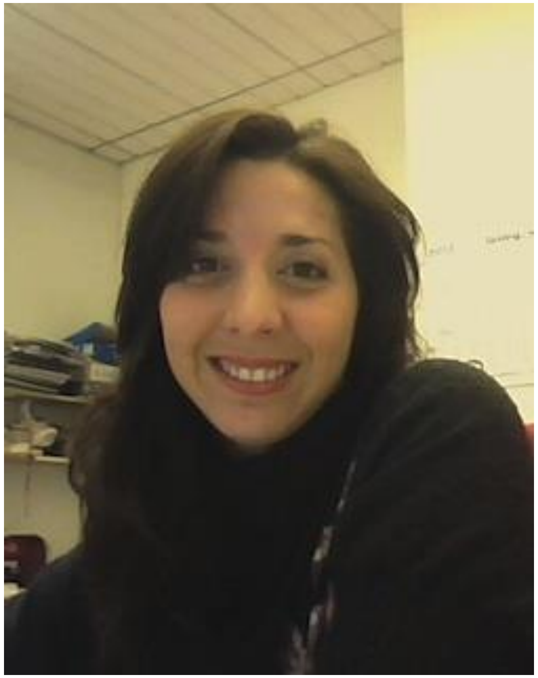
Electronic correlations in Hund metals

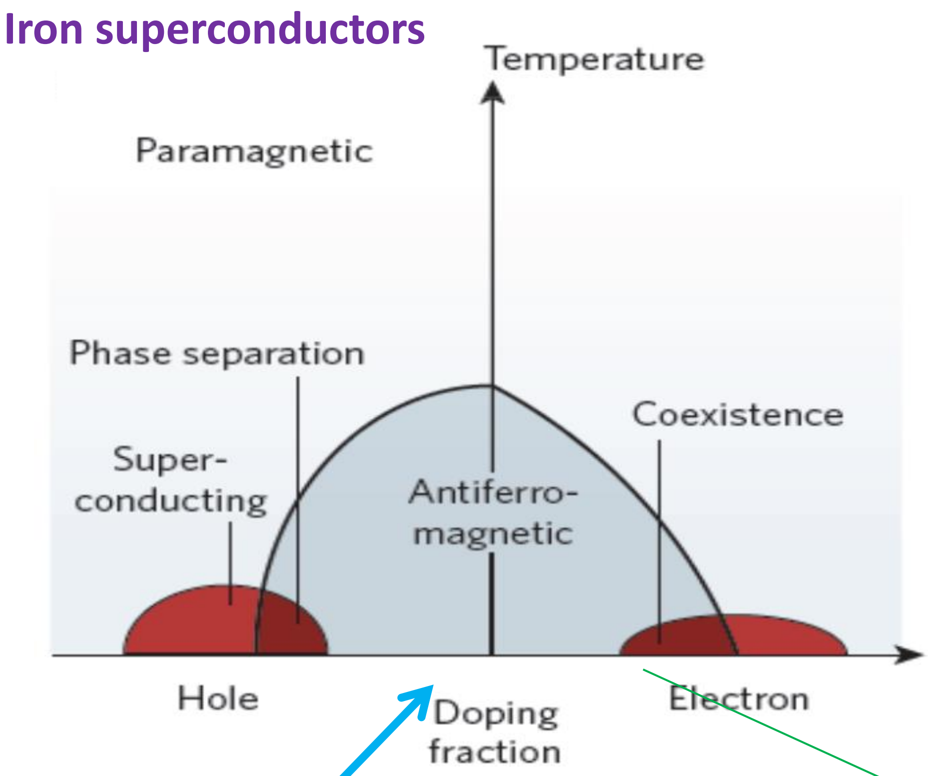
E. Bascones
Instituto de Ciencia de Materiales de Madrid

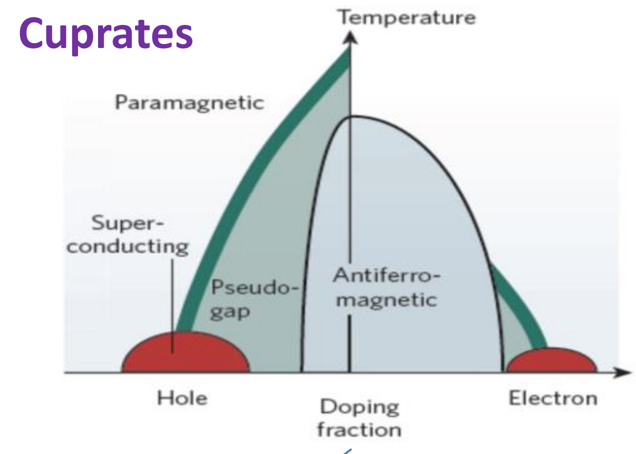


In collaboration with:
Laura Fanfarillo
ICMM-CSIC (now at SISSA, Trieste)

arXiv:1501.04607

Iron superconductors: metallic when "undoped"





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

Discussion on strength of correlations:
weakly correlated (bands, Fermi surface instabilities),
localized spins, Hund metals

Fig: Nature 464,183 (2010)

E. Bascones leni@icmm.csic.es

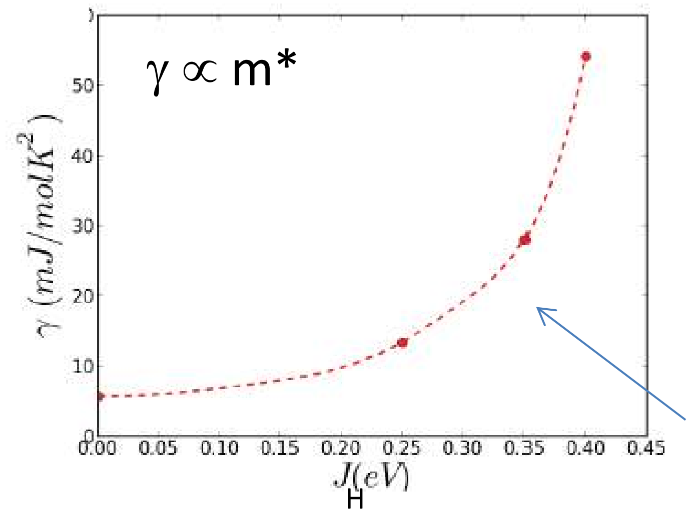
Correlations in multi-orbital systems: Hund's coupling &Hund metals

A definition of 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)

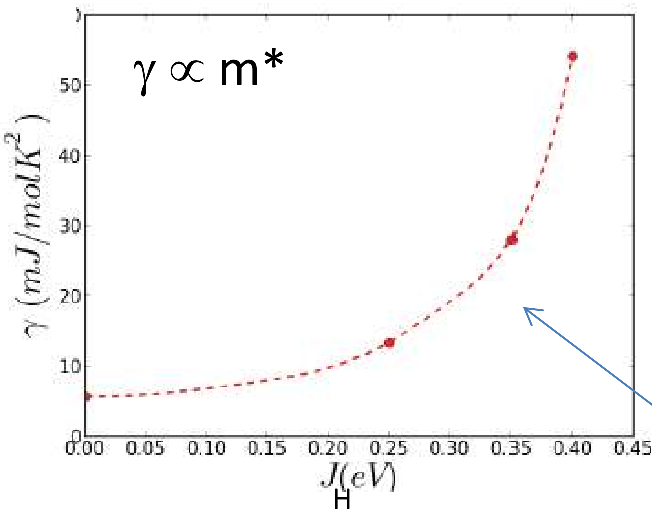
Iron Superconductors
6 electrons in
5 orbitals

Understanding Hund metals:
important not only in the context of iron superconductors but also for many other materials including oxides

Correlations in multi-orbital systems: Hund's coupling &Hund metals

A definition of Hund metals

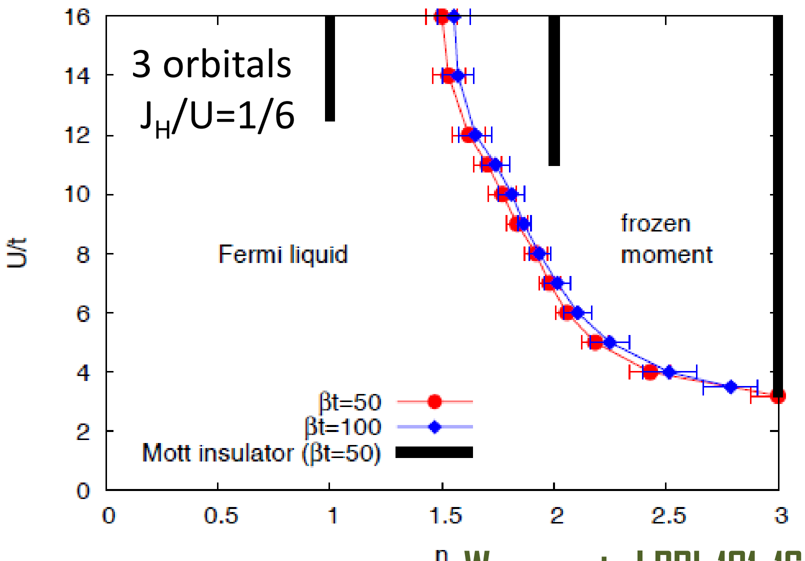
- Correlations driven by Hund J_H weakly dependent on U,
- Not in proximity to a Mott insulator
- Properties essentially different to a doped Mott insulator



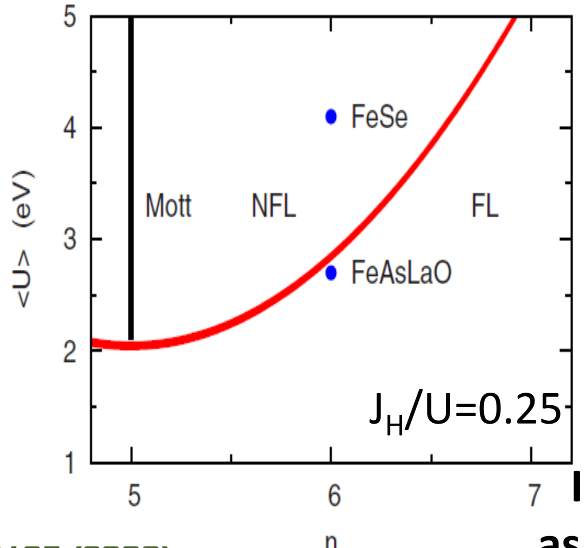
Haule & Kotliar NJP 11,025021 (2009)

Iron Superconductors 6 electrons in 5 orbitals

But correlations controlled by proximity in doping to the half-filled Mott insulator



Werner et al PRL 101, 166405 (2008)



