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Mott Physics: from basic concepts to iron superconductors

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Mott physics: from basic concepts to iron superconductors

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Outline

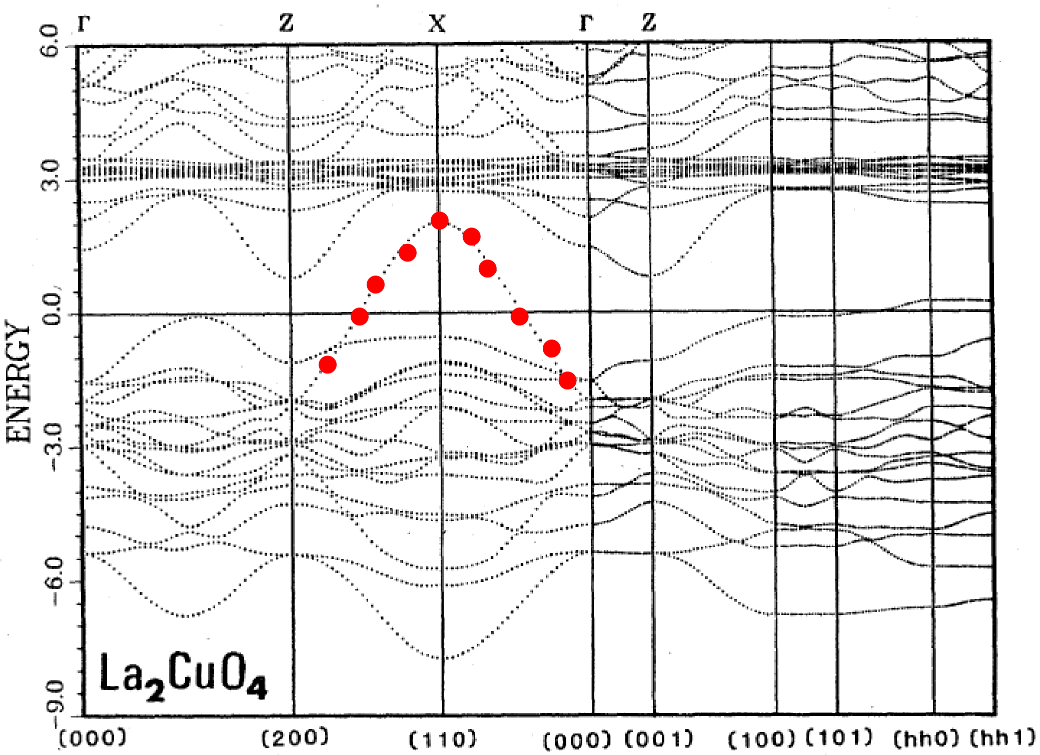
- Mott physics: Basic concepts (single orbital & half filling)
  - Mott transition & breakdown of independent electron picture
  - Insulating state (Hubbard bands)
  - Correlated metallic state (renormalized quasiparticles)
  - Magnetic exchange & metallicity away from half-filling

- Mott physics in Multi-orbital systems (at & away half filling)
  - Degenerate bands
  - Non degenerate bands (OSMT)

  Hund's coupling

- Mott physics in iron superconductors

Mott insulators



Metallic behavior expected

Fig: Pickett, RMP 61, 433 (1989)

Insulating behavior is found

Mott insulator:

Insulating behavior due to electron-electron interactions

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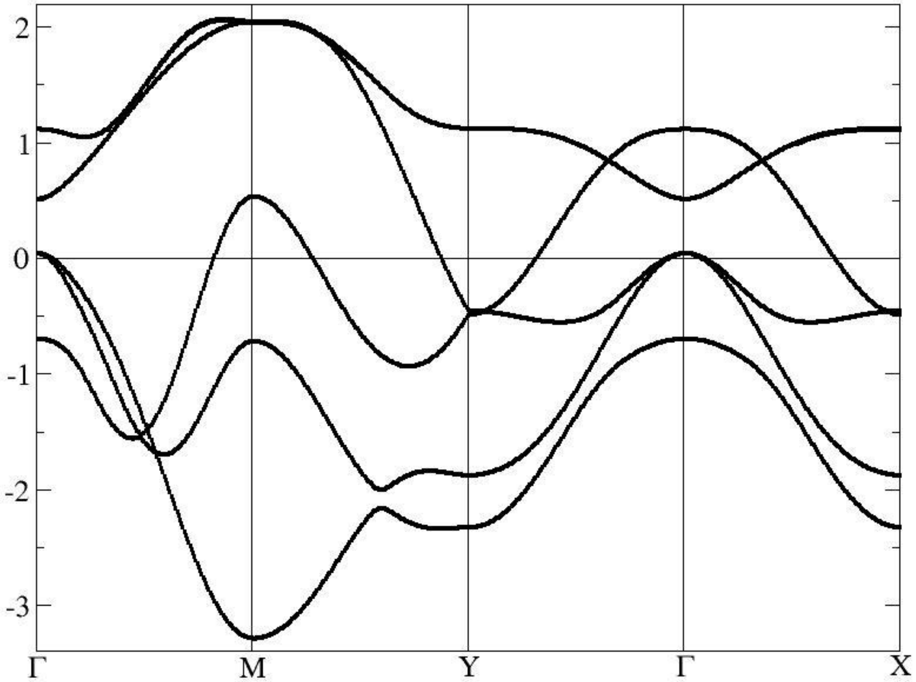
Kinetic energy. Delocalizing effect

$$\sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_{i,\gamma,\sigma}^{\dagger} c_{j,\beta,\sigma} + h.c.$$

Atomic orbital

spin

atomic site (i≠j)



Kinetic energy

Going from one atom to another

↓

Delocalizing effect

Adding electrons → Filling bands (rigid band shift)

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

Interaction energy

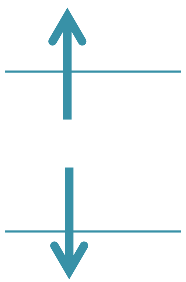
Consider 1 atom with a single orbital

$$U\sum_{j} n_{j,\uparrow} n_{j,\downarrow}$$

1 electron

E =0

2 electron. Gap to add a second electron



To add a second electron
to single filled orbital
costs energy U

Two electrons in the same atom repel each other

Energy states depend
on the occupancy
(non-rigid band shift)

