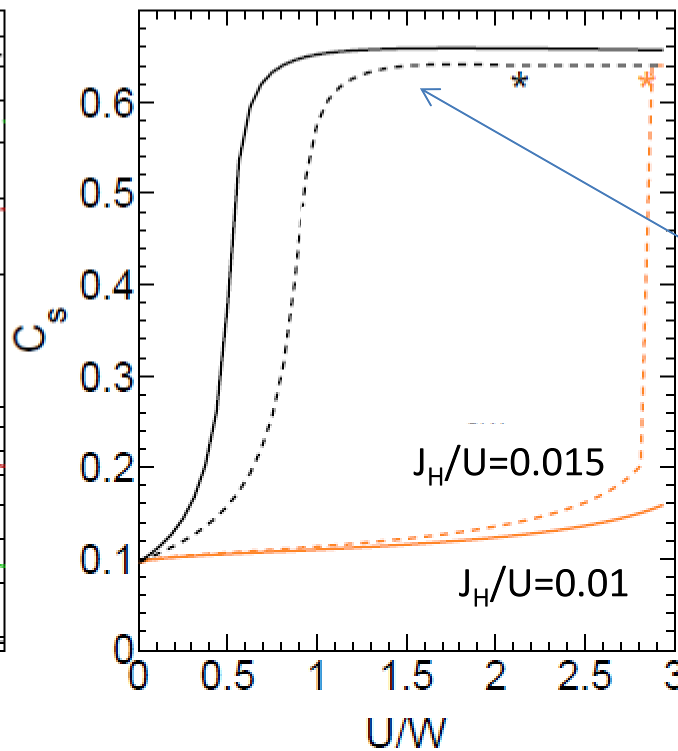
Spin fluctuations

- Single-orbital: Suppression of Z concomitant with the enhancement of spin fluctuations

Multi-orbital: Suppression of Z concomitant
with a very strong enhancement of spin fluctuations







Spin fluctuations
almost saturated
in the Hund metal

L. Fanfarillo, EB arXiv:1501.04607

Hund's rule in a metal → Strong correlations

Charge fluctuations

- Single-orbital: Suppression of Z concomitant with the suppression of charge fluctuations

Mott physics, small Z → Localization

L. Fanfarillo, EB arXiv:1501.04607

Charge fluctuations

- Single-orbital: Suppression of Z concomitant with the suppression of charge fluctuations

Mott physics, small Z → Localization

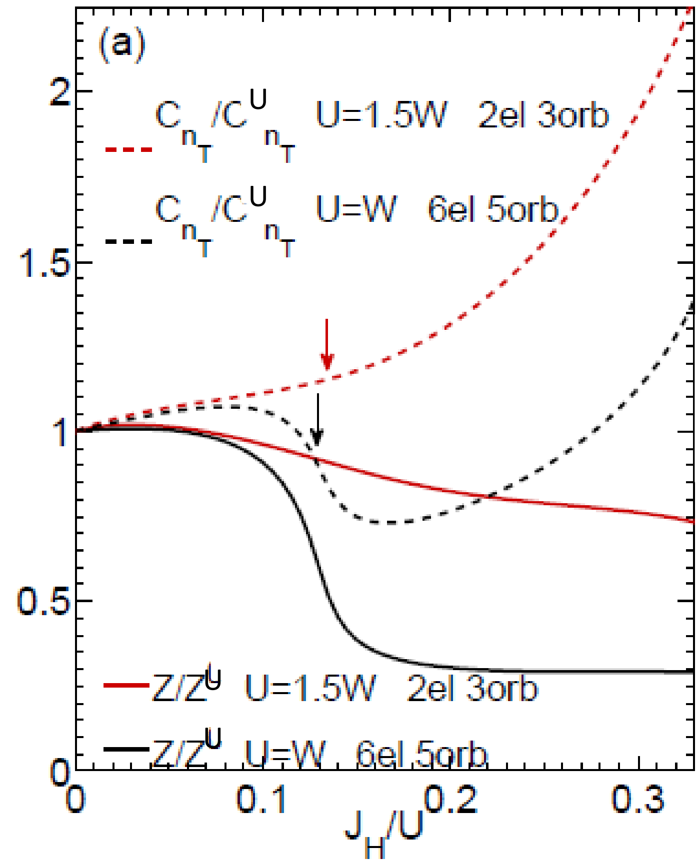
- Multi-orbital: Suppression of Z due to Hund's coupling is not always accompanied by the suppression of charge fluctuations

Hund correlations

↓

Not always localization,
sometimes increases itinerancy

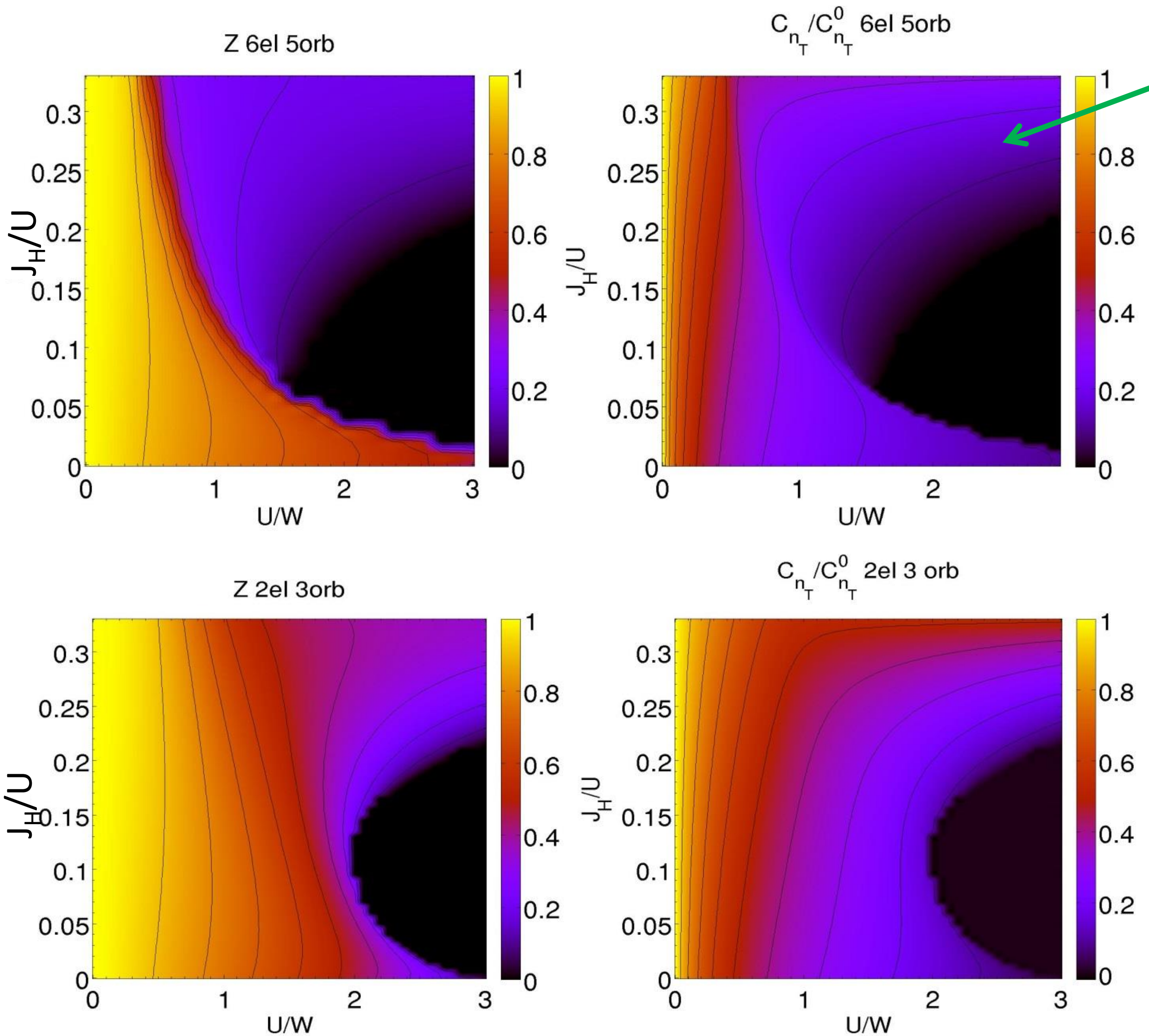
Hund correlations not equal to Mott correlations