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

Iron superconductors as doped Mott insulators

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

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

Pair hopping

$U' = U - 2J_H \quad J' = J_H$

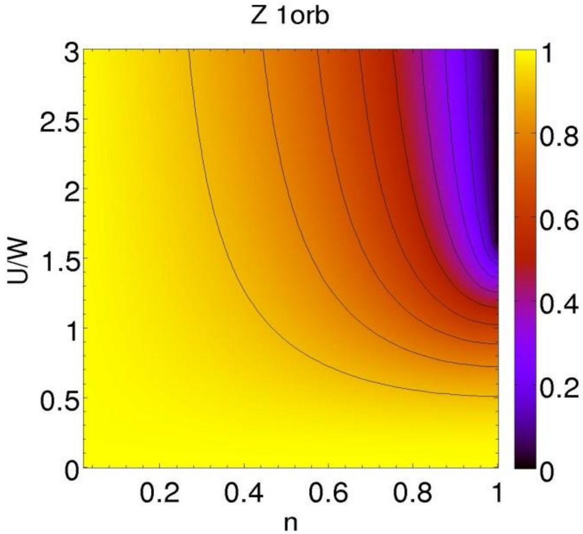
Two interaction parameters: U, J_H

We assume equivalent orbitals (no hybridization between them)

Slave-spin (only density-density terms)

Charge and spin fluctuations in the single-orbital Hubbard model

Quasiparticle weight Z

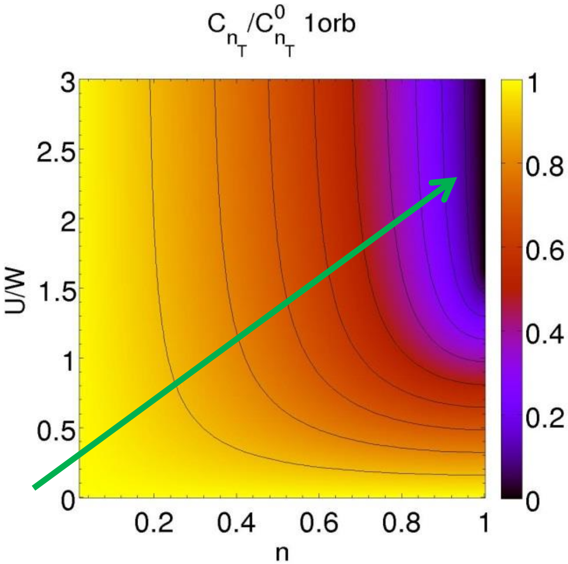


Charge fluctuations

(local &instantaneous)

$C_T = \langle n^2\rangle - \langle n\rangle^2 = \langle(\delta n)^2\rangle$

$n = \langle n\rangle + \delta n$

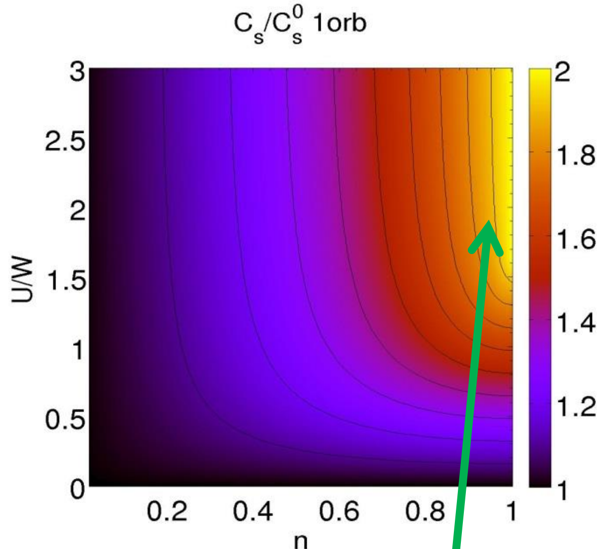


Localization

Spin fluctuations

(local &instantaneous)

$C_S = \langle S^2\rangle - \langle S\rangle^2 = \langle S^2\rangle$



Enhancement of spin fluctuations

Mott insulator:

Suppression of charge fluctuations

n= <n>

Localized spins at each atomic site

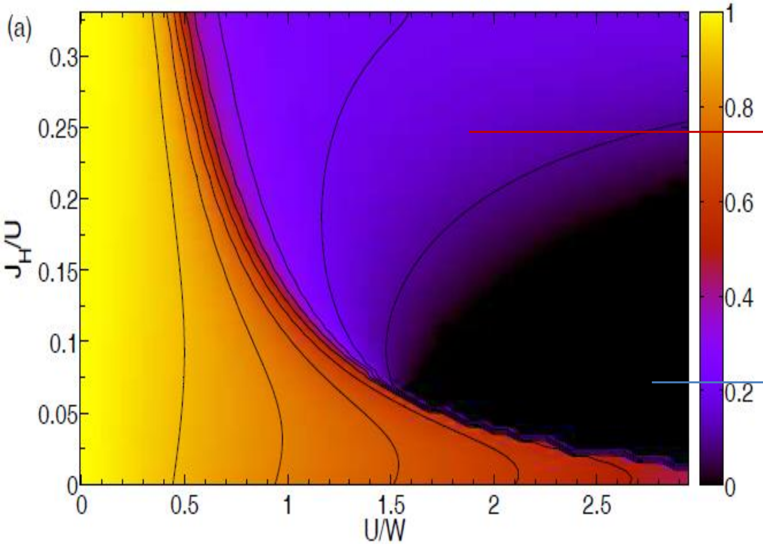
C_s larger when atoms are spin polarized even if there is no long-range order

E. Bascones leni@icmm.csic.es

Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

Colour plots: **Quasiparticle weight Z**



Hund metal

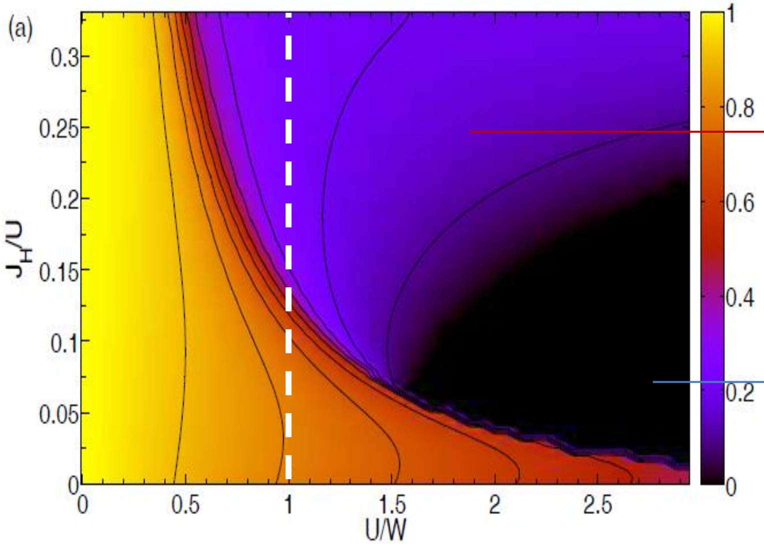
n=6 Mott insulator

Fanfarillo & EB, arXiv:1501.04607

Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

Colour plots: **Quasiparticle weight Z**

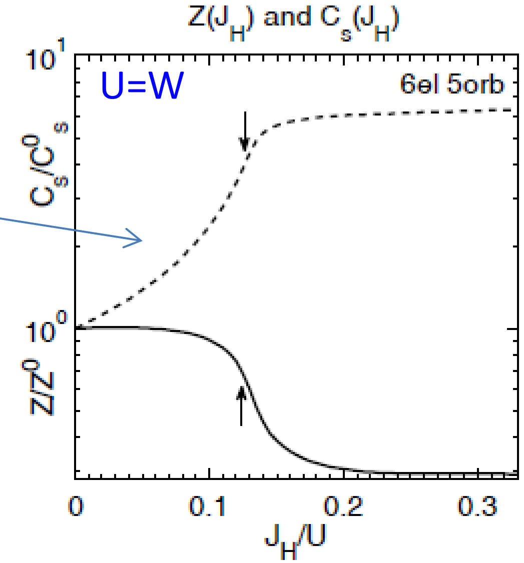


Hund metal

n=6 Mott insulator

Suppression of Z associated to the atomic spin polarization

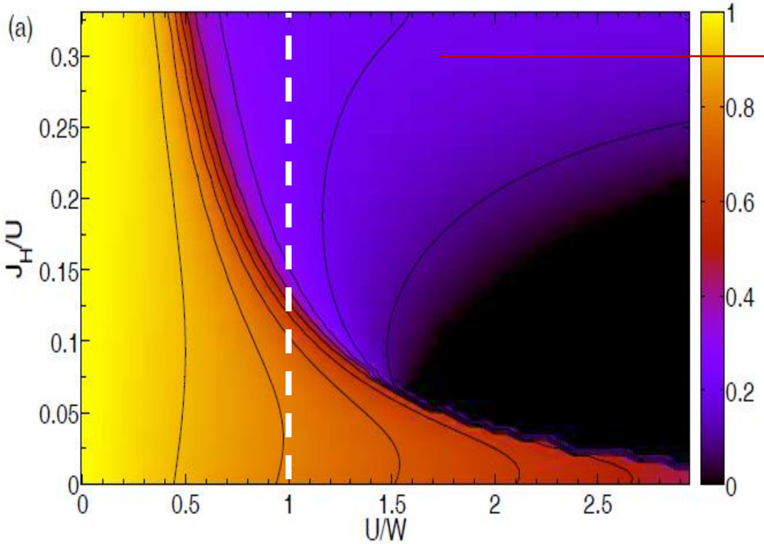
Enhancement of Spin fluctuations



Fanfarillo & EB, arXiv:1501.04607

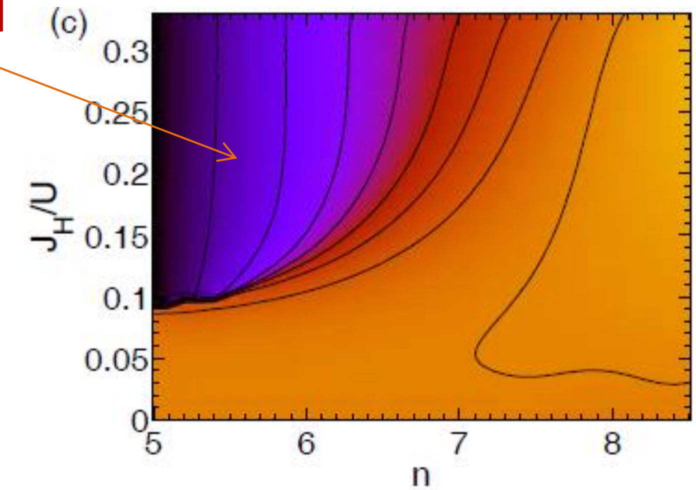
Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals