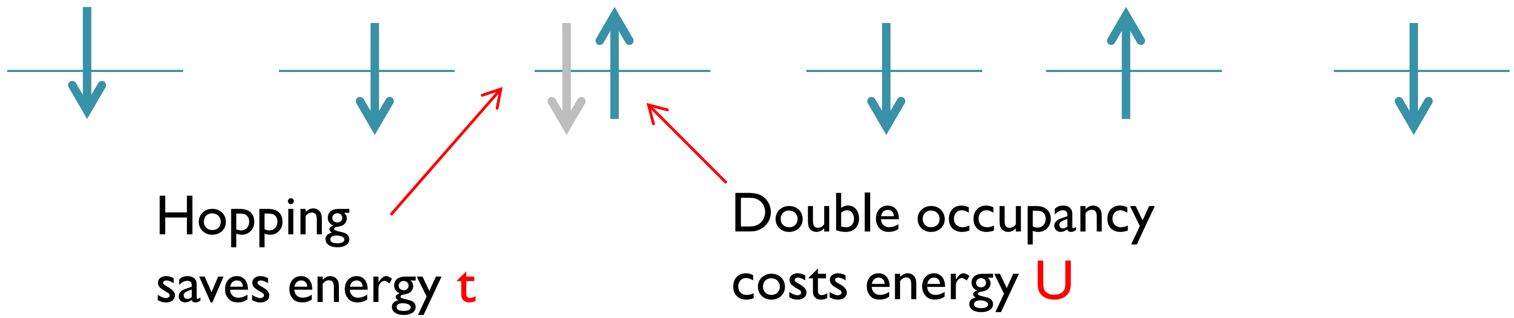
Mott insulators

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

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

The Mott transition

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

Hopping
saves energy t

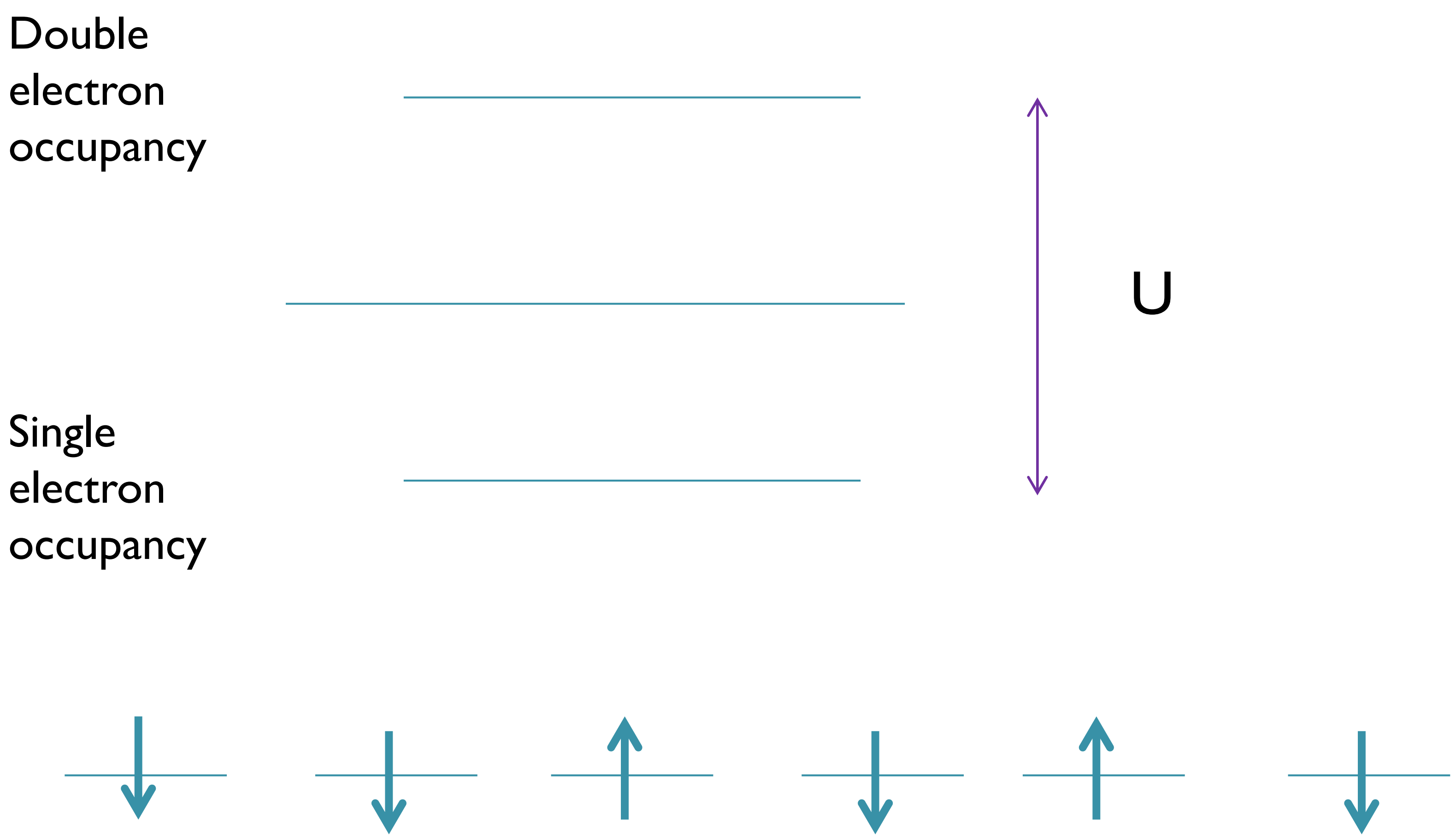
Double occupancy
costs energy U

$\boxed{\text{For } U >> t \text{ electrons localize: Mott insulator}}$

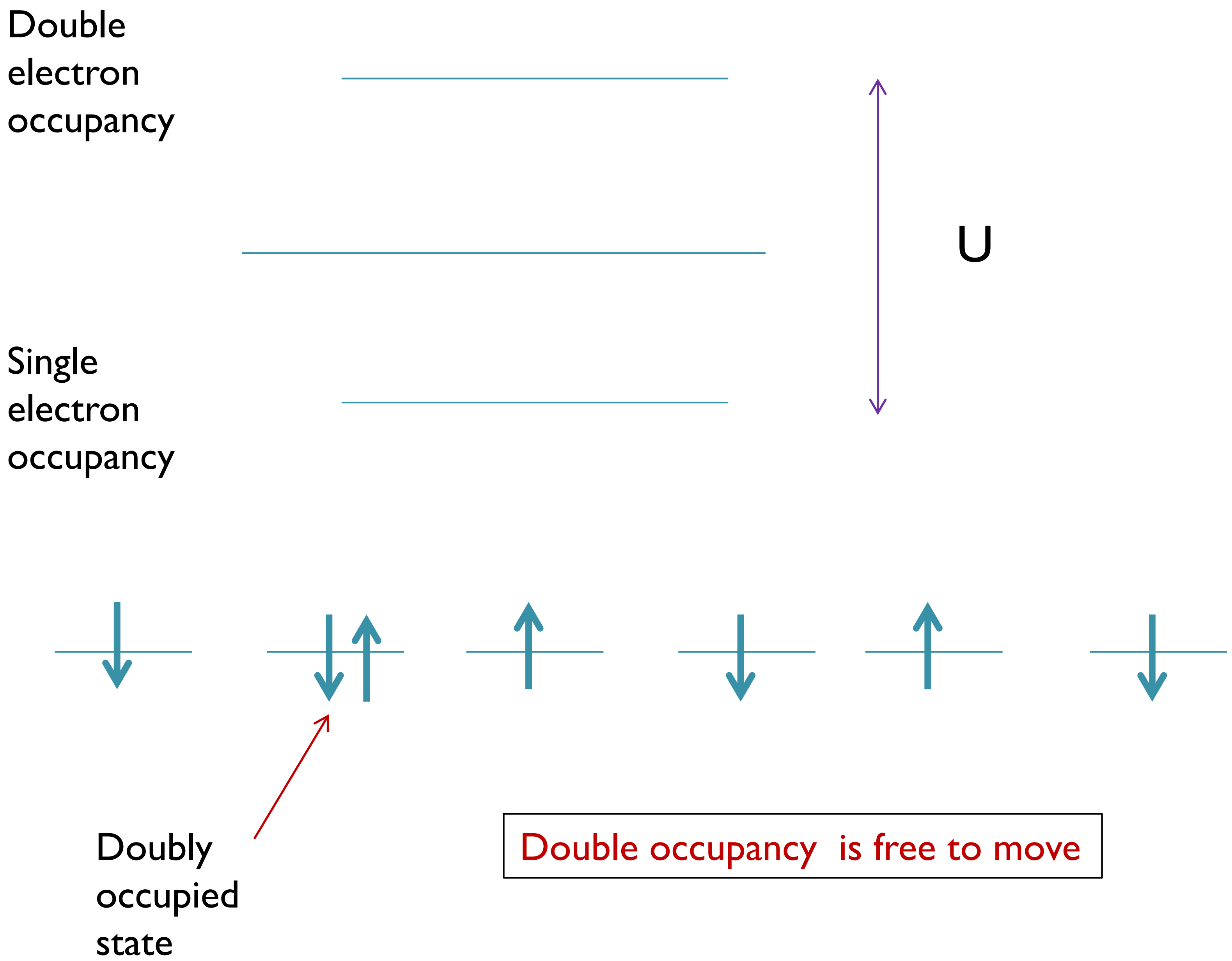
Small U/t	Increasing U/t	Large U/t
Metal	$\longrightarrow$	Insulator