L. Fanfarillo, EB arXiv:1501.04607

Charge fluctuations

Itinerancy



Weaker suppression of charge fluctuations for a given Z, as compared to a single-orbital system or small Hund's coupling

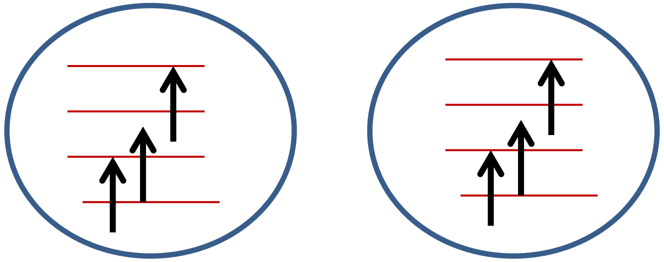
Different dependence of charge fluctuations and quasiparticle weight Z on interactions

L. Fanfarillo, EB arXiv:1501.04607

Understanding the correlations in Hund metals

N orbitals

n electrons



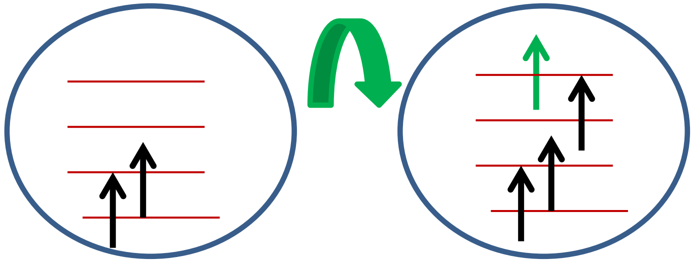
2 spin polarized atoms

Atomic gap: E(n+1)+E(n-1)- 2E(n)
vs
Kinetic Energy

E. Bascones leni@icmm.csic.es

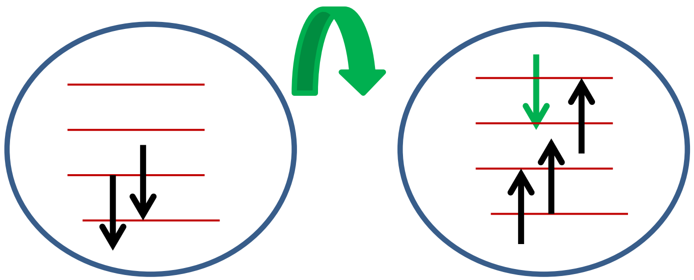
Understanding the correlations in Hund metals

Hopping processes



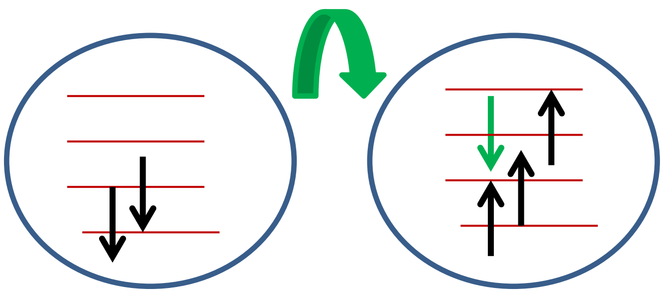
Spin parallel hopping to an empty orbital