Colour plots: **Quasiparticle weight Z**

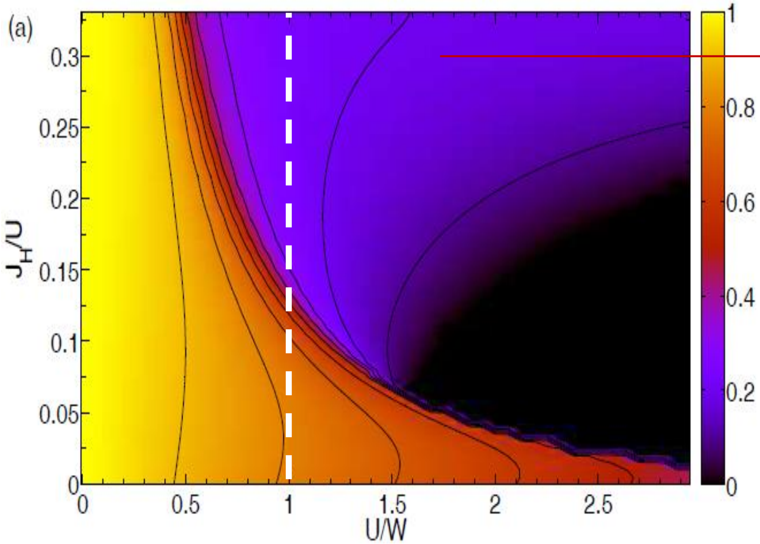
Hund metal



Fanfarillo & EB, arXiv:1501.04607

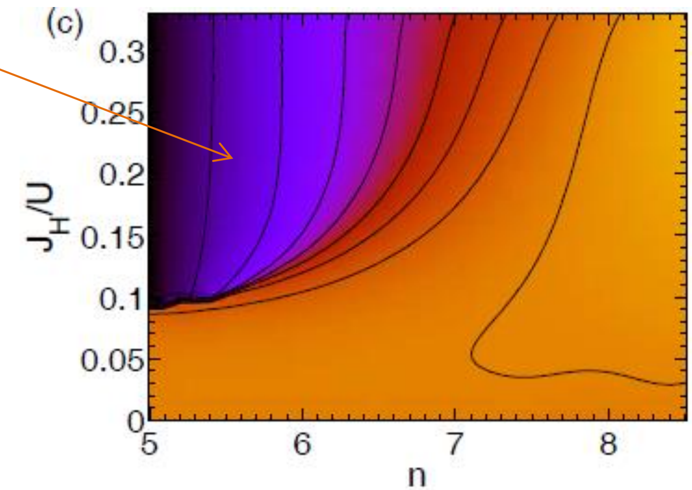
Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

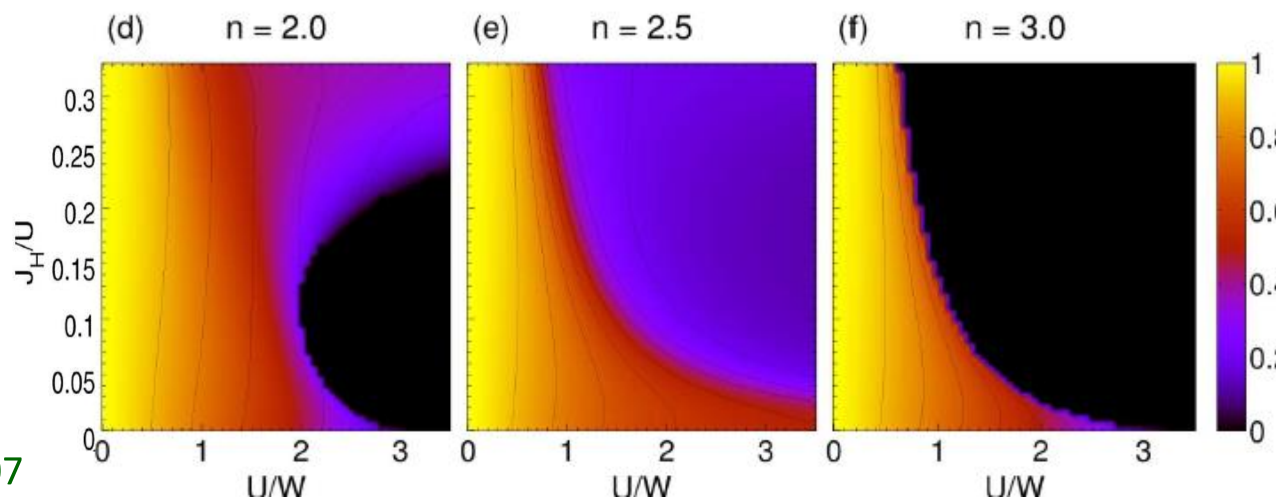


Colour plots: **Quasiparticle weight Z**

Hund metal



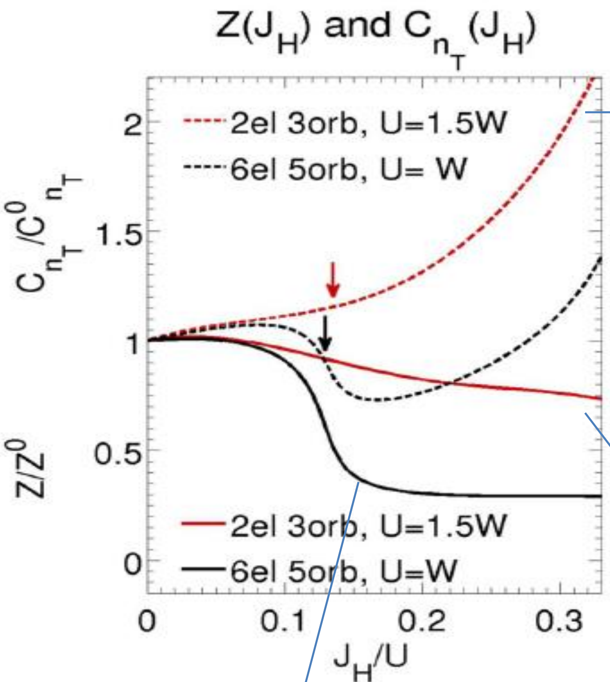
3 orbitals



We confirm that the correlations in Hund metals are directly connected to the half-filled Mott insulator

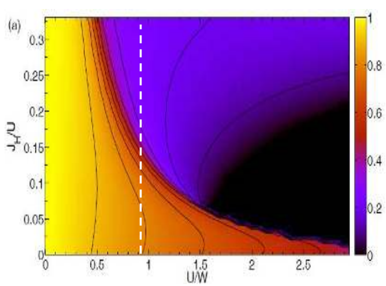
Fanfarillo & EB, arXiv:1501.04607

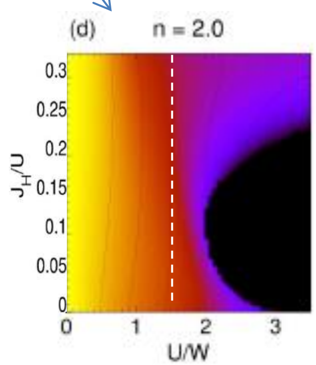
Electronic correlations in multi-orbital systems: Hund metals



Charge fluctuations

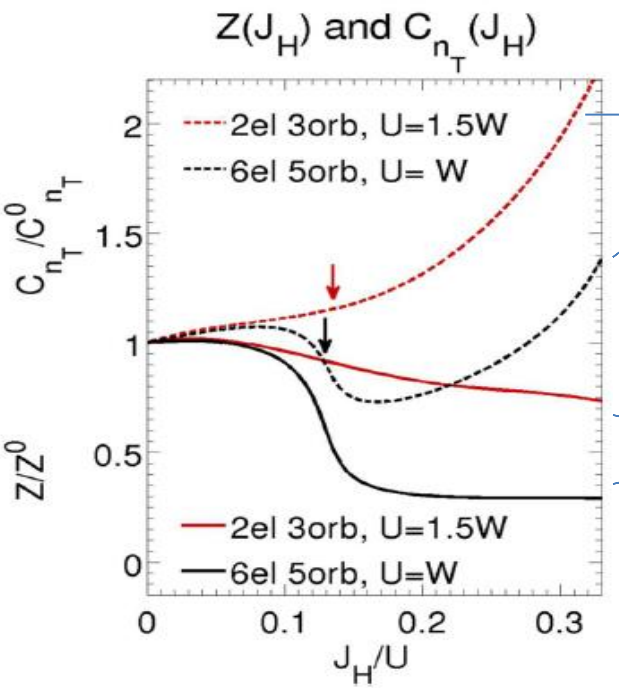
Quasiparticle weight





Fanfarillo & EB, arXiv:1501.04607

Electronic correlations in multi-orbital systems: Hund metals



The quasiparticle weight and the charge fluctuations show different behavior (opposite to what happens In Mott correlated states in the single orbital case)

Contrary to what happens in Mott correlated single-orbital systems,
In Hund metals the quasiparticle weight and the mass enhancement
are not good measures of charge localization

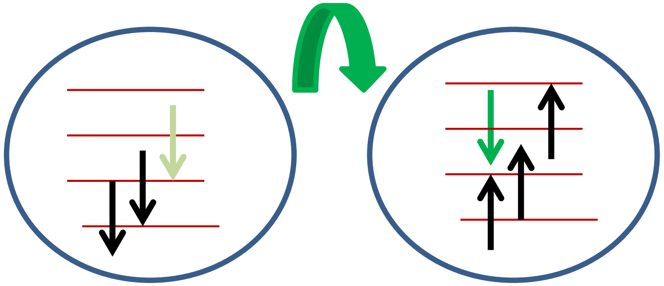
Fanfarillo & EB, arXiv:1501.04607

Electronic correlations in multi-orbital systems: Hund metals

Correlations in Hund metals are directly connected to the half-filled Mott insulator but contrary to what happens in Mott systems, in Hund metals the quasiparticle weight Z can be suppressed on spite of increasing charge correlations

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

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



Key role!

Fanfarillo & EB, arXiv:1501.04607

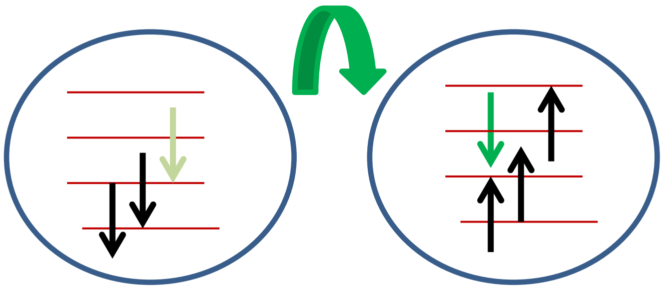
Electronic correlations in multi-orbital systems: Hund metals

Correlations in Hund metals are directly connected to the half-filled Mott insulator but contrary to what happens in Mott systems, in Hund metals the quasiparticle weight Z can be suppressed on spite of increasing charge correlations

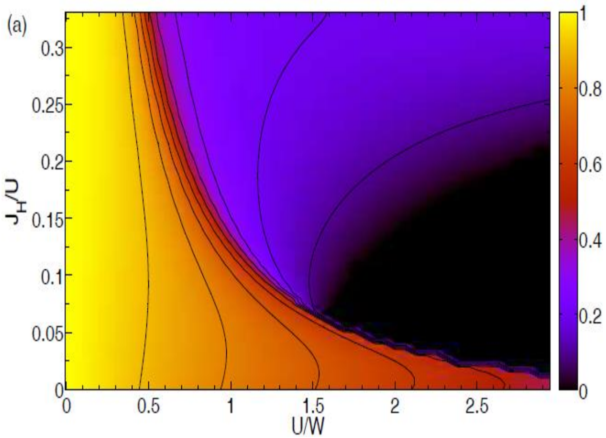
❑ Suppression of coherence due to suppression of hopping processes which involve intraorbital double occupancy