Mott transition

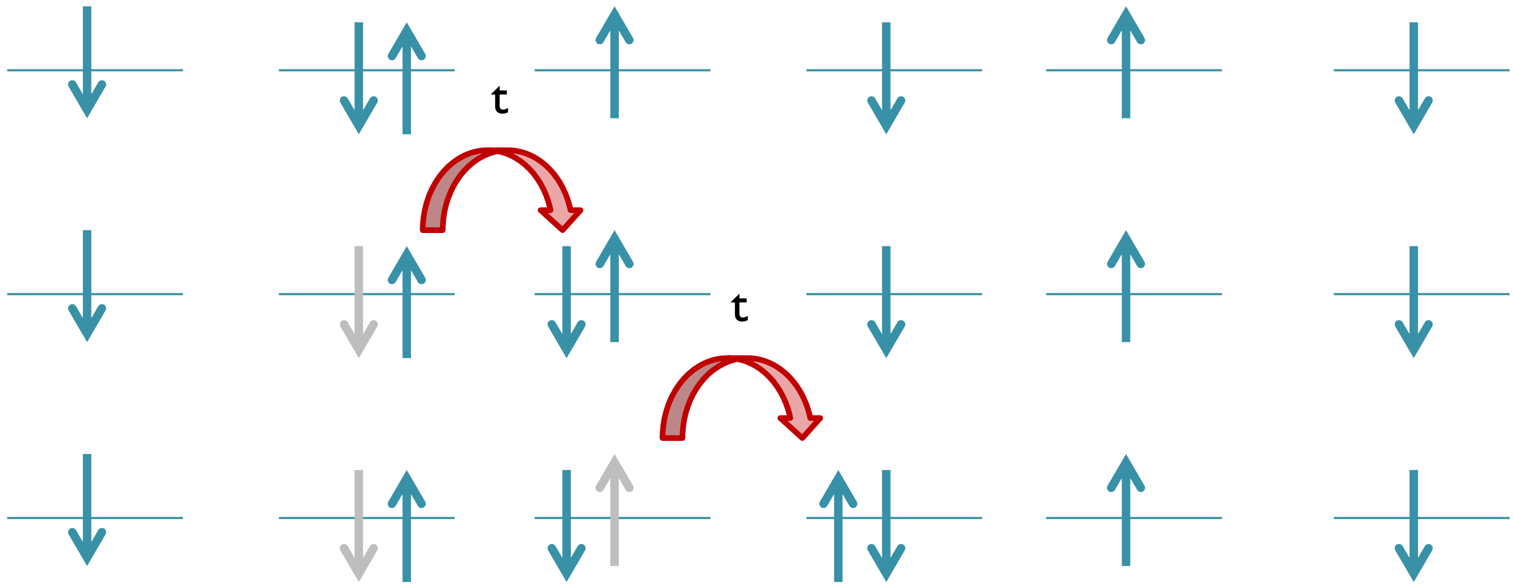
Atomic gap & Hubbard bands

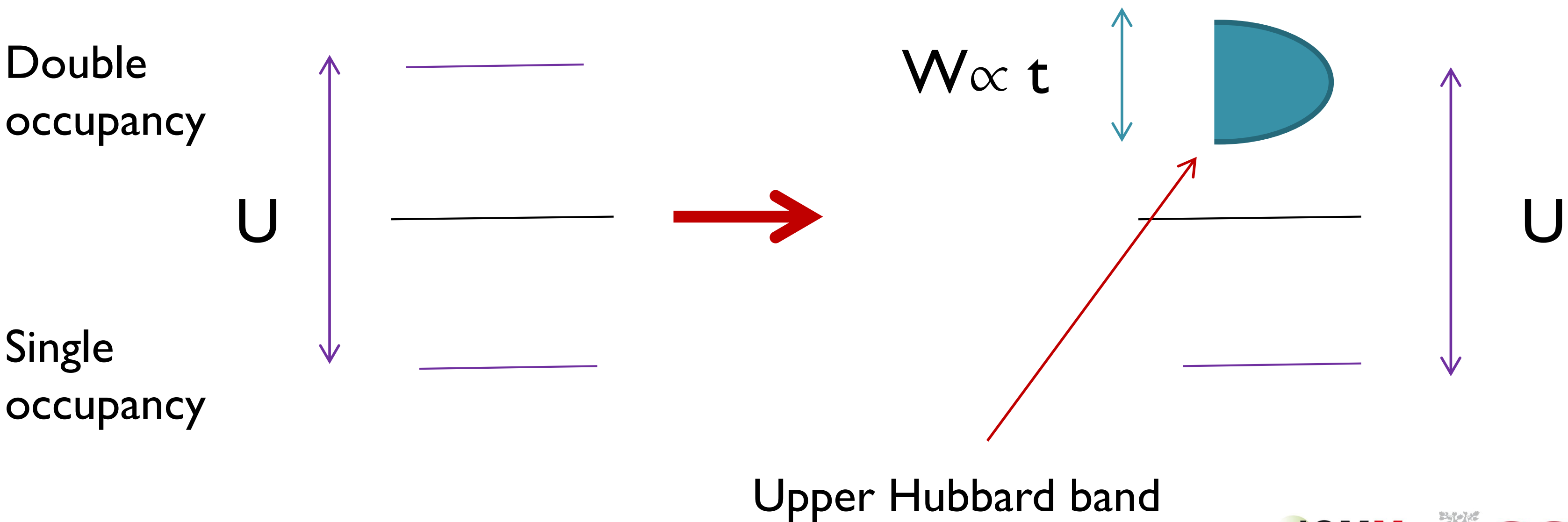


Hubbard bands

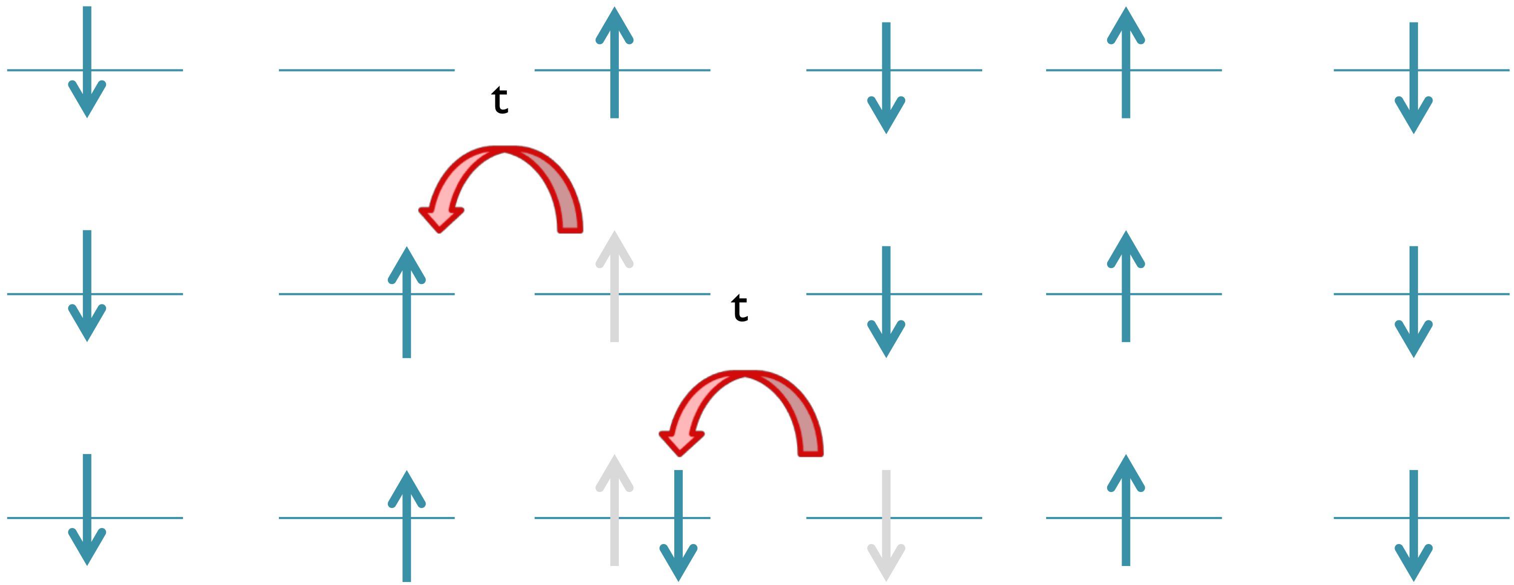


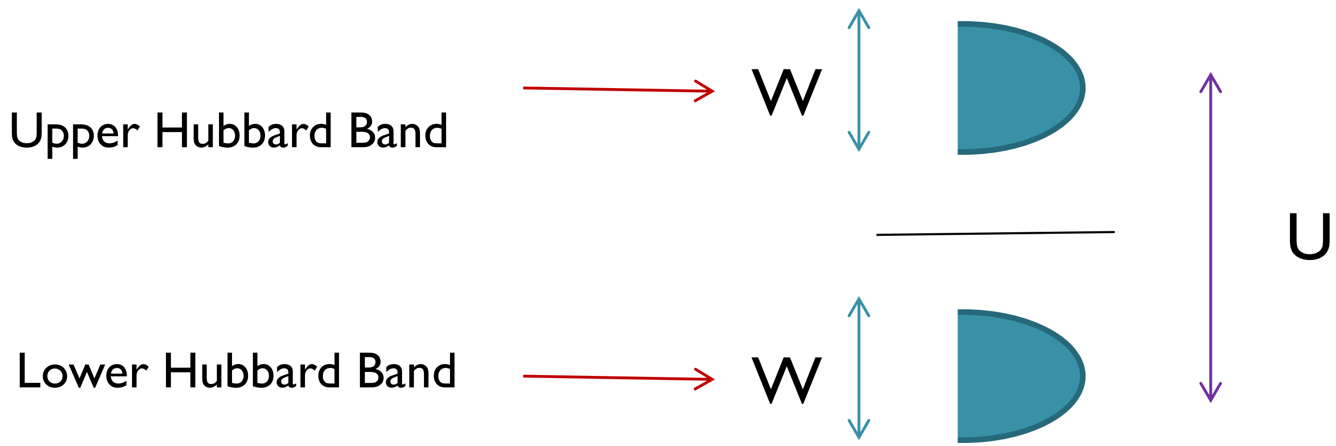
Hubbard bands



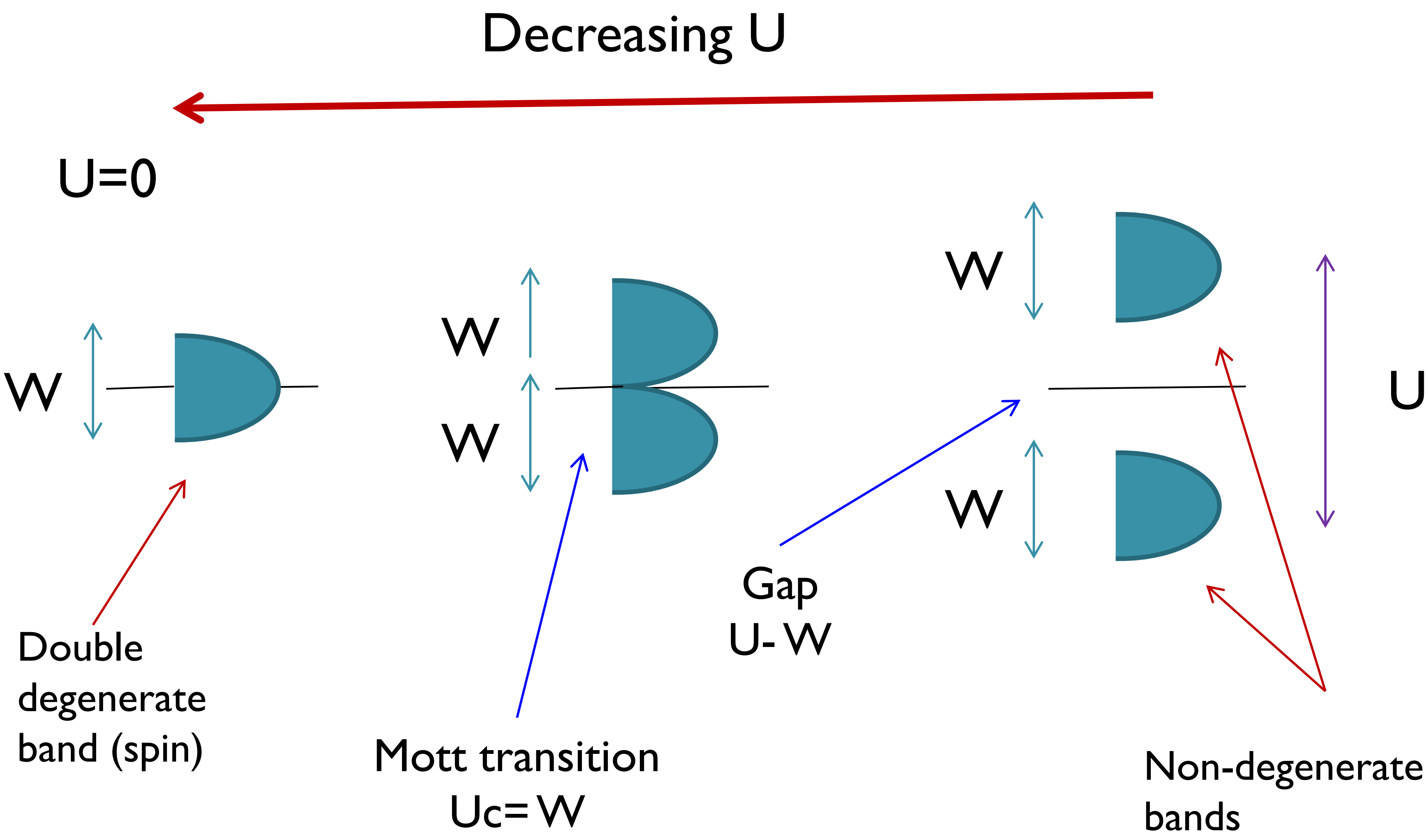


Hubbard bands





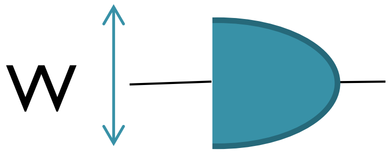
The Mott-Hubbard transition from the insulating state



Gap opens at the Fermi level at Uc

The transition from the metallic state

The uncorrelated metallic state: The Fermi sea |FS>



Spin degenerate

Energy states are filled according to their kinetic energy. States are well defined in k-space

Probability in real space: ¼ for the 4 possible states (half filling)

Cost in interaction energy per particle $\langle U \rangle = U/4$

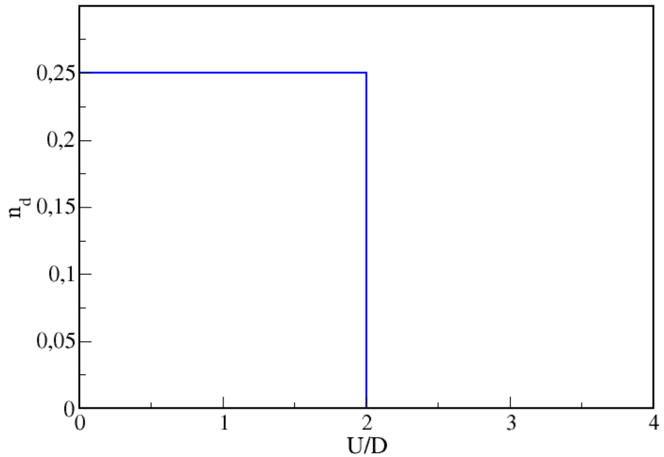
Kinetic energy gain per particle (constant DOS) $\langle K \rangle = -W/4 = -D/2$

The transition from the metallic state

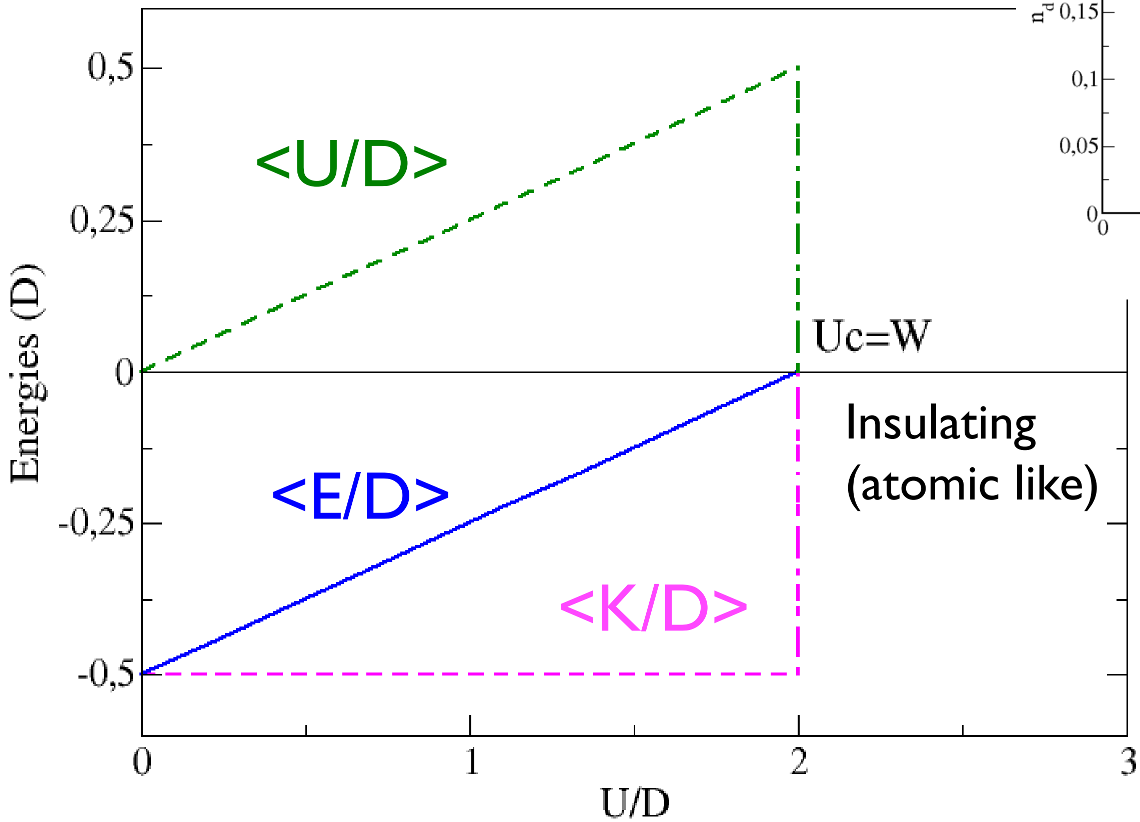
The uncorrelated metallic state: The Fermi sea |FS>

E=K+U

double occupancy



Metallic. Fermi sea



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The transition from the metallic state