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



Spin anti-parallel hopping to an empty orbital

$$E^{inter\uparrow\downarrow} = U + (n-3)J_H$$

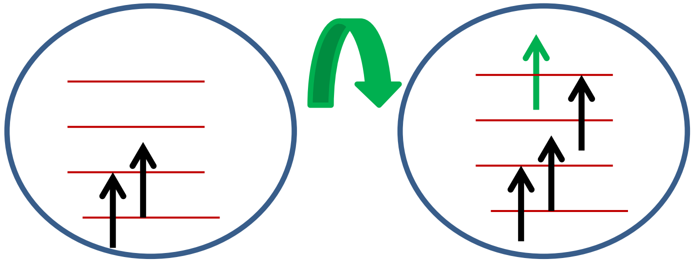


Spin anti-parallel hopping to an occupied orbital

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

Understanding the correlations in Hund metals

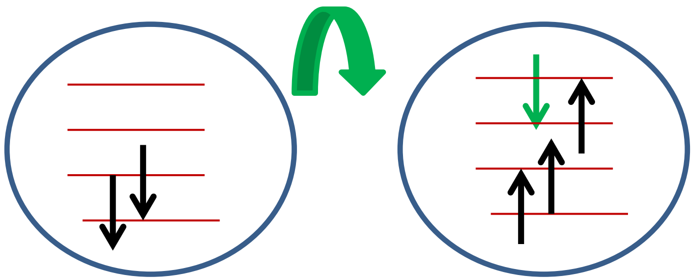
Hopping processes



Spin parallel hopping to an empty orbital

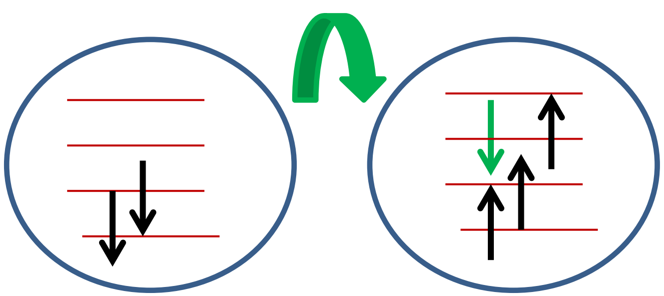
$$E^{\uparrow\uparrow} = U - 3J_H$$

Responsible for the Mott transition away from half-filling



Spin anti-parallel hopping to an empty orbital

$$E^{inter\uparrow\downarrow} = U + (n-3)J_H$$

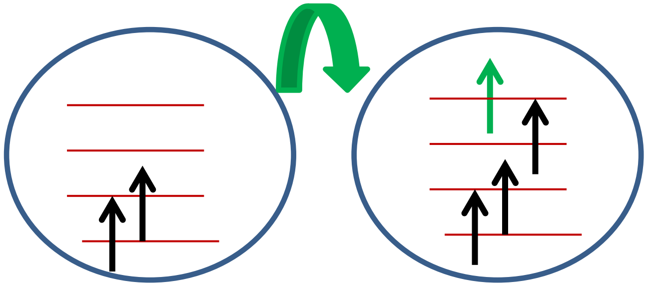


Spin anti-parallel hopping to an occupied orbital

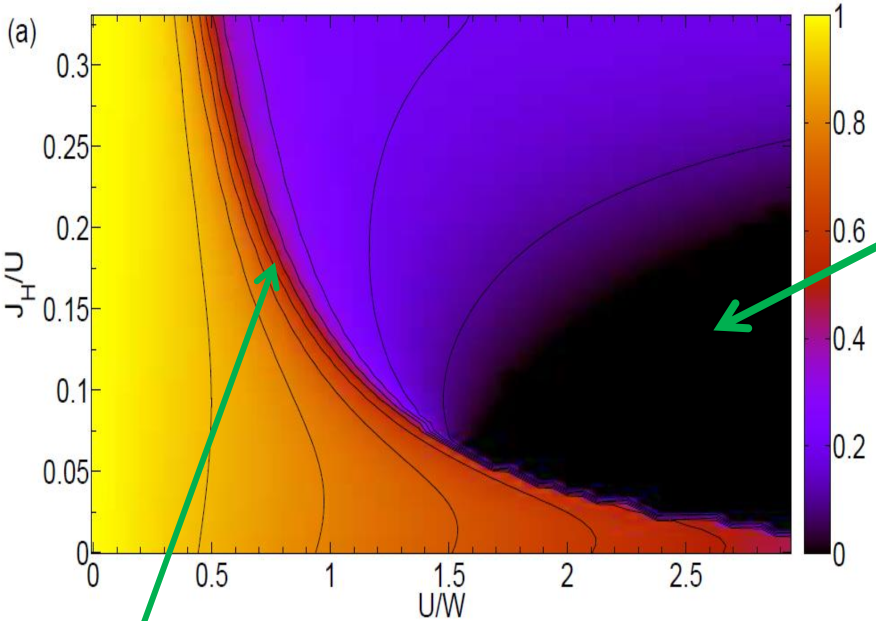
$$E^{intra\uparrow\downarrow} = U + (n-1)J_H$$

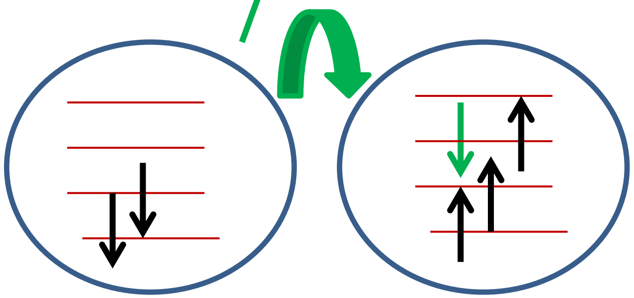
Responsible for the Mott transition at half-filling

Understanding the correlations in Hund metals



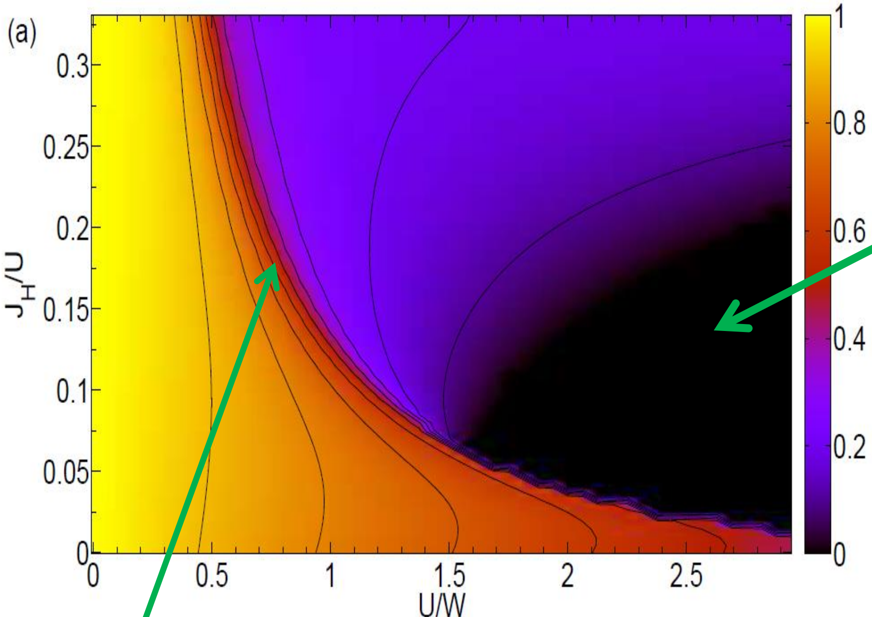
$$E^{\uparrow\uparrow} = U - 3J_H$$

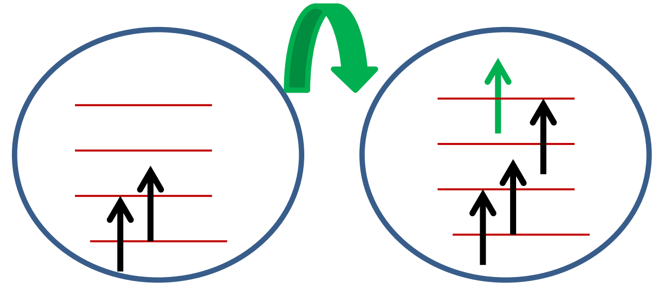




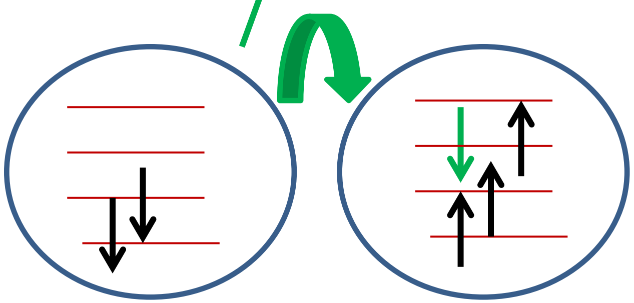
$$E^{intra\uparrow\downarrow} = U + (n-1)J_H$$