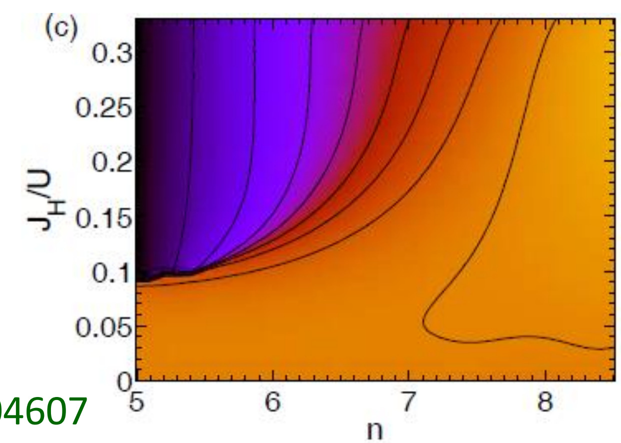
$$E^{intra\uparrow\downarrow} = U + (n-1)J_H$$

Suppressed by Hund's coupling



Links correlations in Hund metals with half-filled Mott insulator





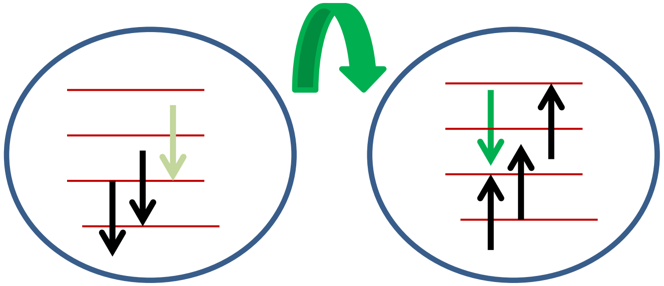
Fanfarillo & EB, arXiv:1501.04607

Electronic correlations in multi-orbital systems: Hund metals

Correlations in Hund metals are directly connected to the half-filled Mott insulator but contrary to what happens in Mott systems, in Hund metals the quasiparticle weight Z can be suppressed on spite of increasing charge correlations

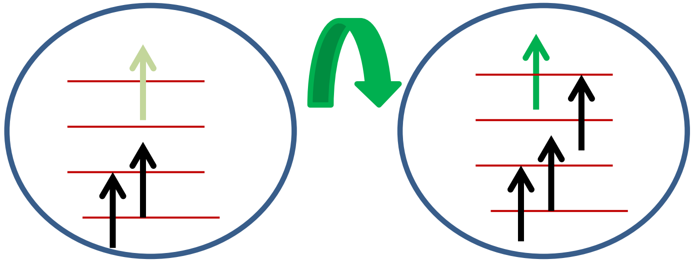
- ❑ Suppression of coherence due to suppression of hopping processes which involve intraorbital double occupancy

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



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

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

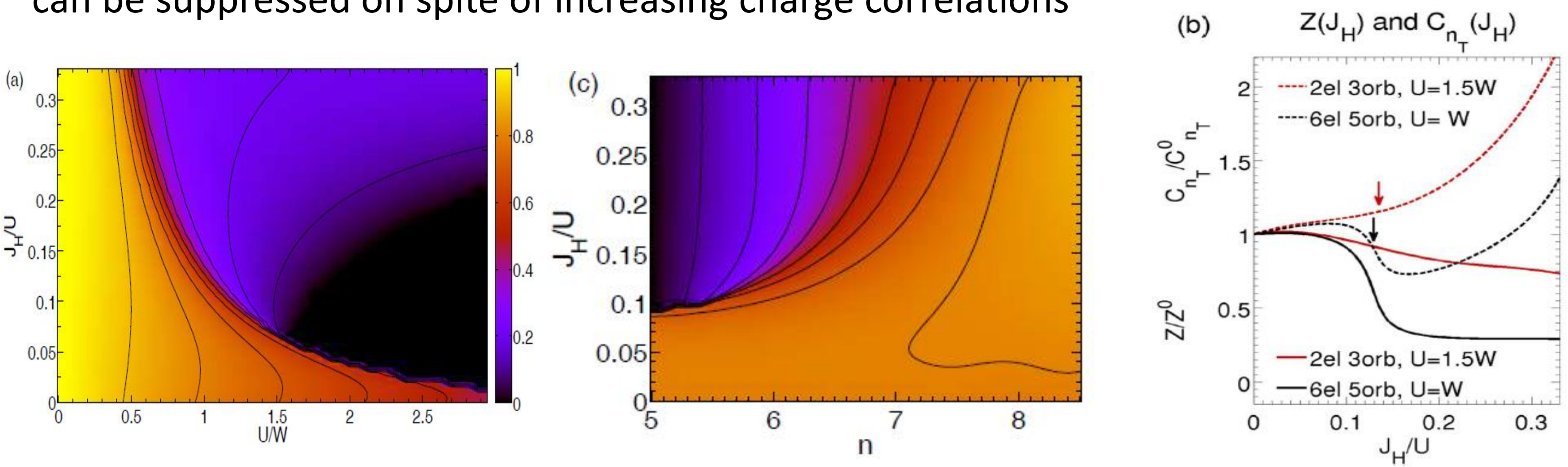


Fanfarillo & EB, arXiv:1501.04607

E. Bascones leni@icmm.csic.es

Summary

Correlations in Hund metals are directly connected to the half-filled Mott insulator but contrary to what happens in Mott systems, in Hund metals the quasiparticle weight Z can be suppressed on spite of increasing charge correlations

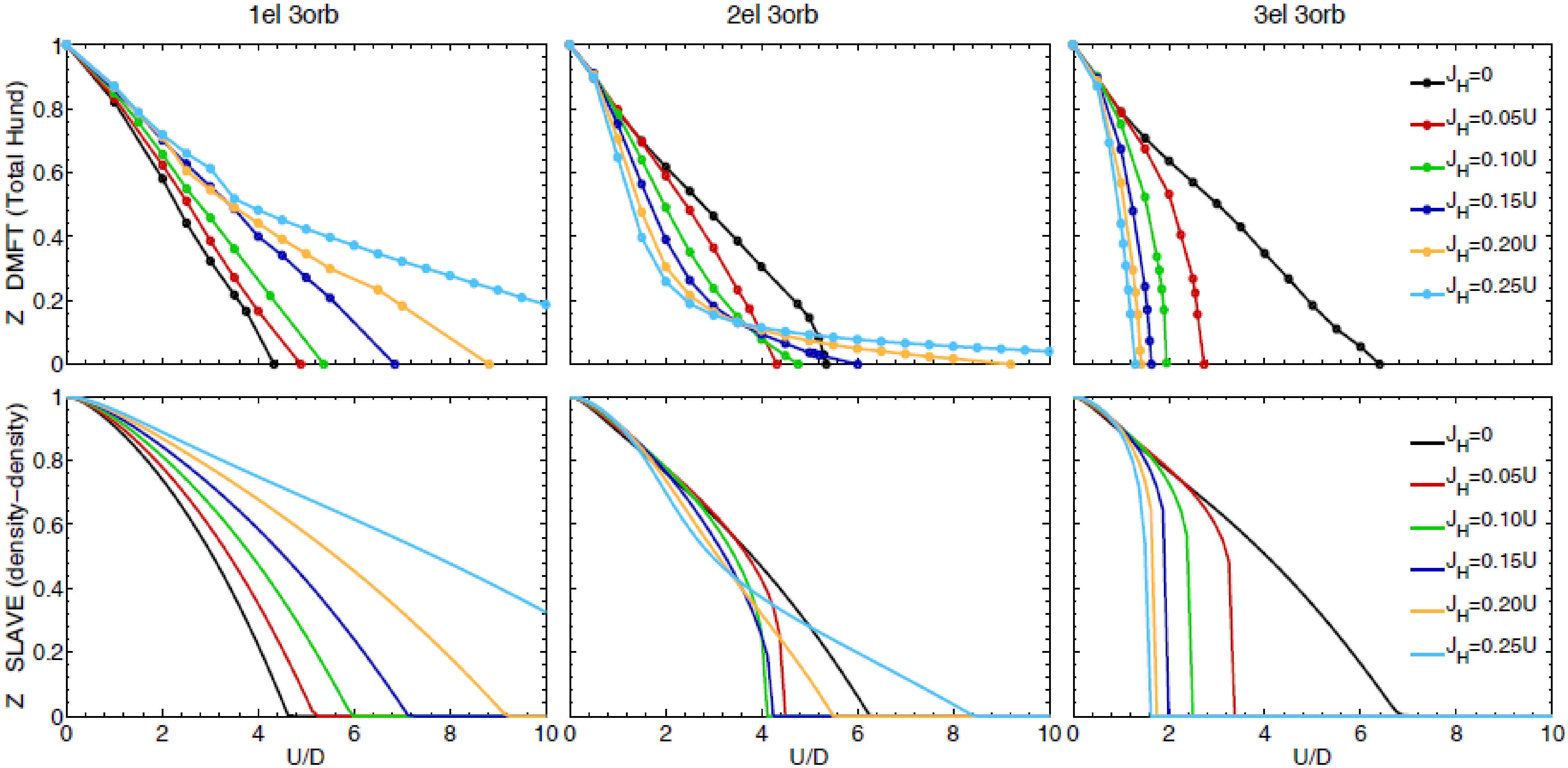


- ❑ Understood in terms of which hopping processes are suppressed (intraorbital double occupancy) or promoted (hopping to an empty orbital with parallel spin)
- ❑ Behavior changes at large U and J_H due to the proximity of non half-filled Mott insulator
- ❑ Understanding of why Hund's coupling promotes orbital decoupling

Fanfarillo & EB, arXiv:1501.04607

Slave spin (Density-density): benchmark

3 orbitals, semi-circular density of states



Fanfarillo & EB, arXiv:1501.04607

The quasiparticle weight in the single-orbital Hubbard model

Z: a way to quantify the correlations

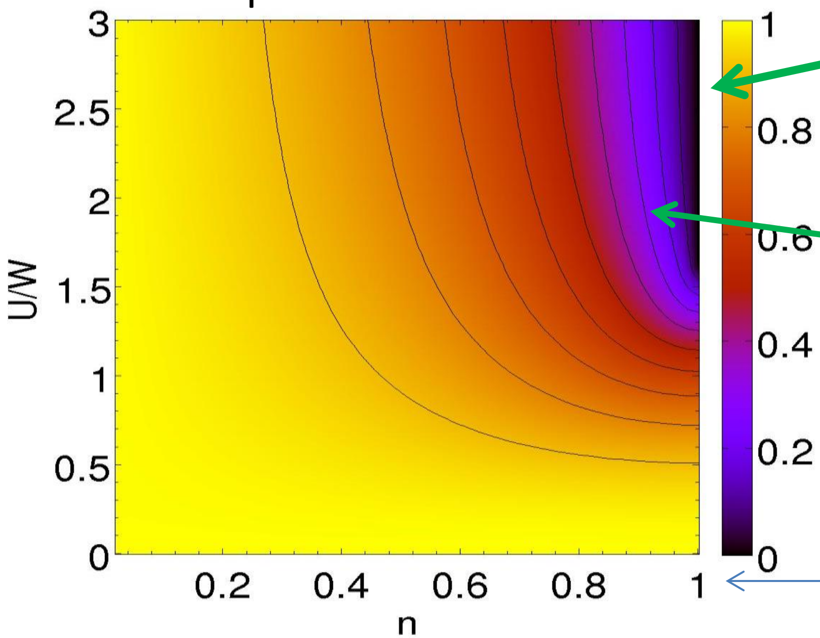
$$0 \leq Z \leq 1$$

Z=1 Single-particle picture (U=0)