The correlated metallic state: Gutzwiller wave function

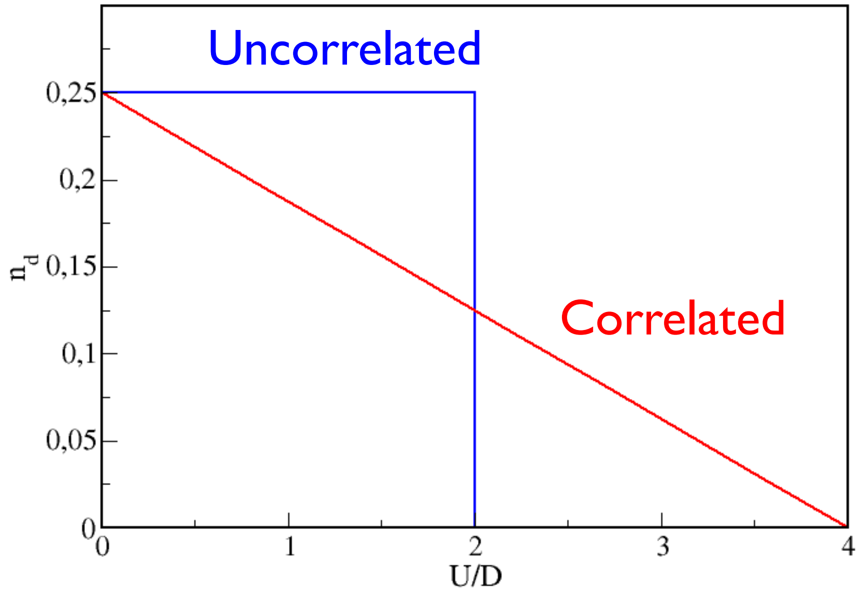
$$|\Psi\rangle = \Pi_j [\, 1-(1-\eta) n_{j\uparrow} n_{j\downarrow}] \, |FS\rangle$$

Variational Parameter

$\eta=1$ U=0

$\eta=0$ U=∞

η uniformly diminishes the concentration of doubly occupied sites



Gutzwiller Approximation. Constant DOS

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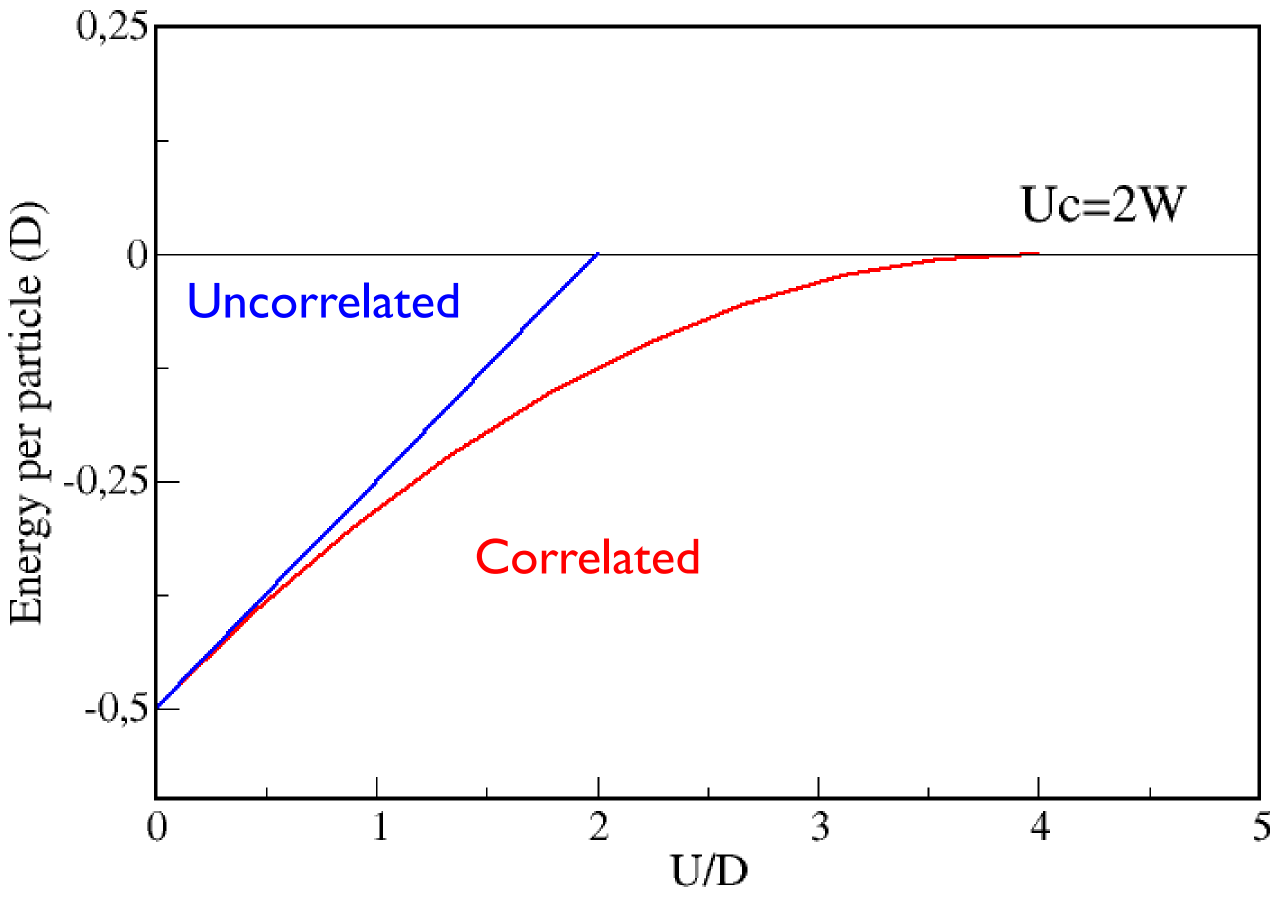
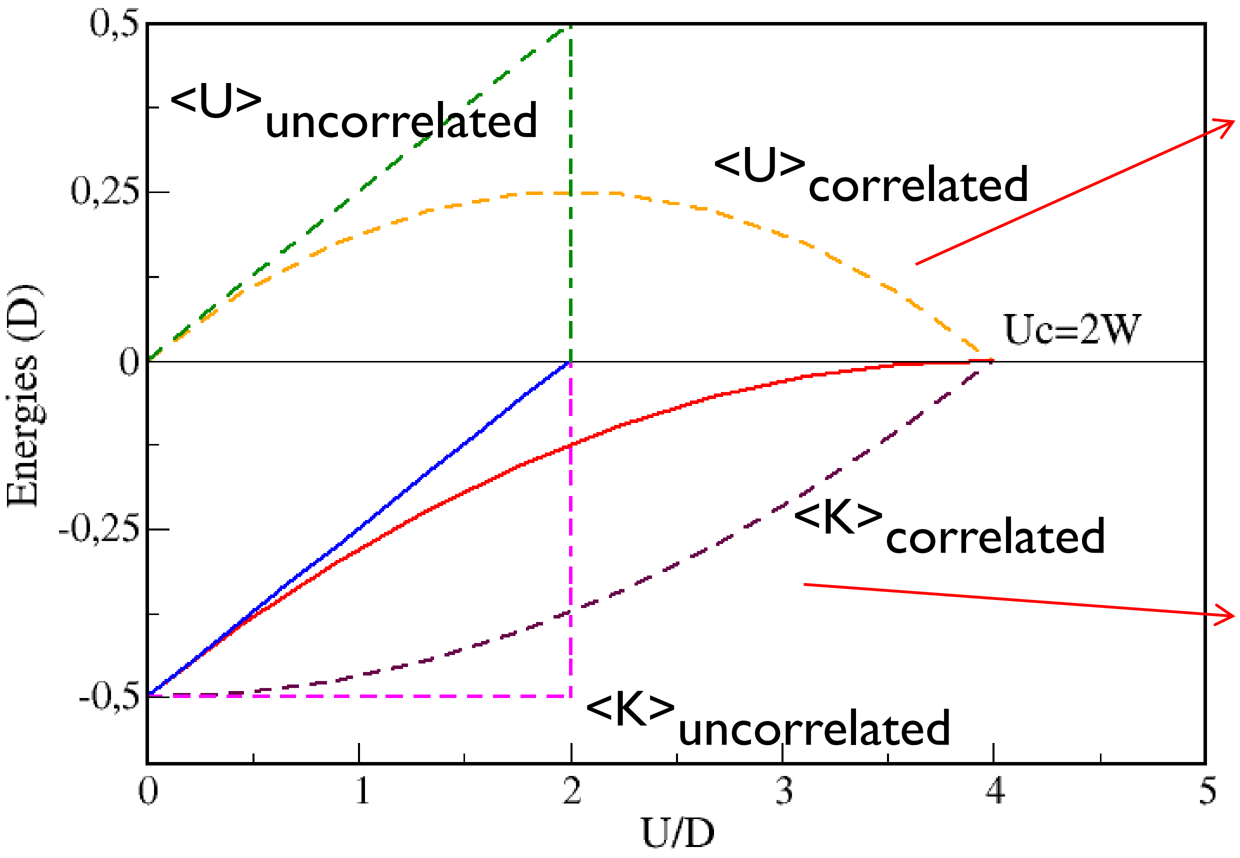
The transition from the metallic state

The correlated metallic state: Gutzwiller wave function



The transition from the metallic state

The correlated metallic state: Gutzwiller wave function



Average potential energy reduced due to reduced double occupancy

Kinetic Energy is reduced

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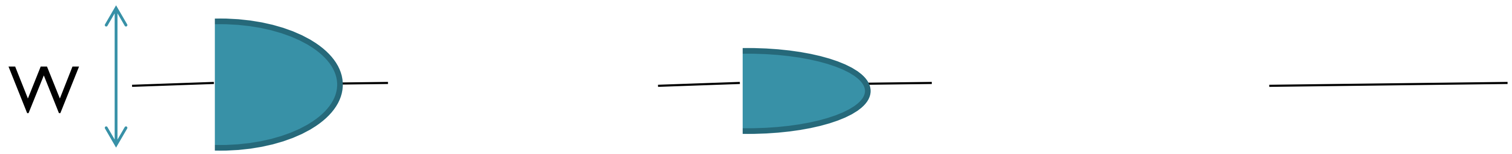
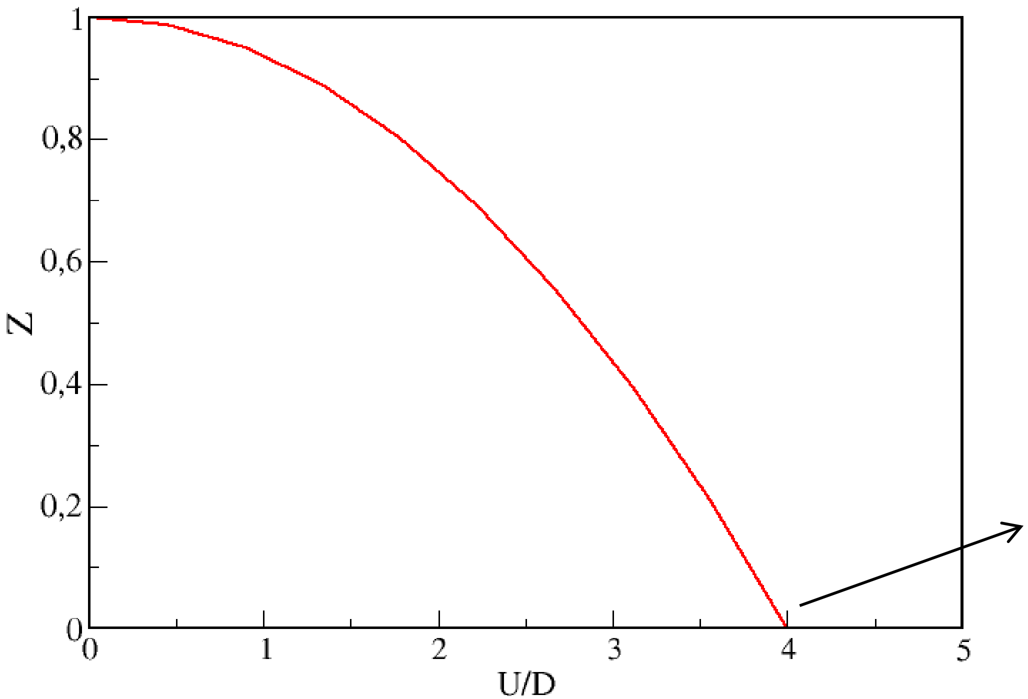
The Brinkman-Rice transition