Understanding the correlations in Hund metals



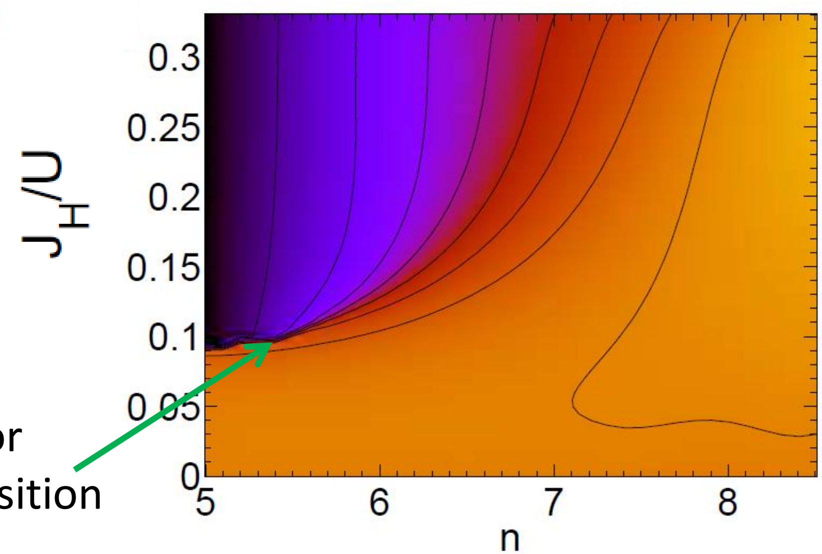


$$E^{\uparrow\uparrow} = U - 3J_H$$

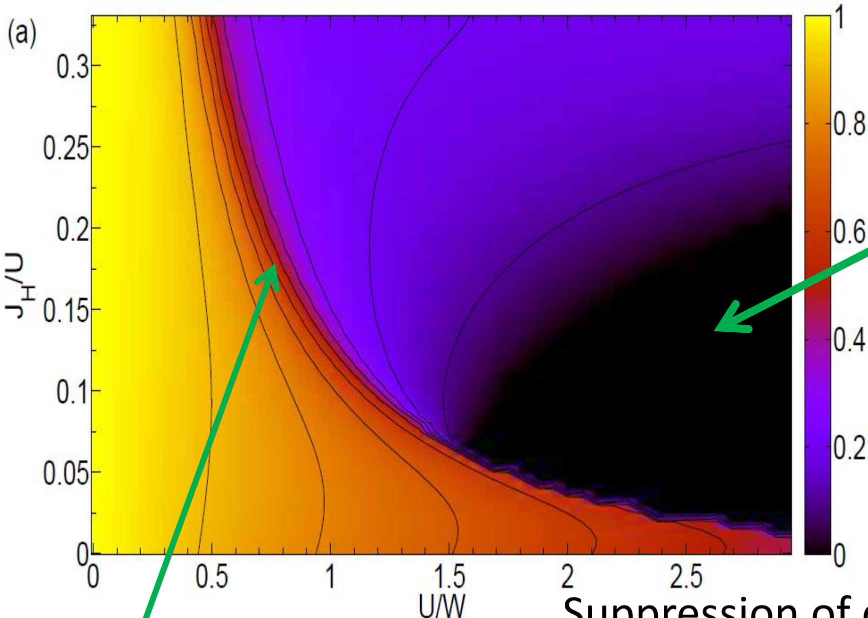


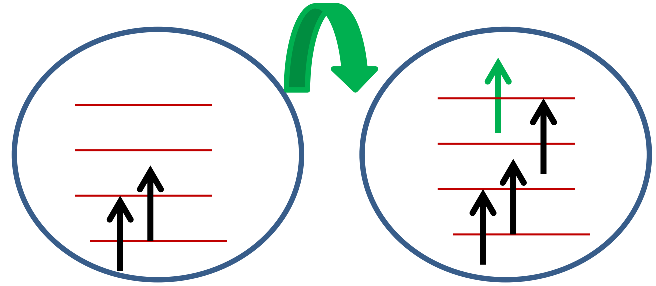
$$E^{intra\uparrow\downarrow} = U + (n-1)J_H$$

Same process responsible for the Mott transition at half-filling

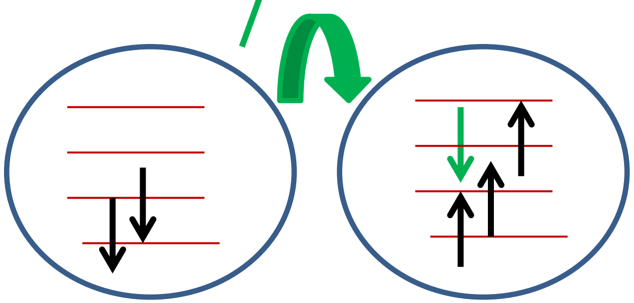


Understanding the correlations in Hund metals



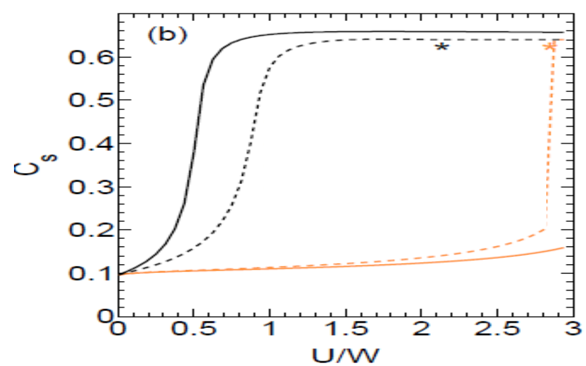


$$E^{\uparrow\uparrow} = U - 3J_H$$

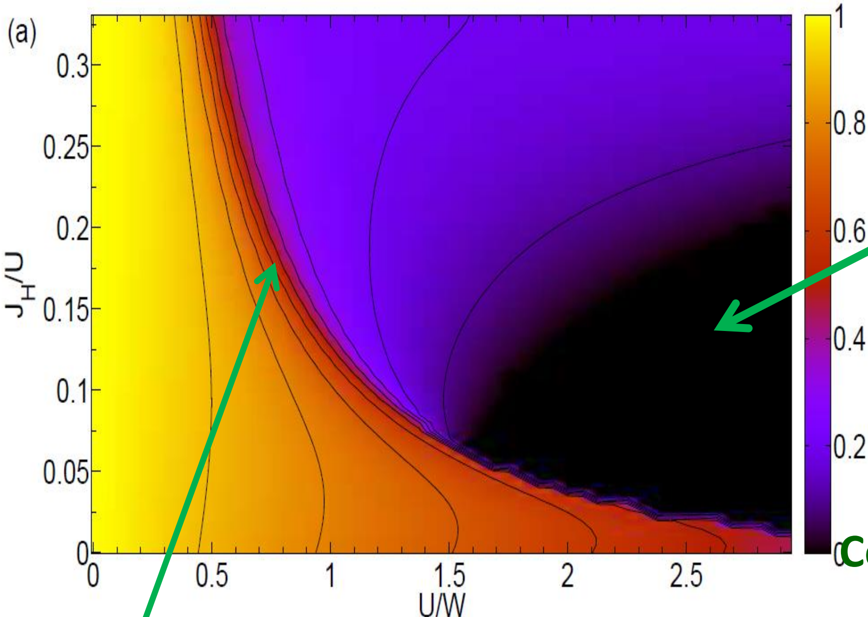


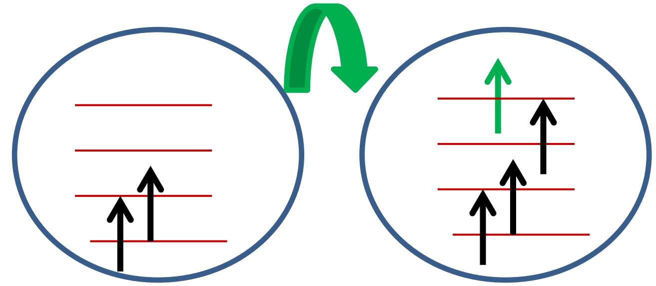
$$E^{intra\uparrow\downarrow} = U + (n-1)J_H$$

Suppression of configurations with double occupancy and for n>2 hopping with antiparallel spins to empty orbitals → **Enhancement of spin fluctuations**



Understanding the correlations in Hund metals





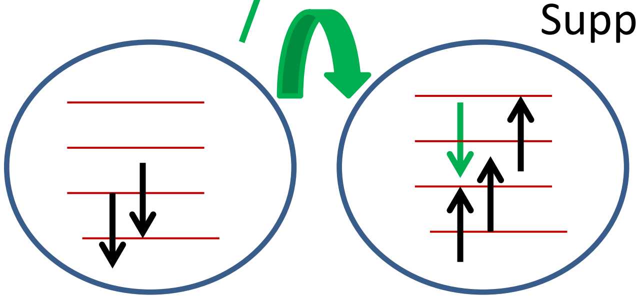
$$E^{\uparrow\uparrow} = U - 3J_H$$

Promoted by Hund

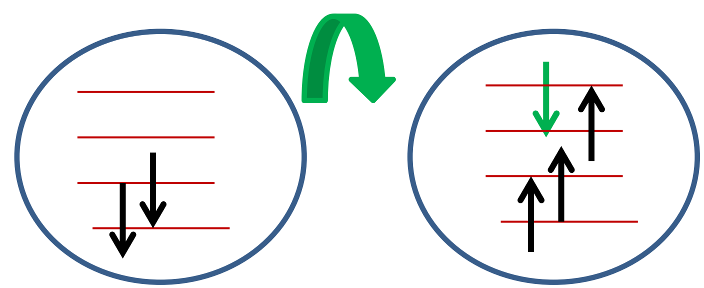
Conflicting behavior in charge fluctuations