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

Simple Fermi liquid 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). Double occupancy of a given orbital is suppressed

Half-filling

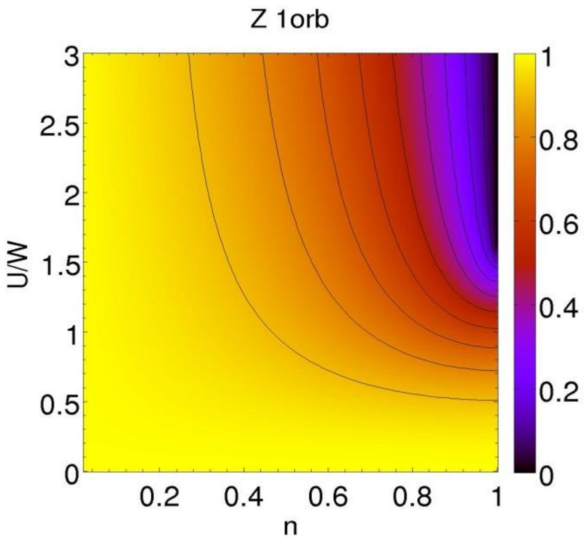
W bandwidth
of non interacting system

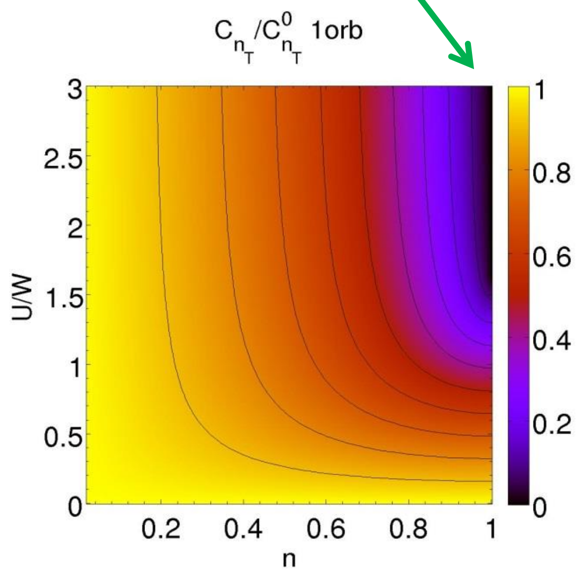
n: number of electrons per atom

Charge and spin fluctuations in the single-orbital Hubbard model

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

Localization





Very often
the quasiparticle weight Z
or the mass enhancement
are taken as a measure
of charge localization

Mott insulator:

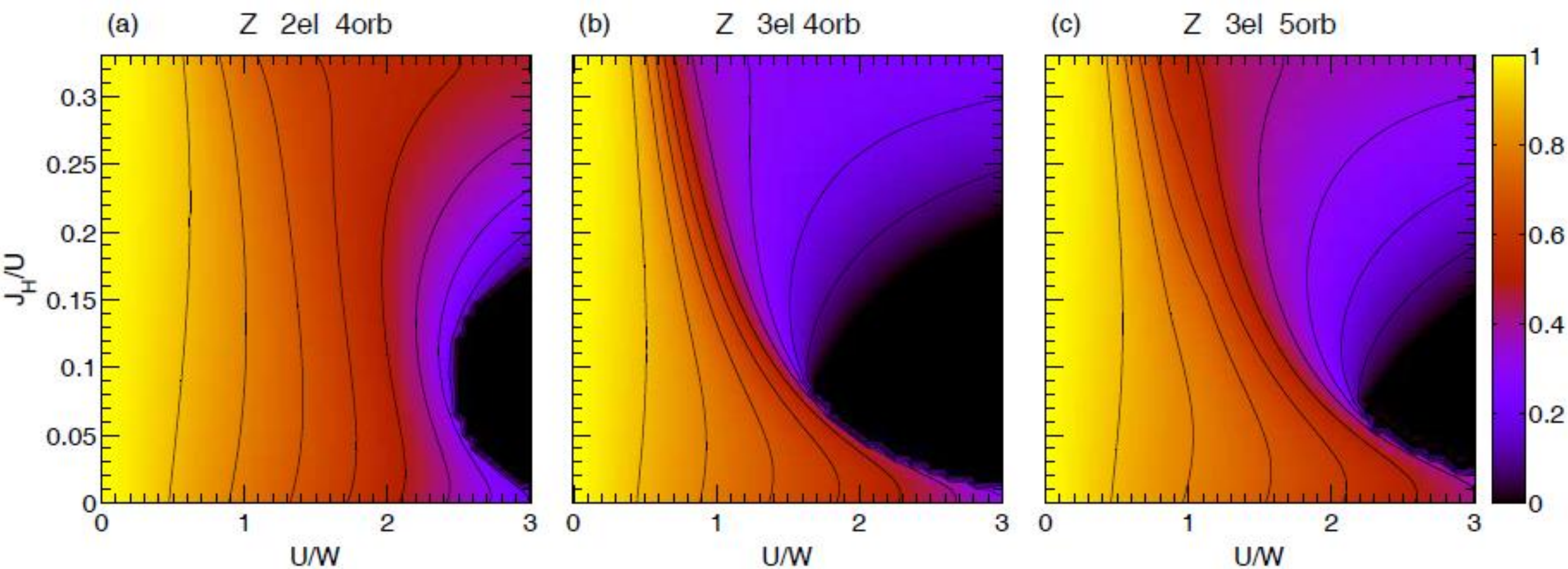
Suppression of charge fluctuations

n= <n>

E. Bascones leni@icmm.csic.es ICMM CSIC

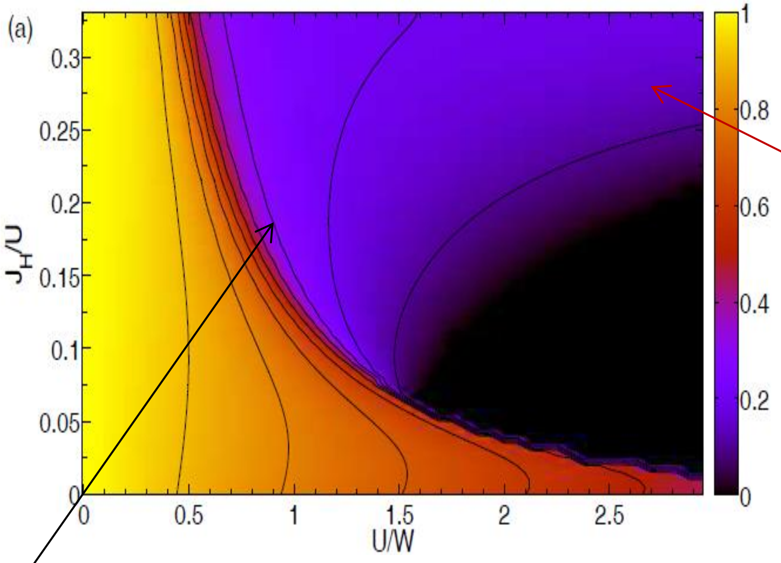
Electronic correlations in Hund metals

Colour plots: **Quasiparticle weight Z**



Fanfarillo & EB, arXiv:1501.04607

Electronic correlations in multi-orbital systems: Hund metals



Behavior of the system controlled by the proximity to the (n=6) Mott insulating phase (Z increases with J_H, Cs decrease with U)

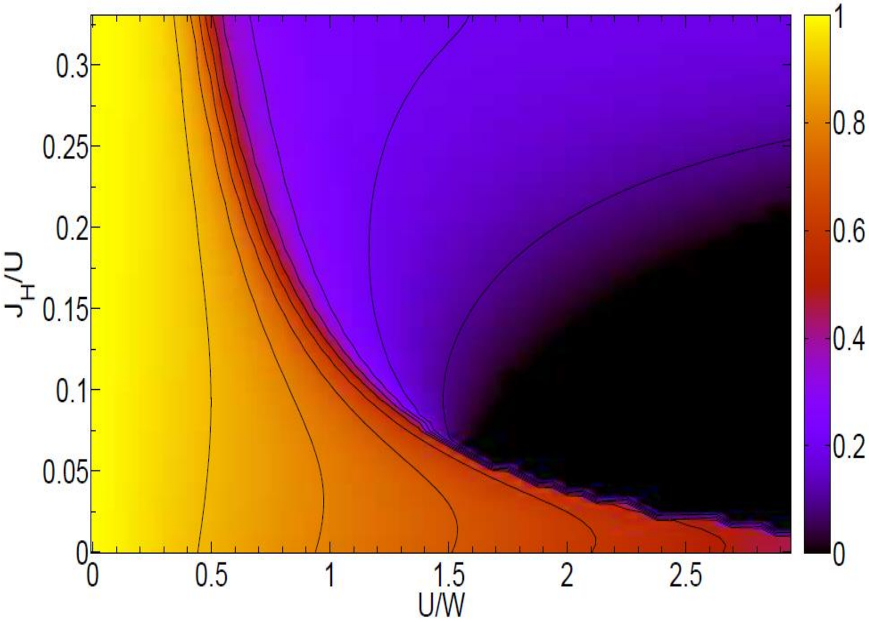
Suppression of coherence due to atomic spin polarization (Z decreases with JH, Cs increase with U)