Correlated metallic state



Heavy quasiparticle
(reduced Kinetic Energy)

Quasiparticle disappears



Reduced quasiparticle residue

Quasiparticle disappears at the Mott transition

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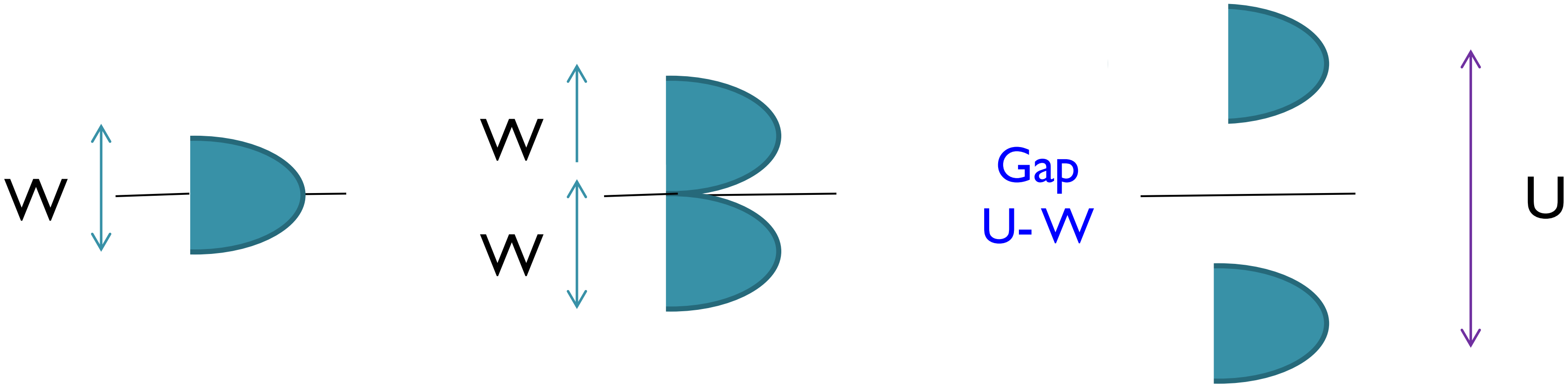
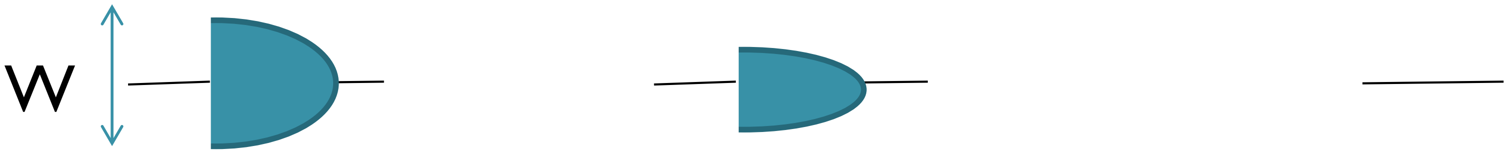
Mott-Hubbard vs Brinkman-Rice transition

The Mott-Hubbard transition (insulator)



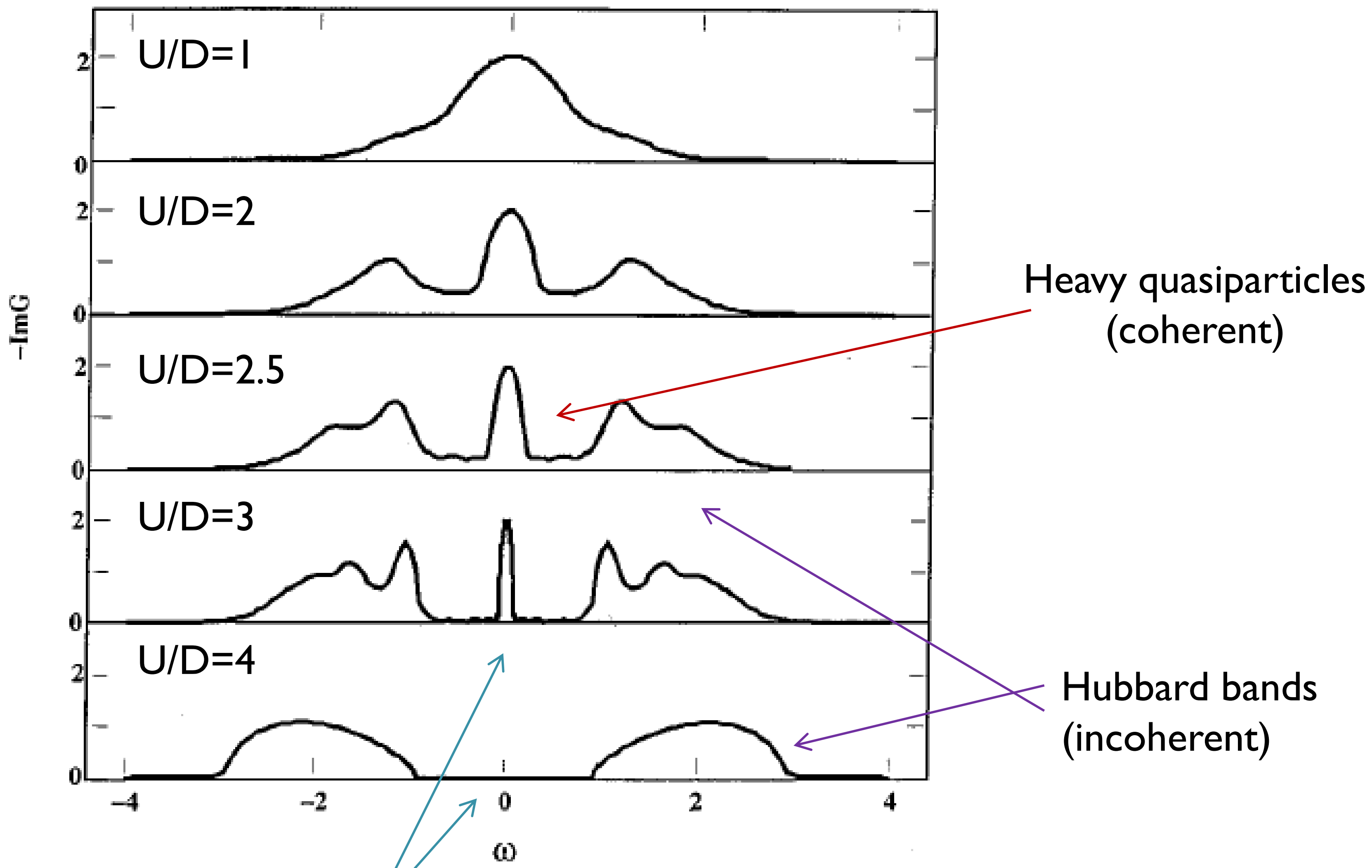
The Brinkman-Rice transition (metallic)



Heavy quasiparticle
(reduced K.E.)
Reduced quasiparticle residue

Quasiparticle disappears

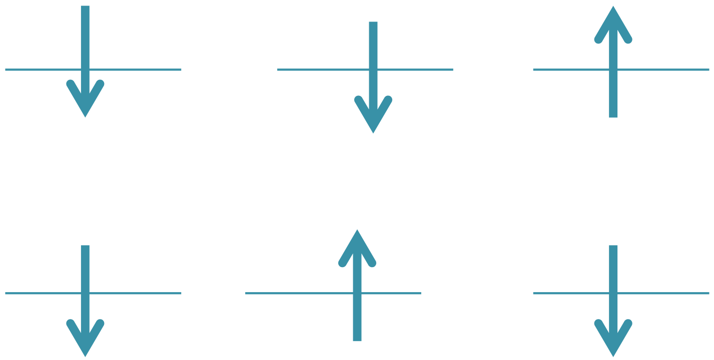
The Mott transition. DMFT picture



Quasiparticles disappear at the Mott transition

Georges et al , RMP 68, 13 (1996)

Large U limit. The Insulator. Magnetic exchange



Mott insulator:
Avoid double occupancy
(no constraint on spin ordering)

Virtual state

t^2/U

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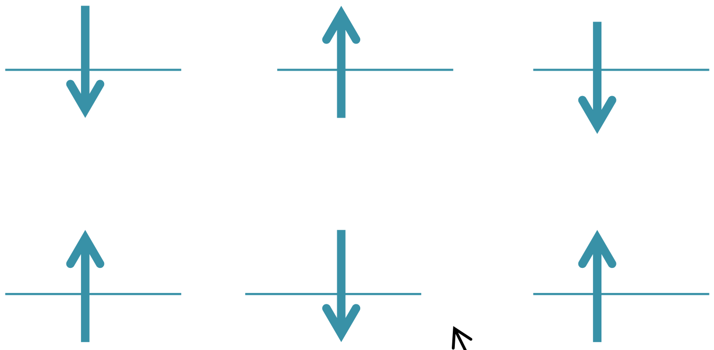
Large U limit. The Insulator. Magnetic exchange



Antiferromagnetic interactions
between the localized spins

Effective exchange interactions

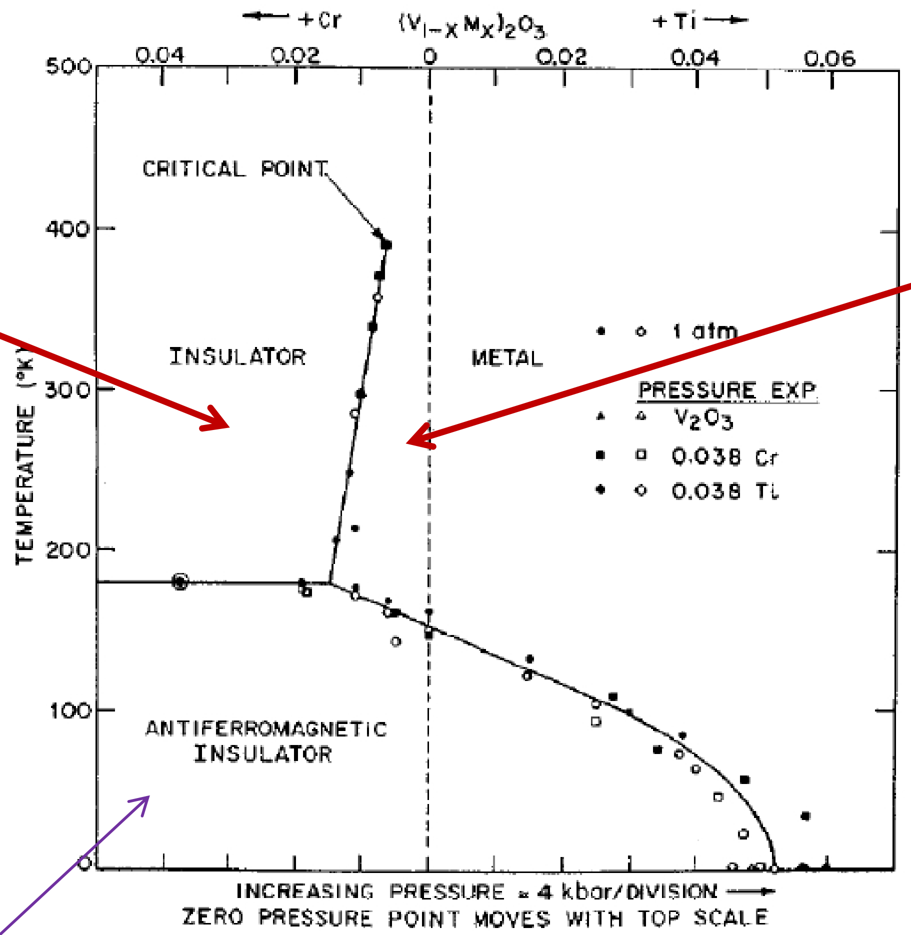
$$J \sim t^2/U$$

Antiferromagnetic ordering can reduce the energy of the localized spins

The phase diagram

Paramagnetic
Mott
Insulator

Metal-Insulator
transition with
decreasing pressure



Increasing Pressure: decreasing U/W

Antiferromagnetism

McWhan et al, PRB 7, 1920 (1973)