Suppressed by Hund

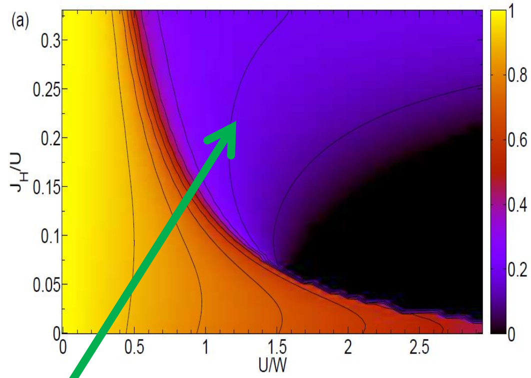
Promoted or suppressed by Hund



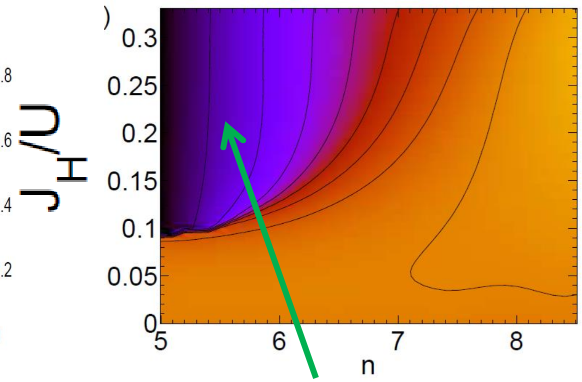
$$E^{intra\uparrow\downarrow} = U + (n-1)J_H$$



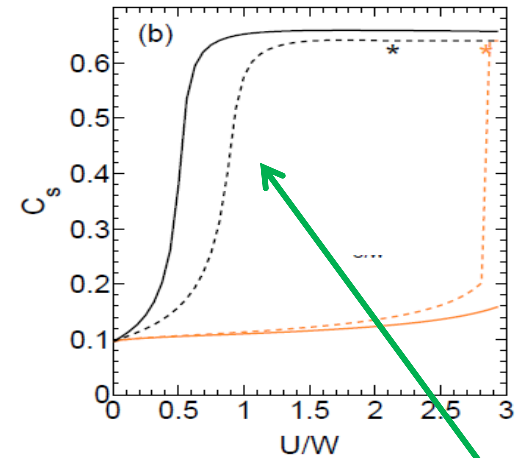
Summary: Strong influence of Hund's coupling on electronic correlations



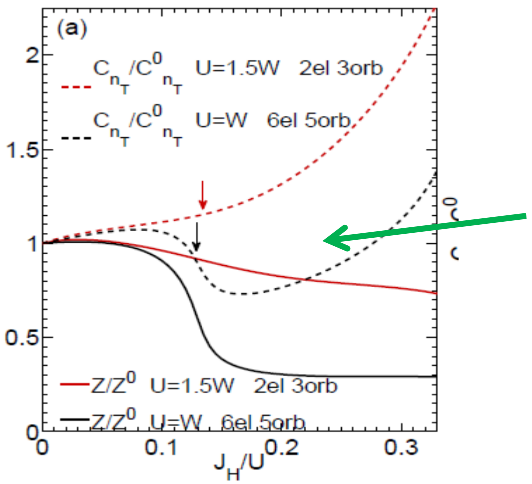
Hund metal with small Qp weight Z: strong correlations



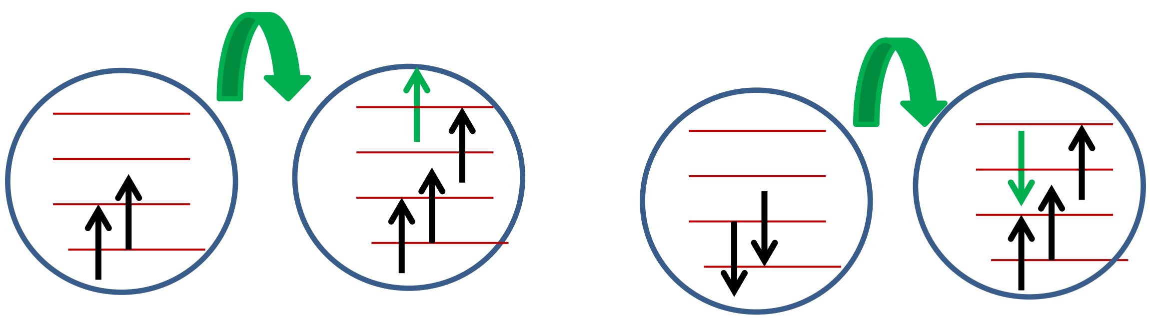
Suppression of Qp weight connected to half-filling Mott insulator



Enhancement of spin fluctuations (atoms polarized)



Charge fluctuations do not follow the behavior expected in Mott systems



Behavior understood in terms of which hopping processes are promoted or suppressed by Hund's coupling

Revisit oxides and other materials

Correlated metals. The quasiparticle weight (Fermi liquid description)

- Write the electron $c^\dagger_{k\sigma}$ in terms of the excitations of the interacting system $a^\dagger_{k\sigma}$

Same charge, momentum & spin

$$c^\dagger{}_{\mathbf{k}\sigma} = \sqrt{Z_\mathbf{k}}\, a^\dagger{}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}_4+\mathbf{k}_3=\mathbf{k}_2+\mathbf{k}} A(\mathbf{k}_4\sigma_4, \mathbf{k}_3\sigma_3; \mathbf{k}_2\sigma_2, \mathbf{k}\sigma)\, a^\dagger{}_{\mathbf{k}_4\sigma_4} a^\dagger{}_{\mathbf{k}_3\sigma_3} a_{\mathbf{k}_2\sigma_2} + \ldots$$

A single particle description of $C^\dagger_{k\sigma}|\Psi^*_g>$ makes sense if Z_k is finite

higher order decay processes

$$Z_k = |<\Psi^*_g|a_{k\sigma} c^\dagger_{k\sigma}|\Psi^*_g>|^2 > 0$$

Quasiparticle weight

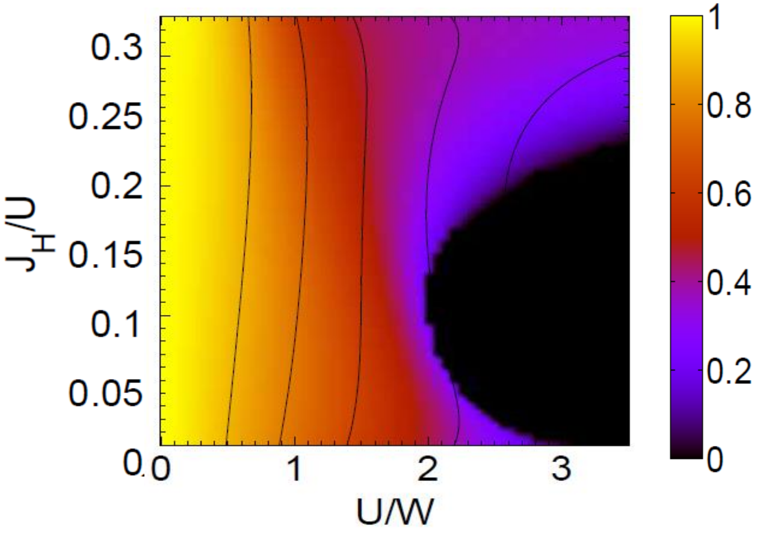
Overlap between the elementary excitations of the interacting and non-interacting system