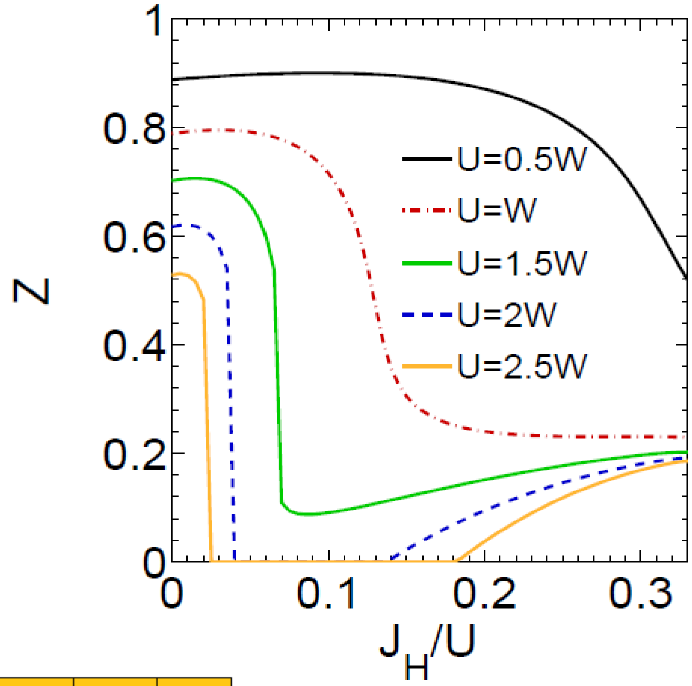
Fanfarillo & EB, arXiv:1501.04607

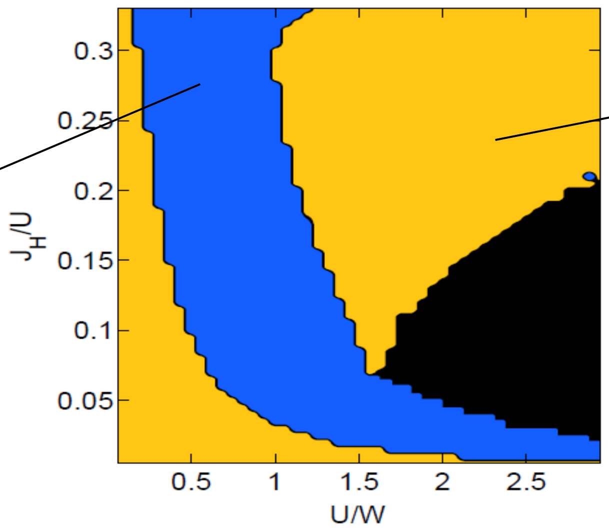
Electronic correlations in Hund metals

Quasiparticle weight Z

6 electrons in 5 orbitals,







Z decreases with J_H

Z increases with J_H

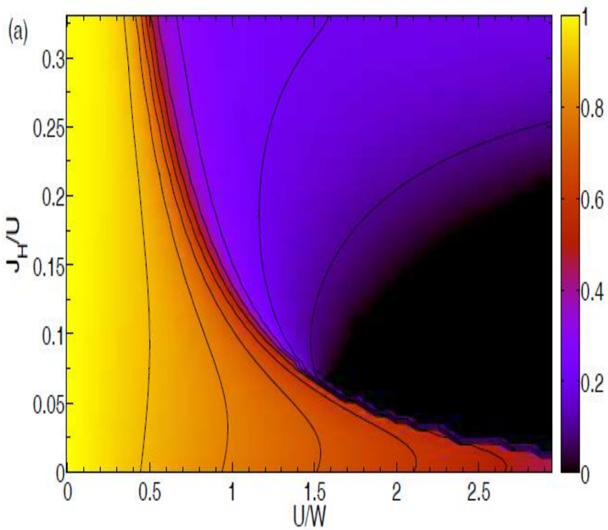
L. Fanfarillo, EB arXiv:1501.04607

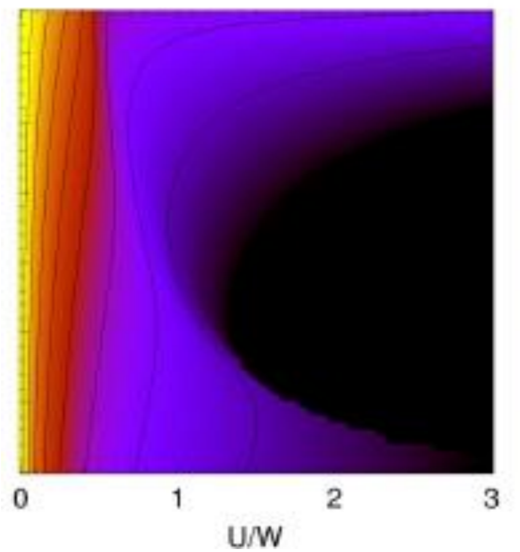
rillo & EB, arXiv:1501.04607

Evolution of charge fluctuations in Hund metals

Quasiparticle Weight Z

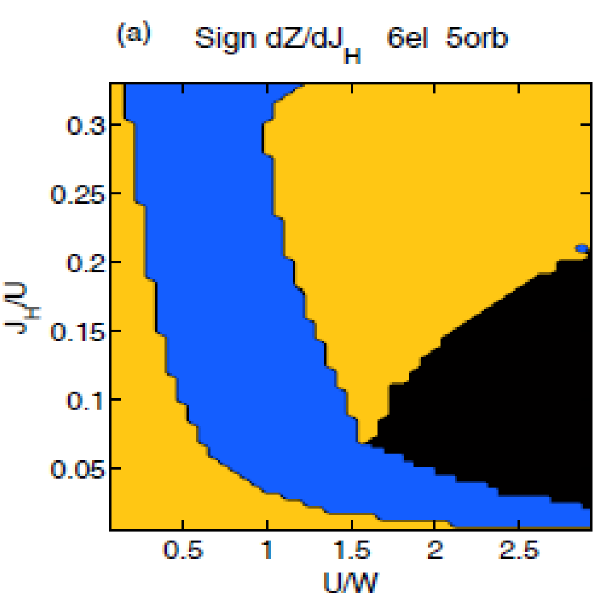
Charge Fluctuations

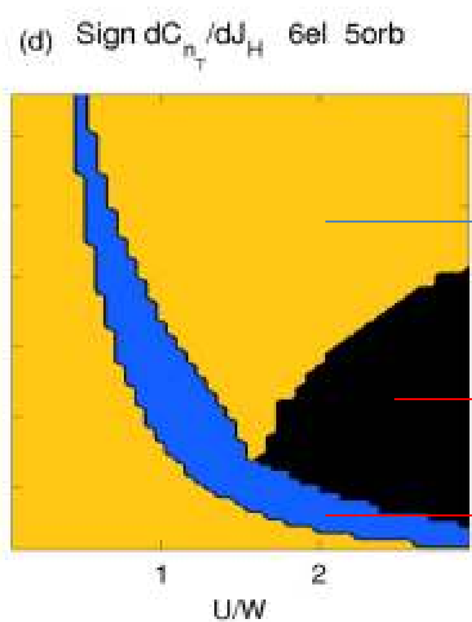




6 electrons in 5 orbitals

The suppression of the quasiparticle weight and the charge fluctuations with interactions follow different patterns





Yellow: increases with J_H

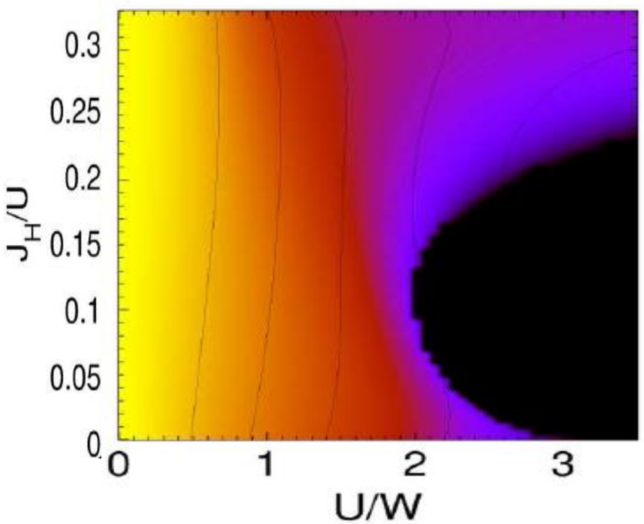
Black: does not change with J_H

Blue: decreases with J_H

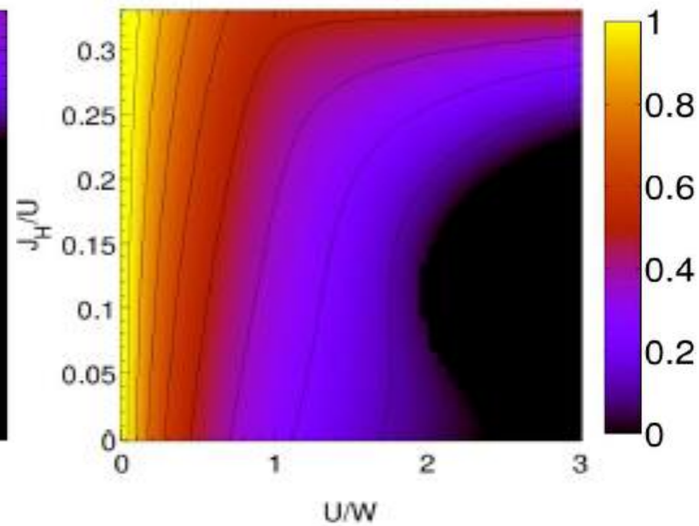
Fanfarillo & EB, arXiv:1501.04607

Evolution of charge fluctuations in Hund metals

Quasiparticle Weight Z

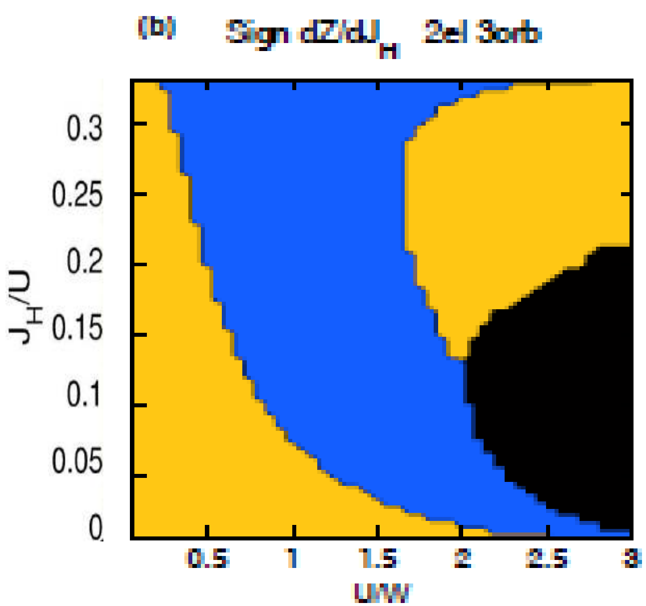


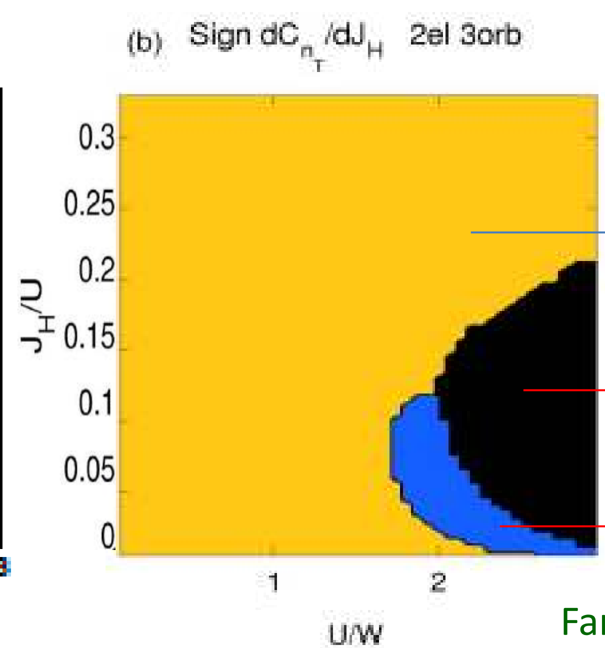
Charge Fluctuations



2 electrons in 3 orbitals

The suppression of the quasiparticle weight and the charge fluctuations with interactions follow different patterns