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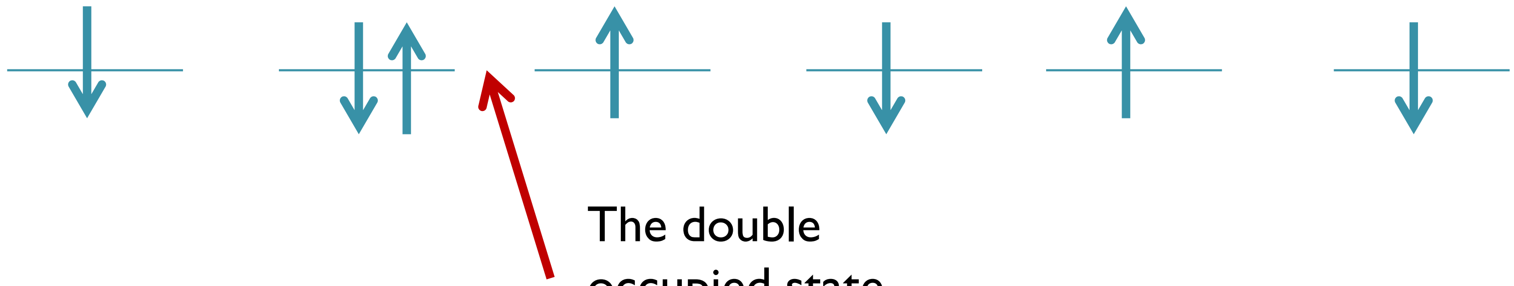
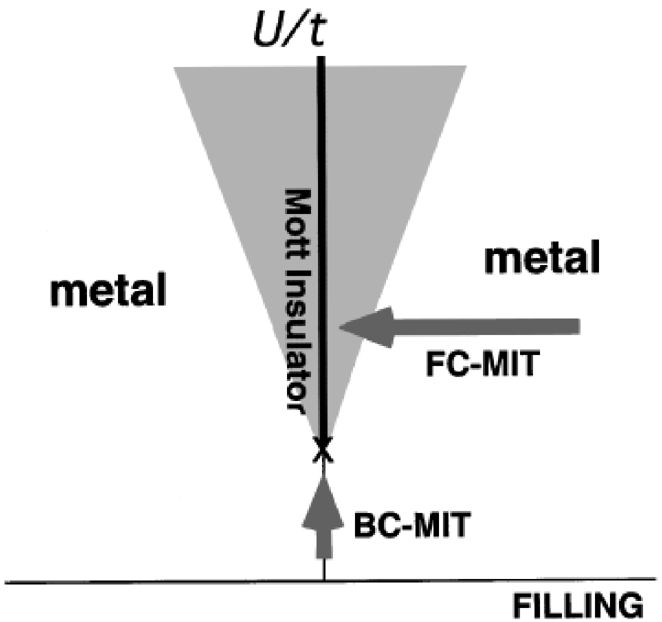
Doping a Mott insulator. Metallicity



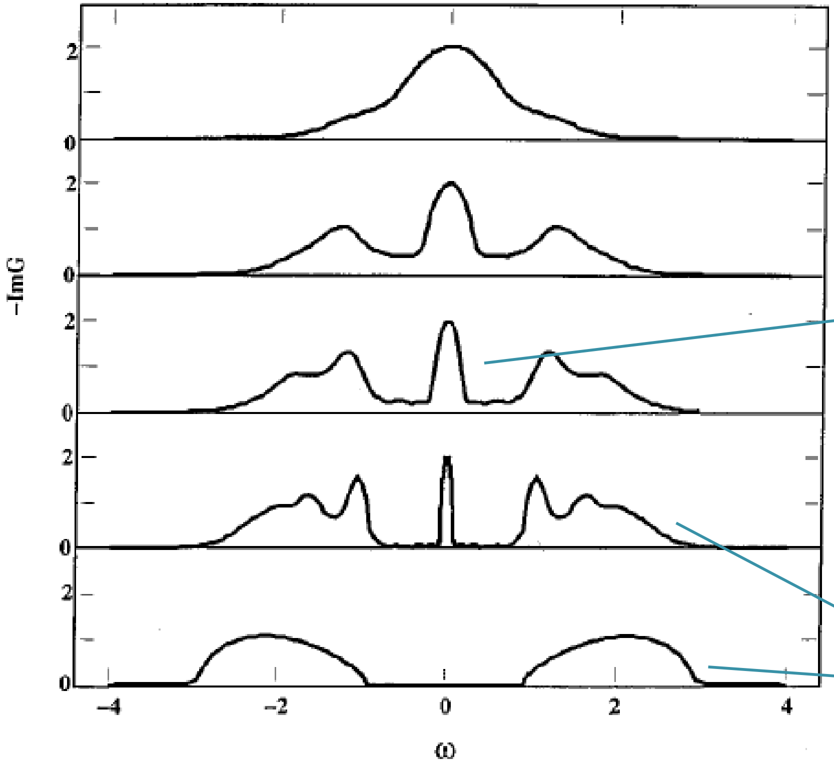
The double
occupied state
can move

A doped Mott insulator has metallic behavior



Tokura et al , RMP 70, 1039 (1998)

Summary: Mott transition in single band systems



MIT transition with increasing interactions

Renormalization of the mass
& reduced quasiparticle weight

Hubbard bands

- ❑ Antiferromagnetic correlations. Exchange $J \sim t^2/U$

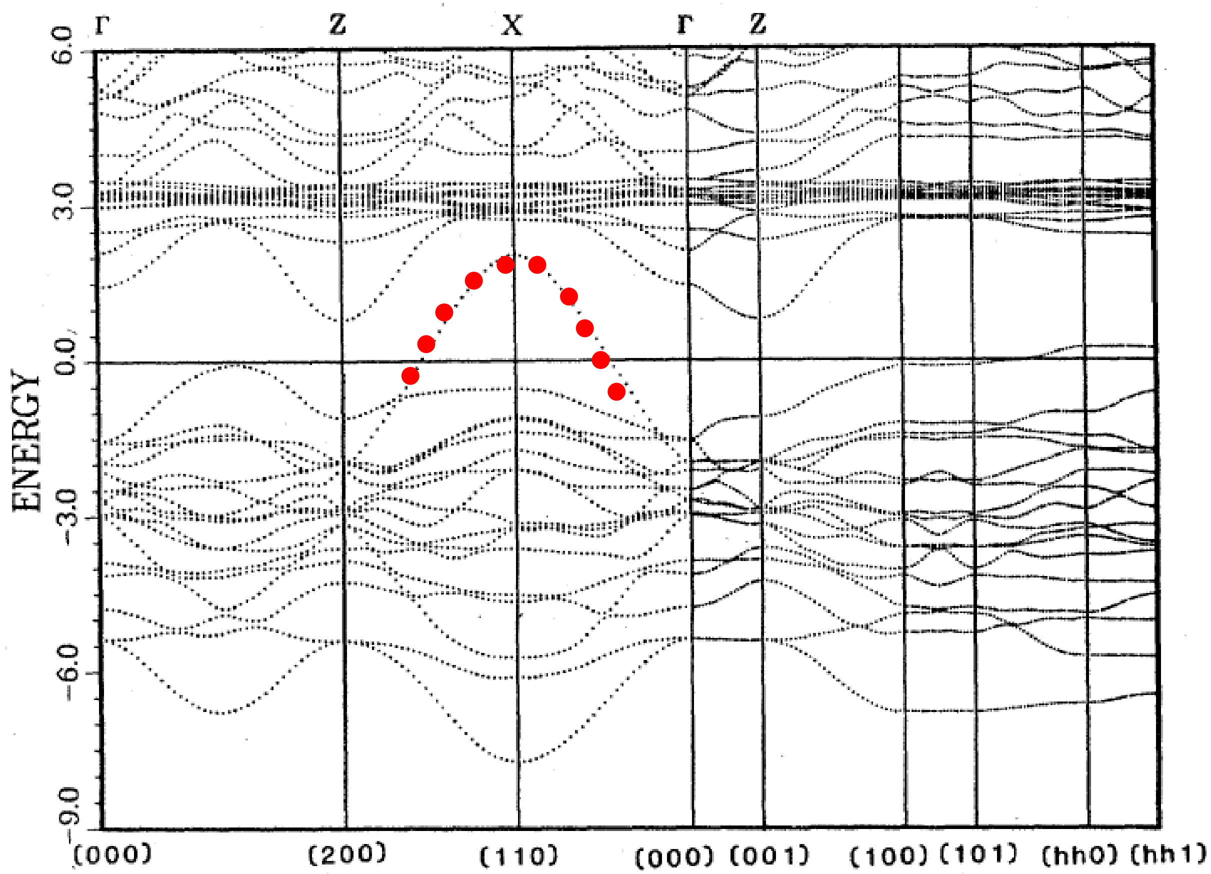
- ❑ Metallicity away from half-filling.

Interactions in one orbital systems

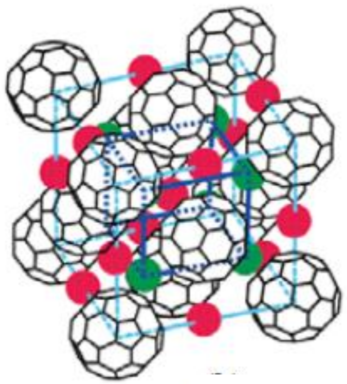
$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c. + U \sum_{j} n_{j,\uparrow} n_{j,\downarrow}$$