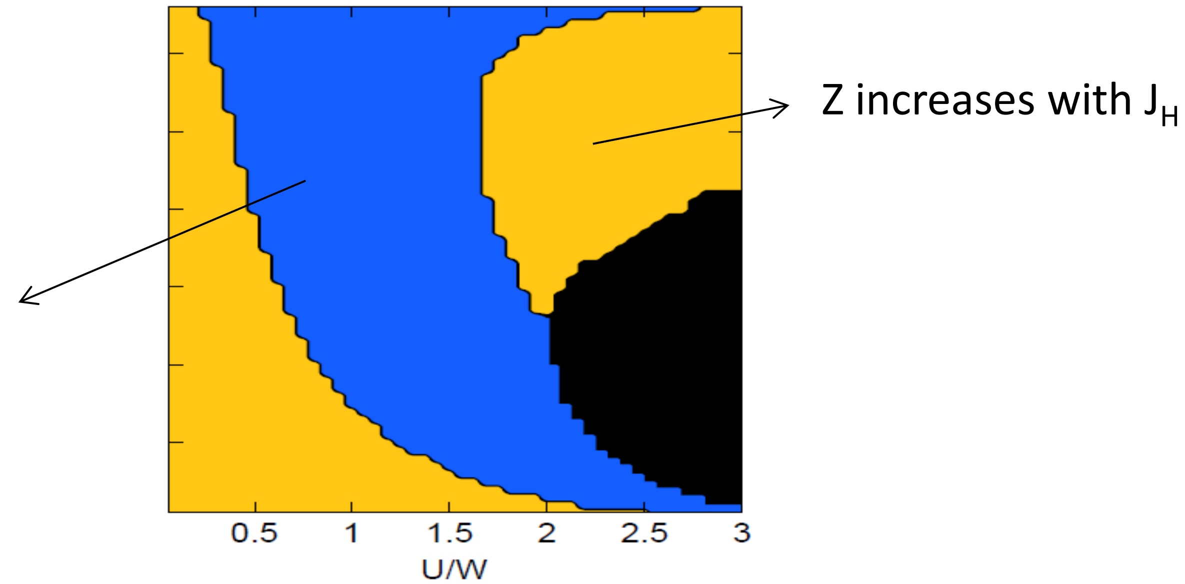
A way to quantify the correlations

See Coleman's book

The quasiparticle weight as a function of interactions

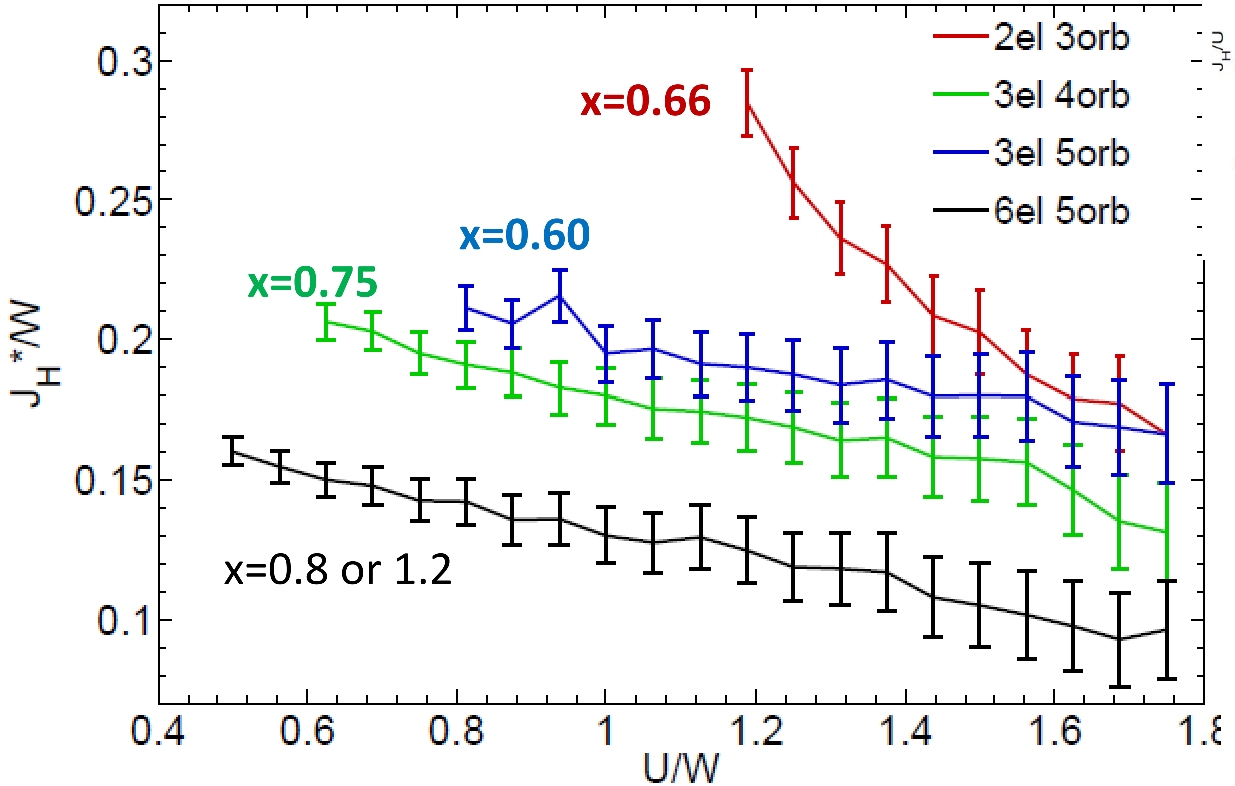
2 electrones en 3 orbitales, x=0.66

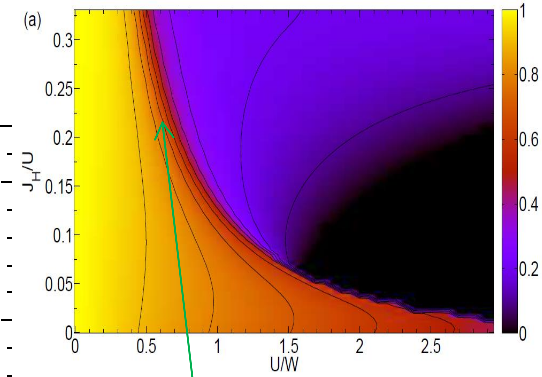




L. Fanfarillo, EB arXiv:1501.04607

The quasiparticle weight as a function of doping

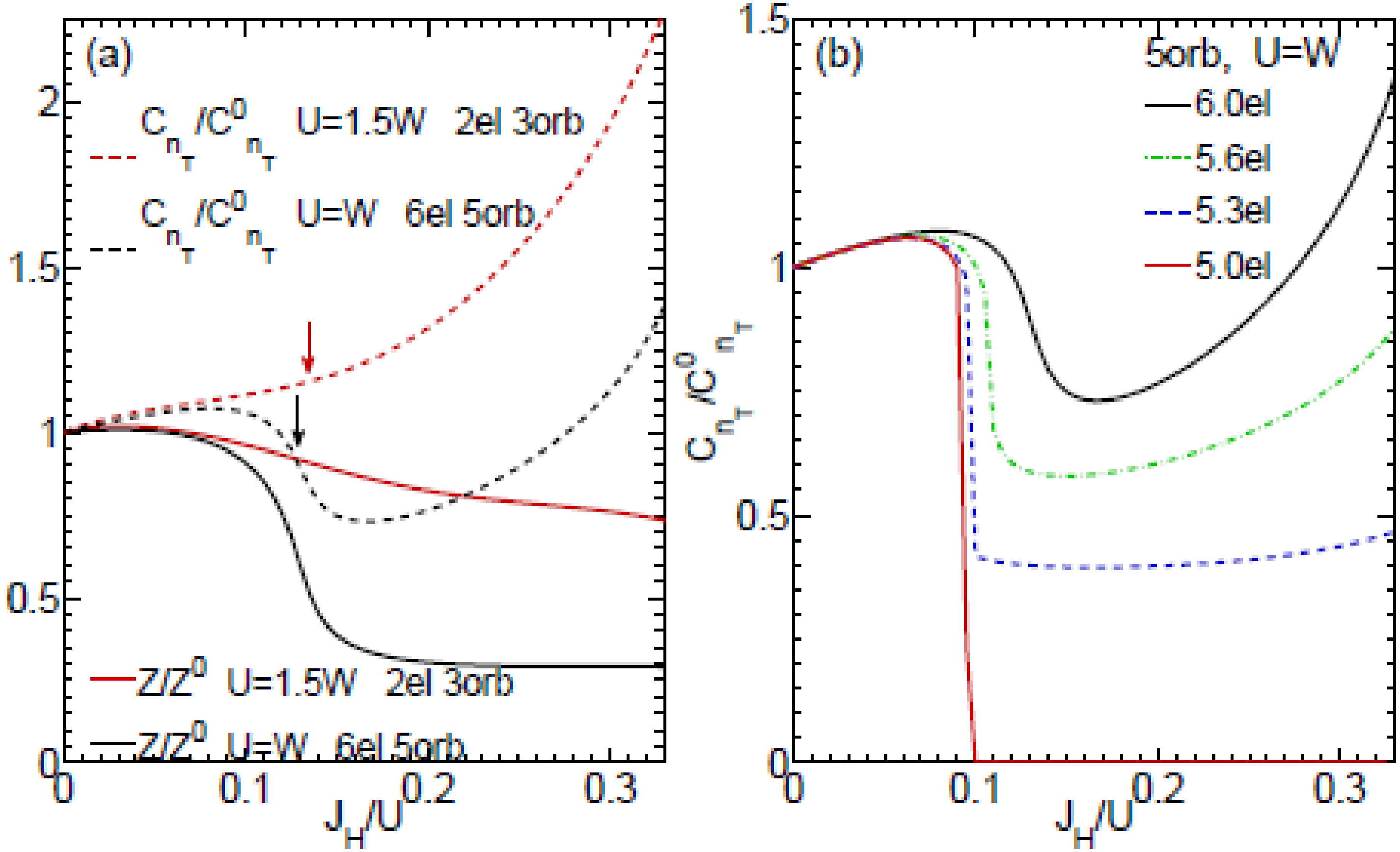




J_H^* crossover

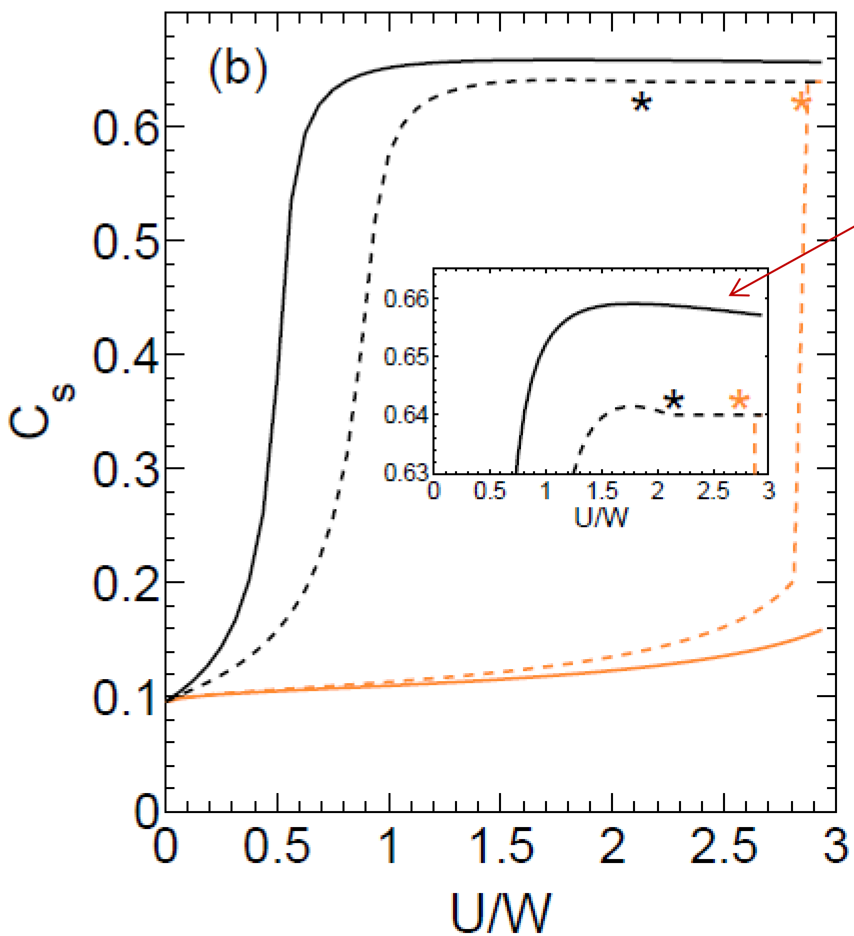
L. Fanfarillo, EB arXiv:1501.04607

Charge correlations in Hund metals



L. Fanfarillo, EB arXiv:1501.04607

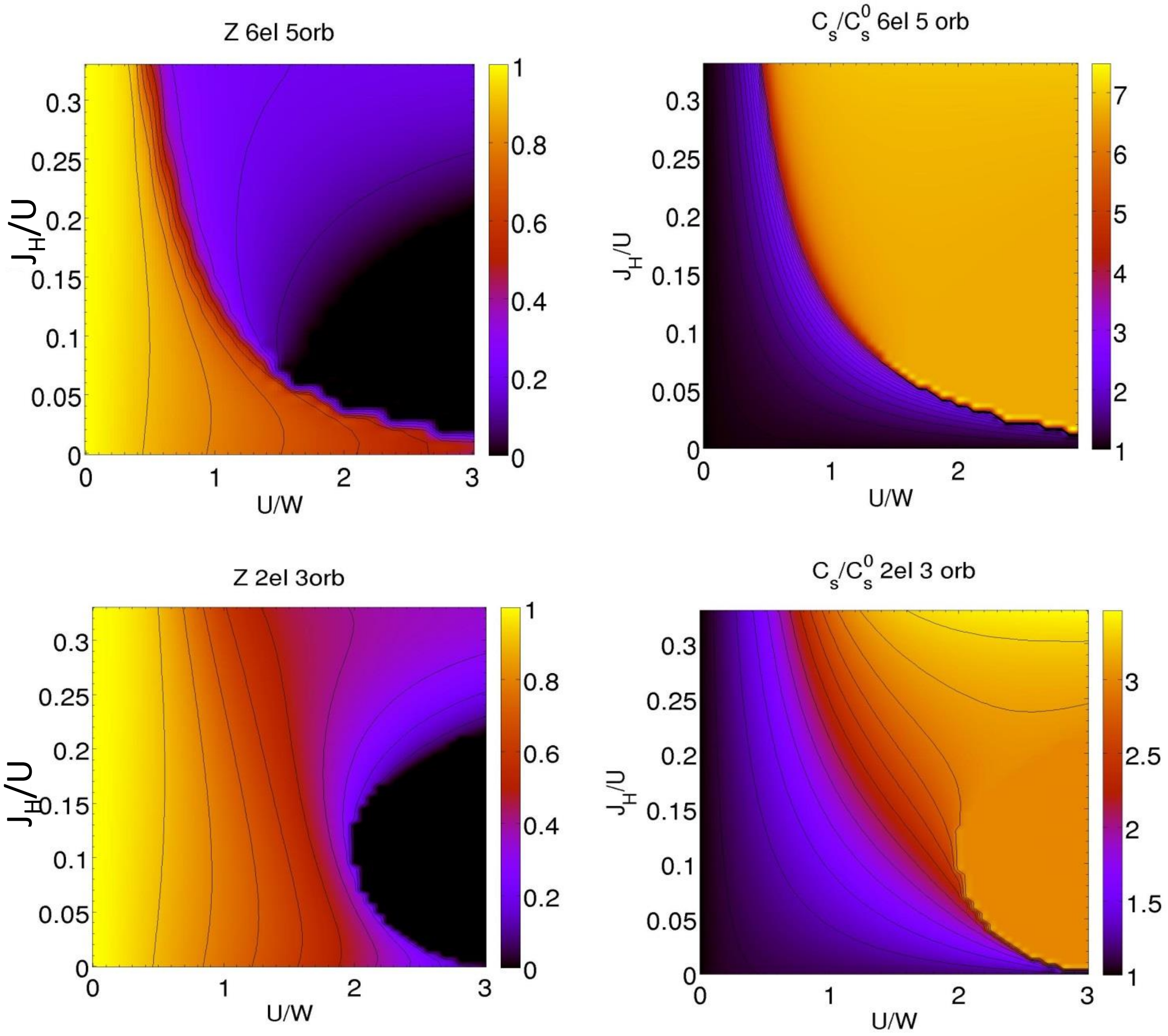
Spin fluctuations in Hund metals



The spin fluctuations are larger in the metal.
U enhances the tendency to localization.

L. Fanfarillo, EB arXiv:1501.04607

Spin fluctuations in Hund metals



Atomic moments are formed in the

L. Fanfarillo, EB arXiv:1501.04607

Z_2- Slave spin technique

$$H= U\sum_m \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U'\sum_{m\neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U'-J_H)\sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma}$$

$n_{m\sigma}=d^{\dagger}_{m\sigma}d_{m\sigma}$

$d_{i\sigma}$ → Auxiliary fermion $f_{i\sigma}$

$d_{i\sigma}$ → Pseudospin variable (slave-spin) $S^z_{i\sigma}$

Physical states

$$|n^d_{i\sigma}=1\rangle \Leftrightarrow |n^f_{i\sigma}=1,\ S^z_{i\sigma}=+1/2\rangle,$$