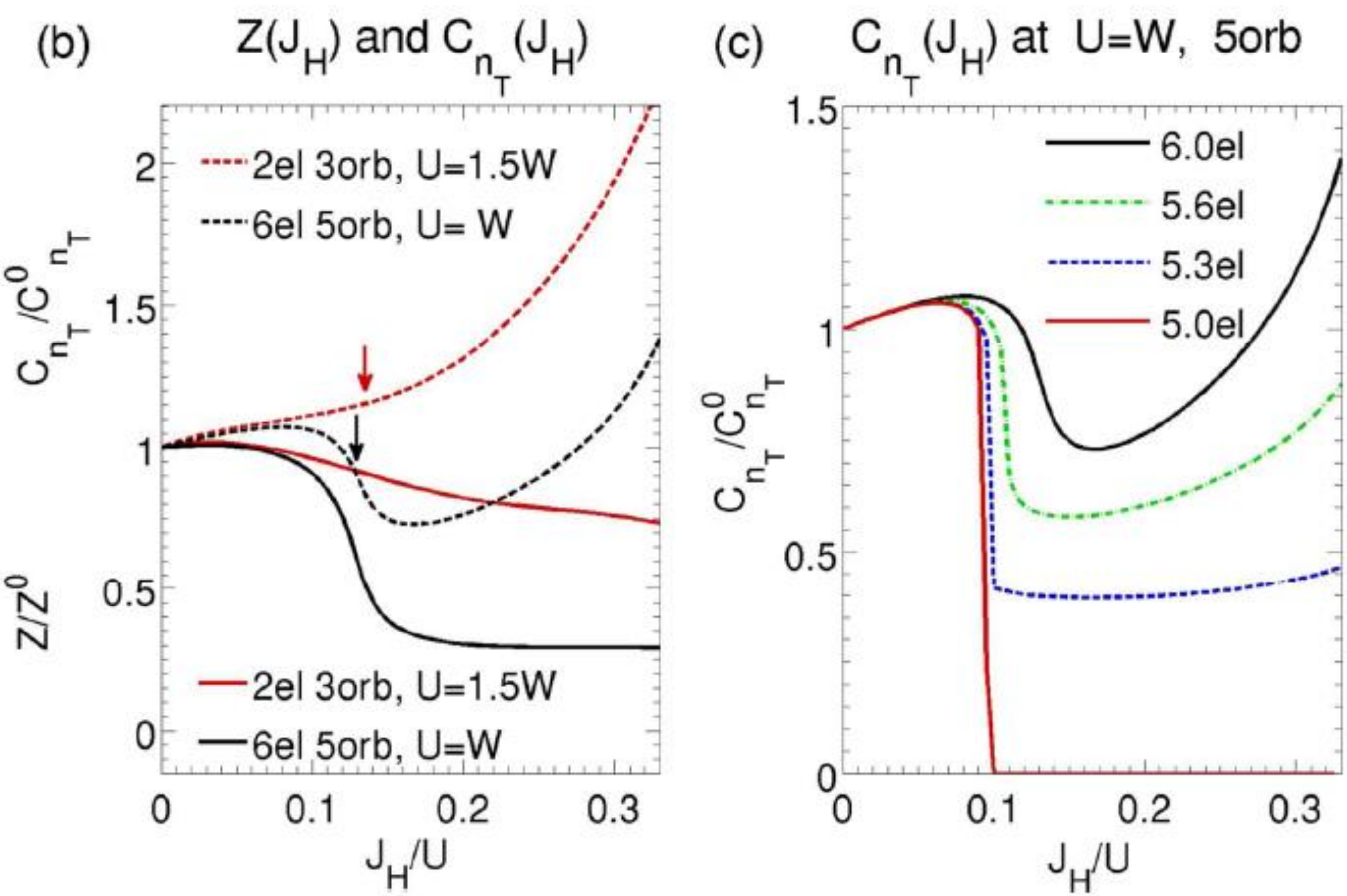
Yellow: increases with J_H

Black: does not change with J_H

Blue: decreases with J_H

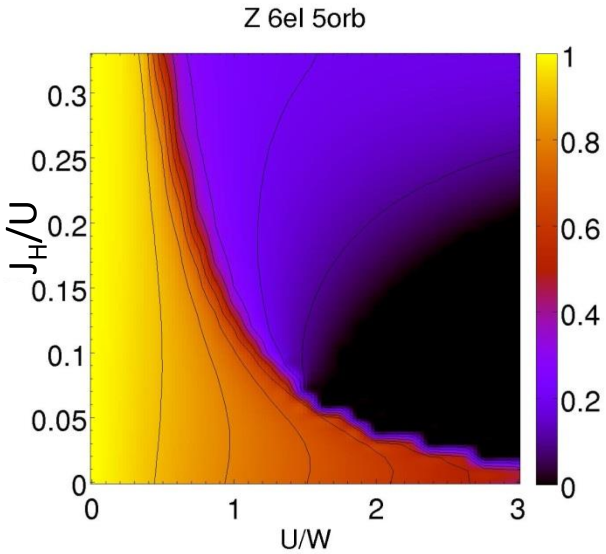
Fanfarillo & EB, arXiv:1501.04607

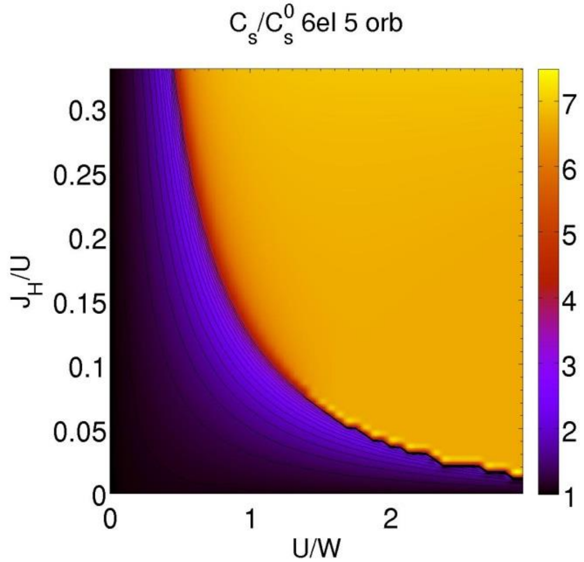
Evolution of charge fluctuations in Hund metals