Kinetic energy

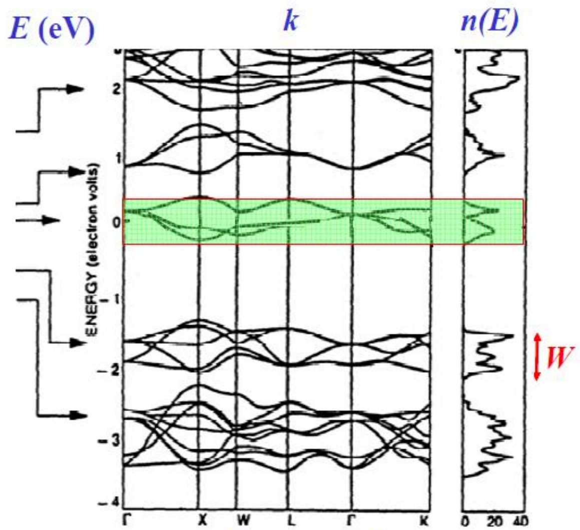
Intra-orbital repulsion

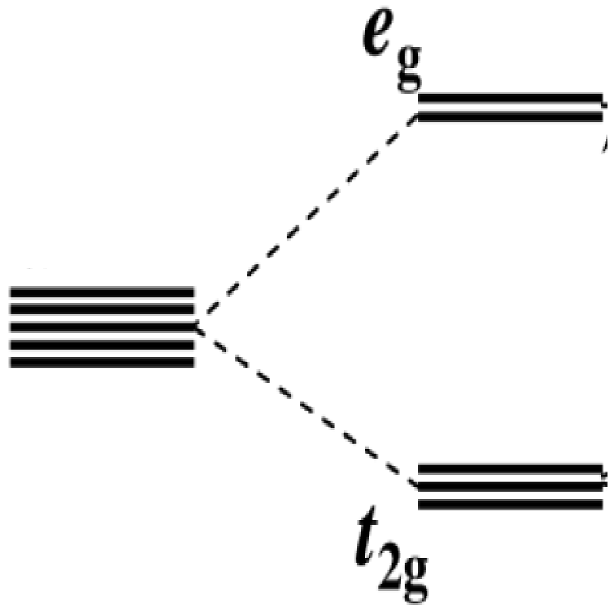


Multi-orbital systems



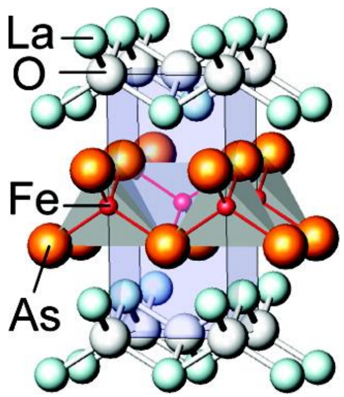
A_3C_{60}

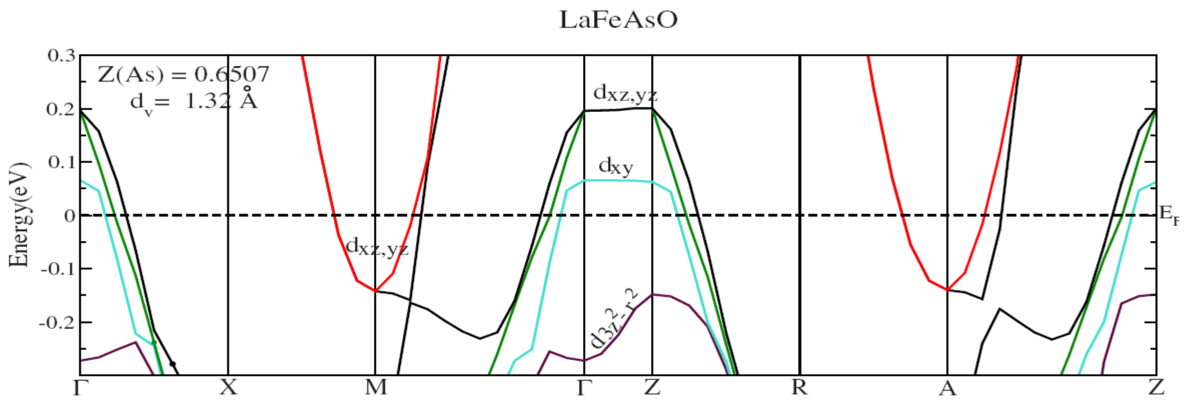




Alloul, EPJ Web of Conf. 23, 15 (2012)

Erwin & Pickett, Science 254, 842 (1991)





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

Vildosola et al, PRB 78, 064518 (2008)

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Interactions in one orbital systems

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

Kinetic energy

Intra-orbital repulsion

Electrons in the same orbital with different spin

Extrapolating to multi-orbital systems:

A Mott transition is expected at half filling (N electrons in N orbitals)

Is there something else?

Outline

- ❑ Multi-orbital systems: interacting Hamiltonian

- ❑ Degenerate multi-orbital systems

  - Mott transition at zero Hund's coupling

  - The effect of Hund's coupling on the Mott transition. Hund metals

- ❑ Non-degenerate multi-orbital systems. Orbital selective Mott transition

- ❑ Is there Mott physics in iron pnictides?

- ❑ Summary

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Interactions in multi-orbital systems

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

Tight-binding (hopping)

Intra-orbital repulsion

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

Inter-orbital repulsion

Hund's coupling

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

Pair hopping

Crystal-field

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

Two parameters: U, J

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Non hybridized & equivalent multi-orbital systems

$$\sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_{i,\gamma,\sigma}^{\dagger} c_{j,\beta,\sigma} + h.c.$$

Assume $t^{\gamma\beta}_{ij} = t\delta^{\gamma\beta}_{ij}$

All bands are equivalent

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Interactions in multi-orbital systems

Intra-orbital repulsion

Inter-orbital Repulsion (different spin)

Inter-orbital Repulsion (same spin)

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

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

Spin flip

Pair hopping

Interactions in multi-orbital systems

Intra-orbital repulsion

Inter-orbital Repulsion (different spin)

Inter-orbital Repulsion (same spin)

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

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

Spin flip

Pair hopping

Density-density interactions in multi-orbital systems

Intra-orbital repulsion

Inter-orbital Repulsion (different spin)

Inter-orbital Repulsion (same spin)

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

Zero Hund's coupling

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

U' =U – 2J= U

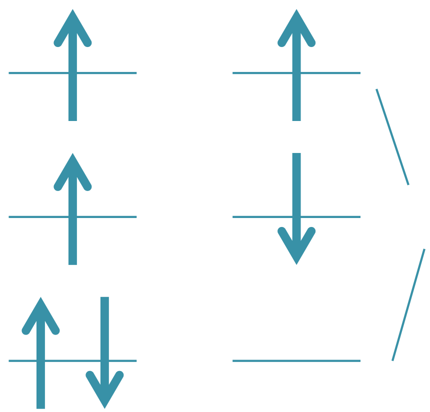
Equal intra- and inter-orbital interactions

Equivalent bands. Zero Hund. Half filling

$$U' = U - 2J = U$$

Equal intra- and inter-orbital interactions

2 orbitals, 2 electrons



Same energy

N orbitals, half filling

Atomic gap:

$$E(N+1)+E(N-1)-2\,E(N) = U$$

In absence of orbital hybridization the non-interacting bandwidth W does not depend on the number of orbitals

$$t^{\gamma\beta}_{ij} = t\,\delta^{\gamma\beta}_{ij}$$

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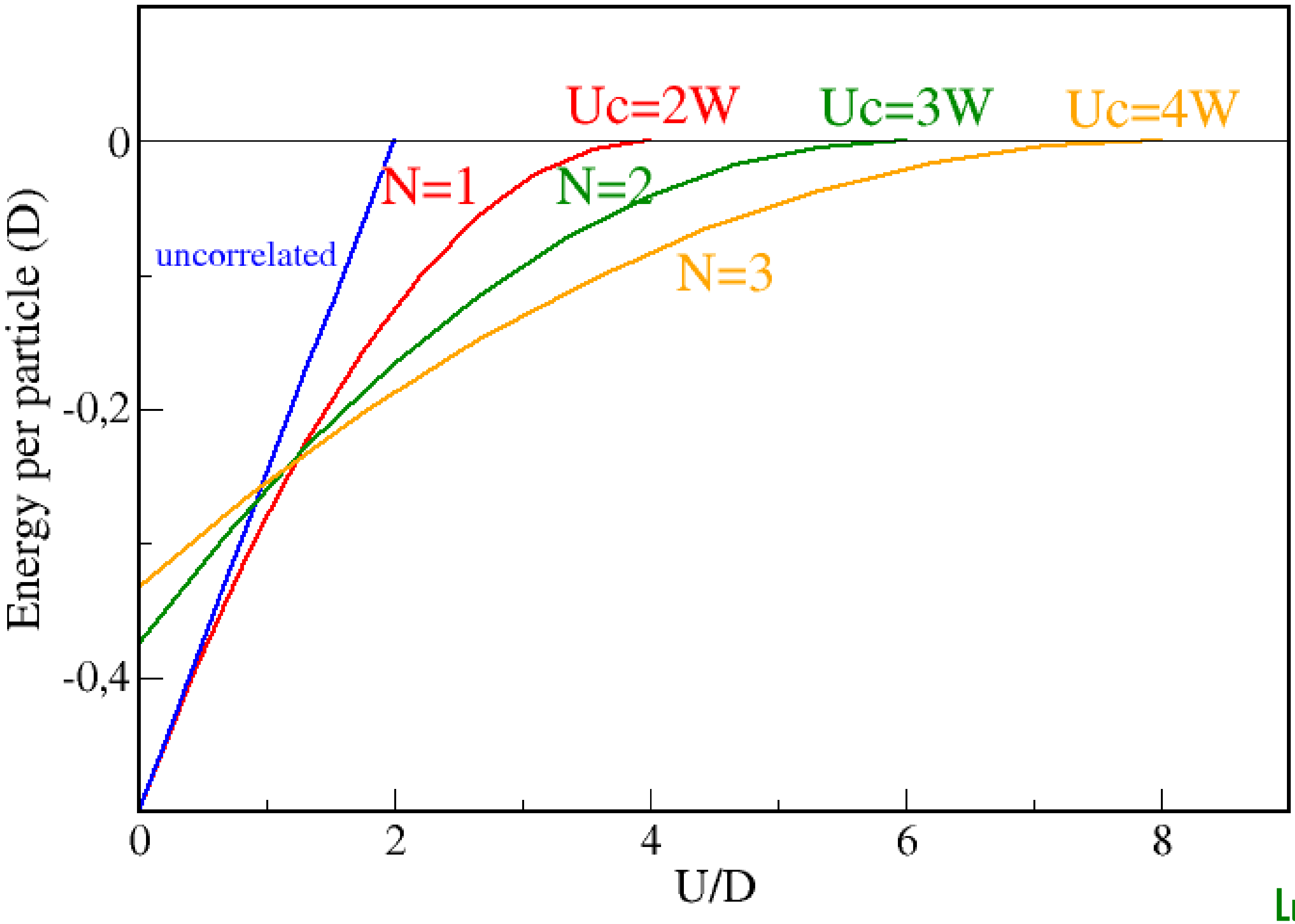
Zero Hund. Half filling

Uc depends on the number of orbitals

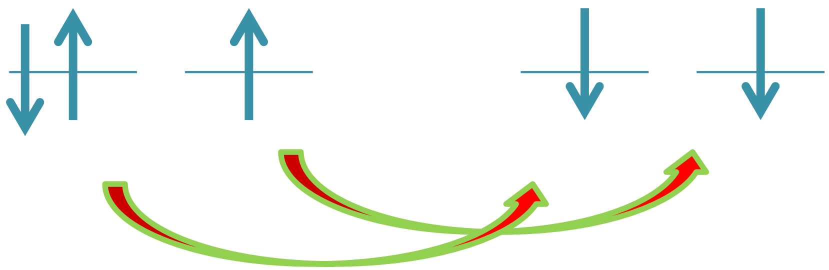


Lu PRB 49, 5687 (1994)