$$|n^d_{i\sigma}=0\rangle \Leftrightarrow |n^f_{i\sigma}=0,\ S^z_{i\sigma}=-1/2\rangle.$$

Unphysical states

$$|n^f_{i\sigma}=0,\ S^z_{i\sigma}=+1/2\rangle$$

$$|n^f_{i\sigma}=1,\ S^z_{i\sigma}=-1/2\rangle$$

→

Constraint

$$f^{\dagger}_{i\sigma}f_{i\sigma} = S^z_{i\sigma} + \frac{1}{2}$$

de Medici et al, PRB 72, 205124 (2005)
Hassan & de Medici, PRB 81, 035106 (2010)

Z_2- Slave spin technique

$$d_{i\sigma} = f_{i\sigma} O_{i\sigma}, \quad d^\dagger_{i\sigma} = f^\dagger_{i\sigma} O^\dagger_{i\sigma}$$

For non- diagonal operators

$$O_{i\sigma} = \begin{pmatrix} 0 & c_{i\sigma} \\ 1 & 0 \end{pmatrix} \qquad c = \frac{1}{\sqrt{n(1-n)}} - 1.$$

$$H_0 = -\sum_m t_m \sum_{<ij>,\sigma} O^\dagger_{im\sigma} O_{jm\sigma} (f^\dagger_{im\sigma} f_{jm\sigma} + h.c) + \sum_{i,m\sigma} (\epsilon_m - \mu) f^\dagger_{im\sigma} f_{im\sigma}$$

$$\frac{U}{2}\sum_i \left(\sum_{m,\sigma} S^z_{im\sigma}\right)^2 + \frac{U'}{2}\sum_i (\sum_{m,\sigma} S^z_{im\sigma})^2 + J\sum_{i,m}(\sum_\sigma S^z_{im\sigma})^2 - \frac{J}{2}\sum_{i,\sigma}(\sum_m S^z_{im\sigma})^2$$

$$H_{int}[\{\vec{S}_{im\sigma}\}]$$

de Medici et al, PRB 72, 205124 (2005)
Hassan & de Medici, PRB 81, 035106 (2010)

Z_2- Slave spin technique

- Constraint treated on average with static and site independent Lagrange multiplier λ_m. Spin variables and auxiliary fermions are decoupled