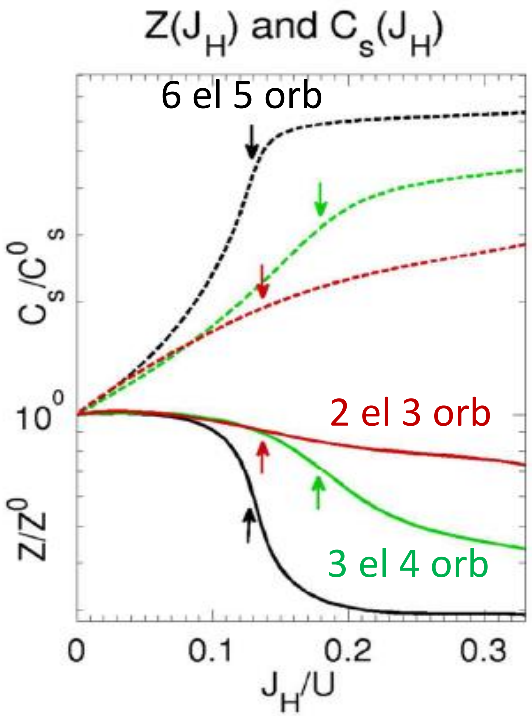
Fanfarillo & EB, arXiv:1501.04607

Spin fluctuations in Hund metals





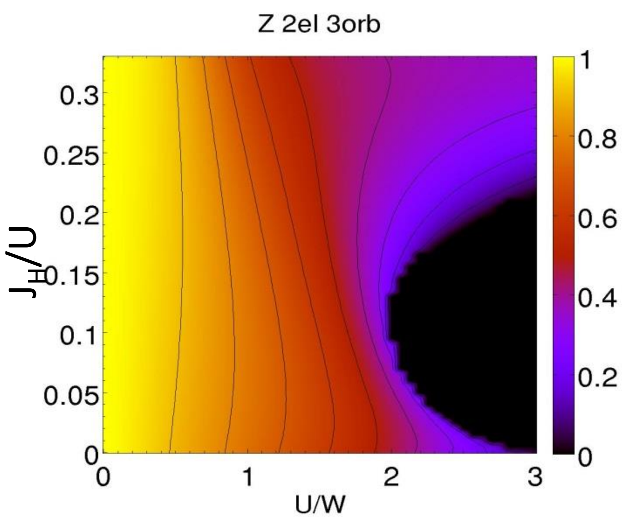
6 electrons in 5 orbitals

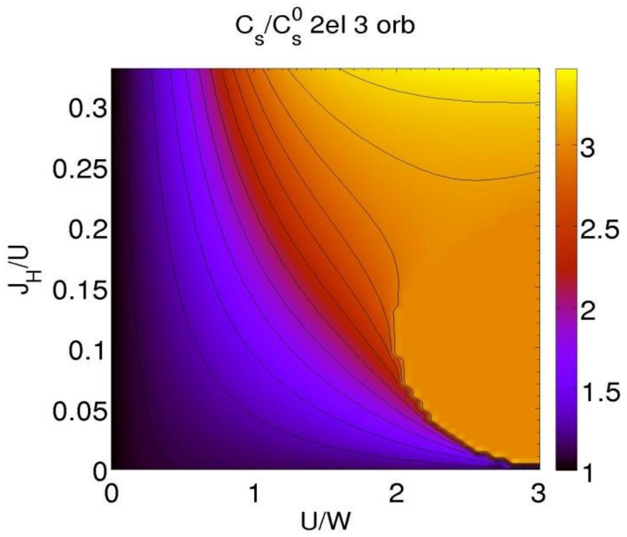


Atomic moments are formed in the Hund metal

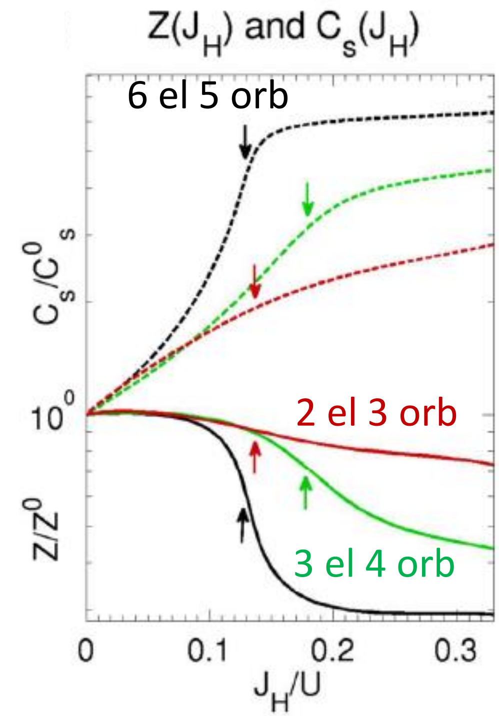
Fanfarillo & EB, arXiv:1501.04607

Spin fluctuations in Hund metals





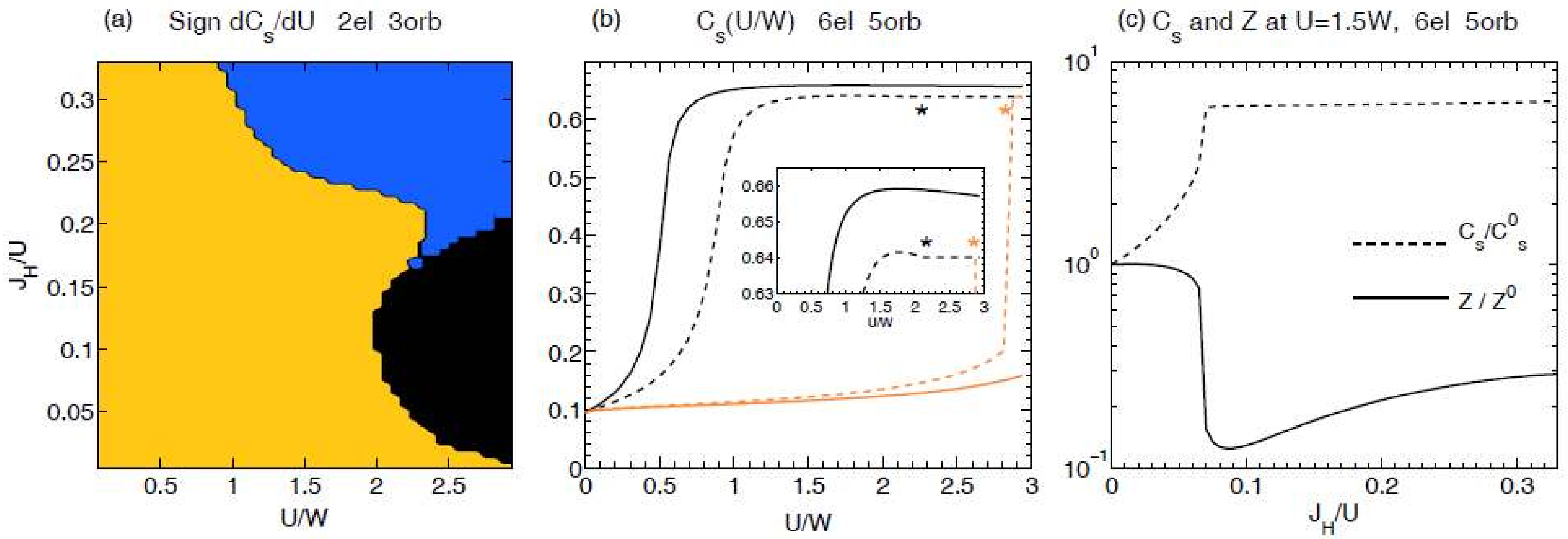
2 electrons in 3 orbitals



Atomic moments are formed in the Hund metal

Fanfarillo & EB, arXiv:1501.04607

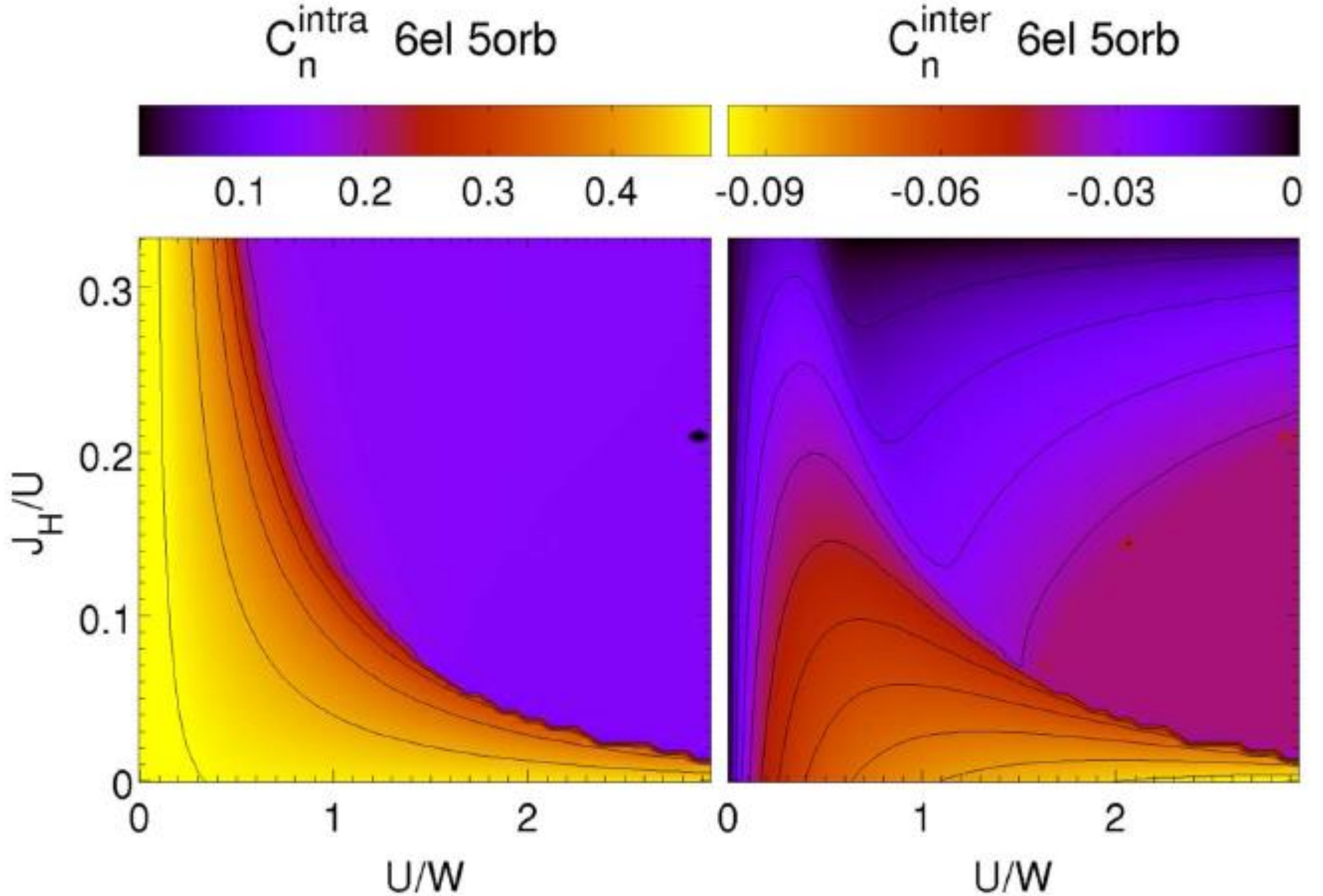
Spin fluctuations in Hund metals



Fanfarillo & EB, arXiv:1501.04607

Electronic correlations in multi-orbital systems: Hund metals

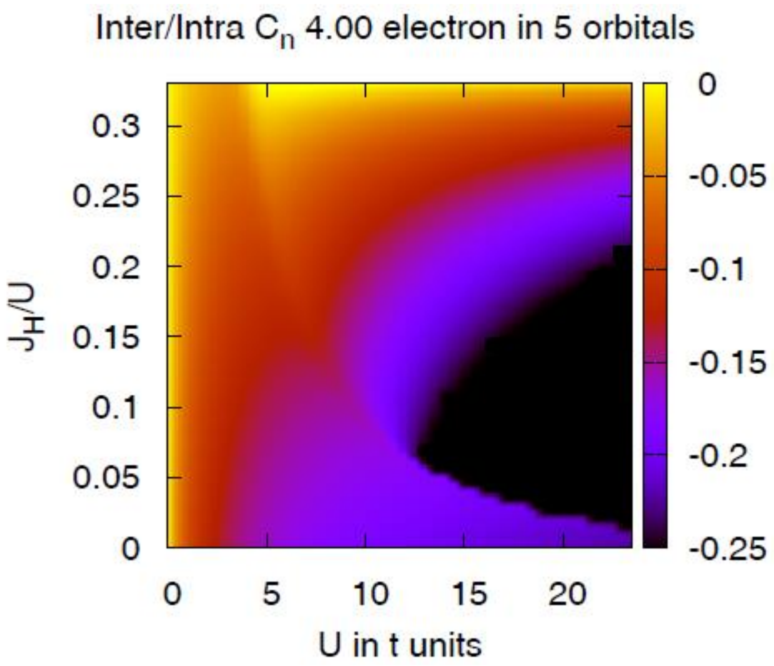
$C_n^{\rm intra} = < n_a^2 > - < n_a >^2 = < (\delta n_a)^2 >$ $\qquad$ $C_n^{\rm inter} = < n_a n_b > - < n_a >< n_b > = < \delta n_a \delta n_b >$



$$C_{n_T} = N\left(C_n^{\rm intra} + (N-1)C_n^{\rm inter}\right)$$

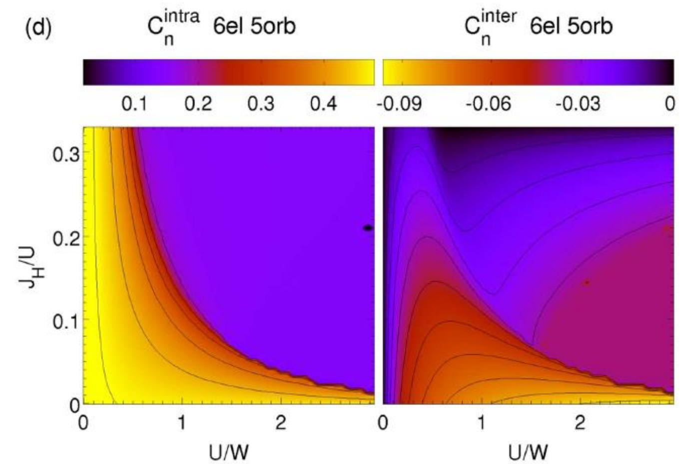
Fanfarillo & EB, arXiv:1501.04607

Electronic correlations in multi-orbital systems: Decoupling



$$C_n^{\mathrm{inter}} = < n_a n_b > - < n_a >< n_b > = < \delta n_a \delta n_b >$$

$$C_n^{\mathrm{intra}} = < n_a^2 > - < n_a >^2 = < (\delta n_a)^2 >$$



The atomic spin polarization effectively reduces the interaction between electrons in different orbitals to $U'-J_H=U-3J_H$

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

$U'=U-2J_H$

Fanfarillo & EB, arXiv:1501.04607

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)

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

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

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

Hubbard-Kanamori hamiltonian

$$H_{\rm int} = U\sum_{a} n_{a\uparrow}n_{a\downarrow} + (U' - J_H)\sum_{a<b,\sigma} n_{a\sigma}n_{b\sigma}$$
$$+ U'\sum_{a\neq b} n_{a\uparrow}n_{b\downarrow} - J_H\sum_{a\neq b} c^{\dagger}_{a\uparrow}c_{a\downarrow}c^{\dagger}_{b\downarrow}c_{b\uparrow}$$
$$+ J'\sum_{a\neq b} c^{\dagger}_{a\uparrow}c^{\dagger}_{a\downarrow}c_{b\downarrow}c_{b\uparrow}$$

This terms are neglected
in our calculation
(Ising approx)

$U' = U - 2J_H$

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 $f_{i\sigma}$

Pseudospin variable $S^{z}_{i\sigma}$
(slave-spin)

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

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

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

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

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

$$\underbrace{\frac{U}{2}\sum_i \left(\sum_{m,\sigma} S^z_{im\sigma}\right)^2 + \frac{U'}{2}\sum_i (\sum_{m,\sigma} S^z_{im\sigma})^2 + J\sum_{i,m}(\sum_\sigma S^z_{im\sigma})^2 - \frac{J}{2}\sum_{i,\sigma}(\sum_m S^z_{im\sigma})^2}_{H_{int}[\{\vec{S}_{im\sigma}\}]}$$

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

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

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

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

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

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

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

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)
Hassan & de Medici, PRB 81, 035106 (2010)