$$H^f_{eff} = -\sum_m t^{eff}_m \sum_{<ij>,\sigma} (f^\dagger_{im\sigma} f_{jm\sigma} + h.c.)$$

$$+ \sum_{i,m\sigma} (\epsilon_m - \mu - \lambda_m) f^\dagger_{im\sigma} f_{im\sigma}$$

$$H^S_{eff} = -\sum_m J^{eff}_m \sum_{<ij>,\sigma} O^\dagger_{im\sigma} O_{jm\sigma}$$

$$+ \sum_{i,m\sigma} \lambda_m (S^z_{im\sigma} + \frac{1}{2}) + H_{int}[\{\vec{S}_{im\sigma}\}]$$

$$t_m^{eff} = t_m < O^\dagger_{im\sigma} O_{jm\sigma} >$$

$$J^{eff}_m = t_m \langle f^\dagger_{im\sigma} f_{jm\sigma} + f^\dagger_{jm\sigma} f_{im\sigma} \rangle$$

de Medici et al, PRB 72, 205124 (2005)
Hassan & de Medici, PRB 81, 035106 (2010)

Z_2- Slave spin technique

- Spin hamiltonian treated at a single site mean field level

$$H^f_{eff} = \sum_{\mathbf{k},m\sigma} (Z_m \epsilon_{\mathbf{k}m} + \epsilon_m - \mu - \lambda_m) f^\dagger_{\mathbf{k}m\sigma} f_{\mathbf{k}m\sigma}$$

$$H_s = \sum_{m\sigma} h_m \, O^\dagger_{m\sigma} + \sum_{m\sigma} \lambda_m (S^z_{m\sigma} + \frac{1}{2}) + H_{int}[\vec{S}_{m\sigma}]$$

$$h_m = \langle O_{im\sigma} \rangle \frac{1}{\mathcal{N}} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}m} \langle f^\dagger_{\mathbf{k}m\sigma} f_{\mathbf{k}m\sigma} \rangle$$

$$Z_m = \langle O^\dagger_{im\sigma} \rangle^2$$

- Solve self-consistently both coupled equations to calculate λ_m, h_m, Z_m

de Medici et al, PRB 72, 205124 (2005)
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