Gutzwiller like wave function. N, N+1,N-1 occupancy allowed

Zero Hund. Half filling

The number of channels for hopping increases with orbital degeneracy



Enhanced Kinetic Energy due to ground state degeneracy increases Uc

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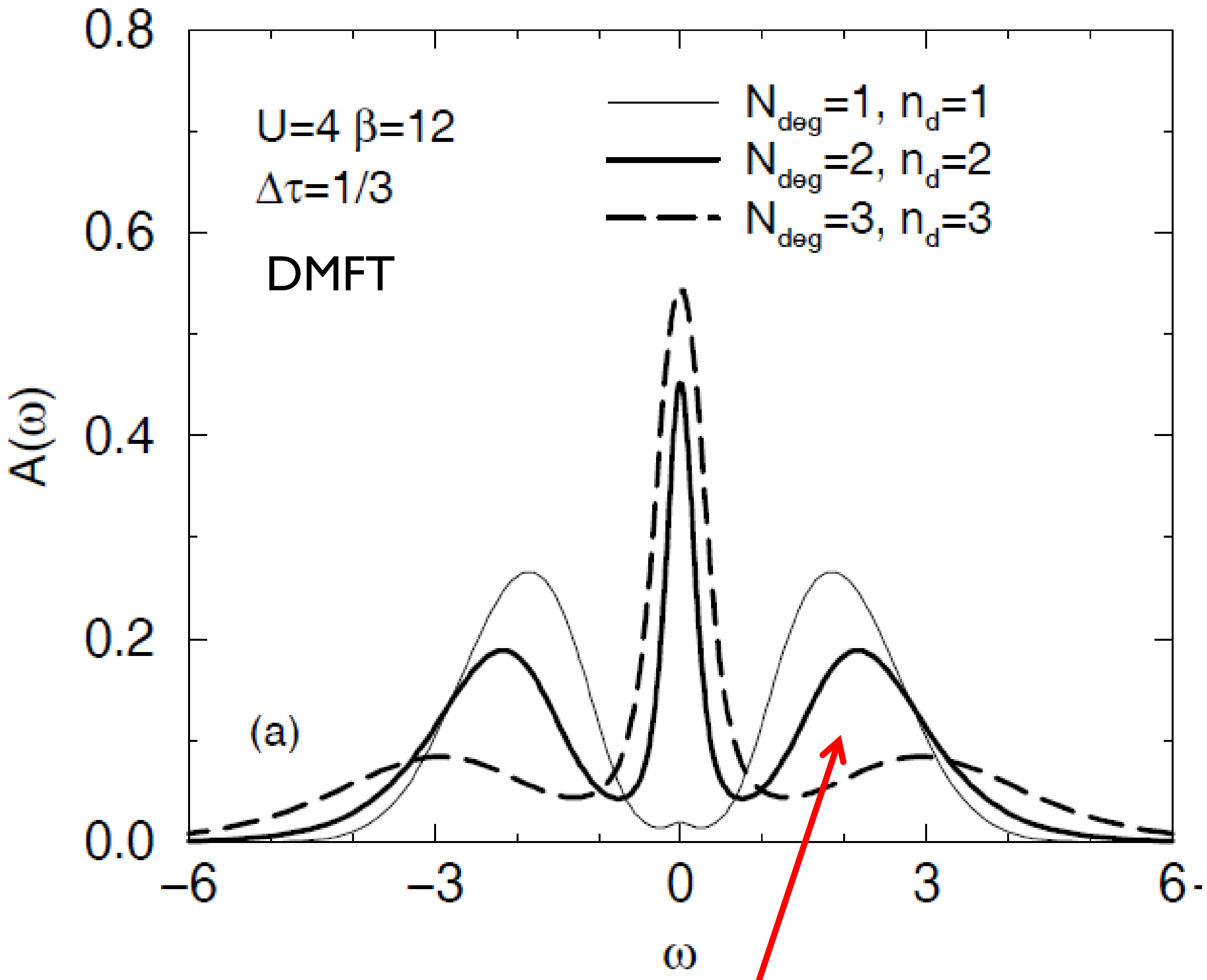
Zero Hund. Mott transition at half filling



Han et al PRB 58, R4199 (1998)

Wider Hubbard bands with increasing degeneracy

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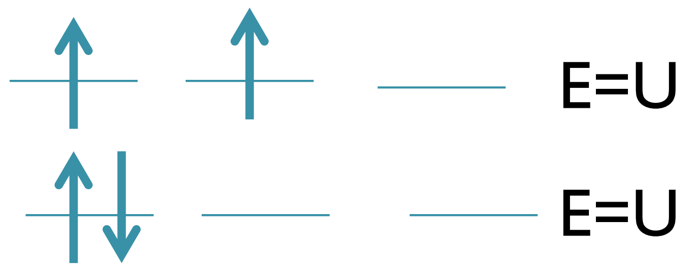
Zero Hund. Mott transition away from half filling

3 orbitals, 1 electrons

3 orbitals, 2 electrons

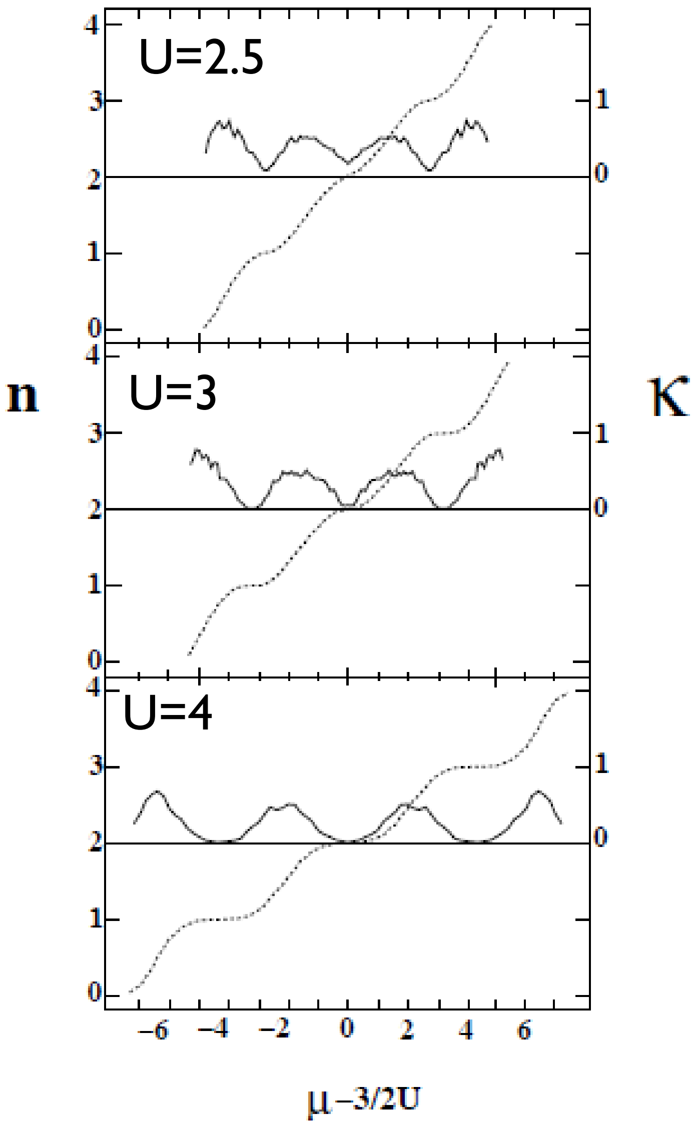


Atomic gap:

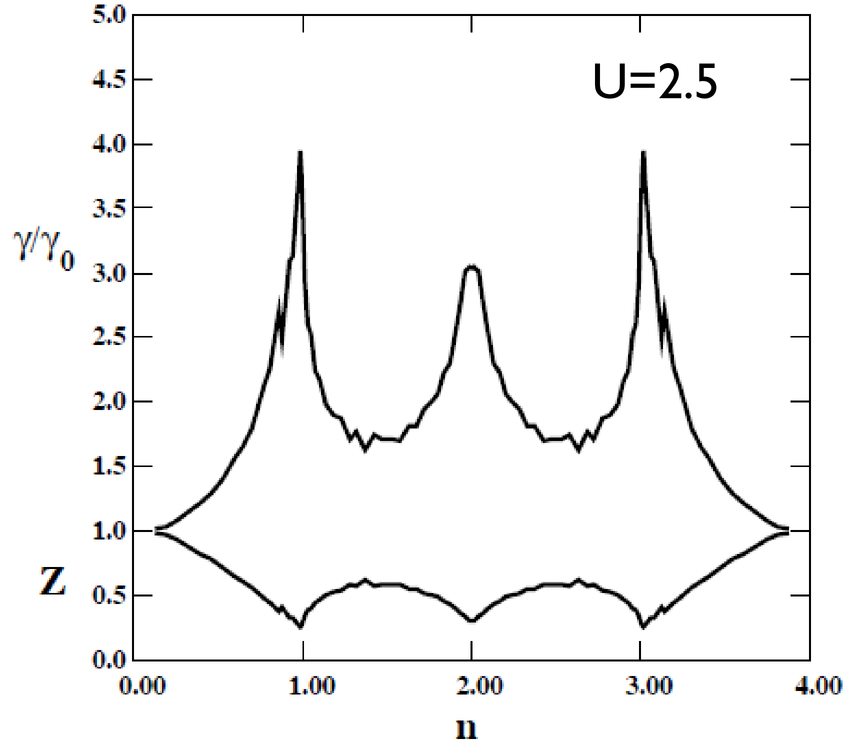
E(N+1)+E(N-1)-2 E(N)= U

A Mott transition is expected at integer atomic occupation away from half filling

Zero Hund. Mott transition away from half filling

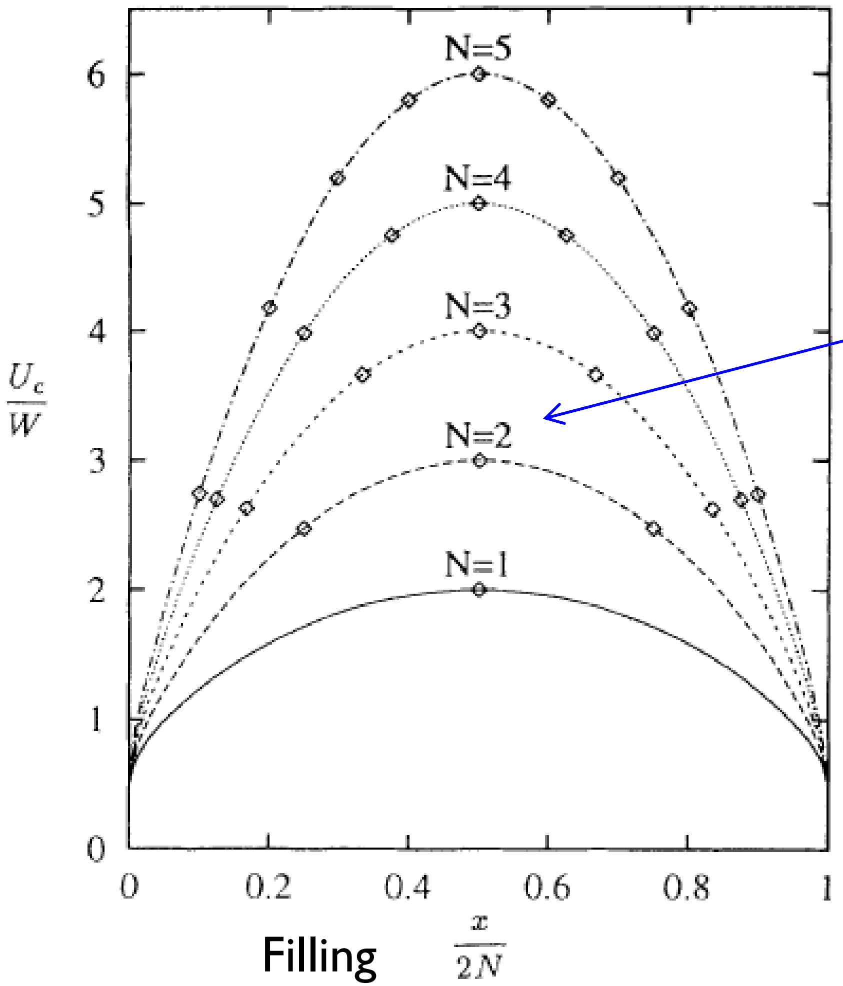


2 band degenerate Hubbard Model. DMFT



Rozenberg, PRB 55, R4855 (1997)

Zero Hund. Mott transition away from half filling



Gutzwiller

N: number of degenerate bands

Uc larger at half filling

Lu PRB 49, 5687 (1994)

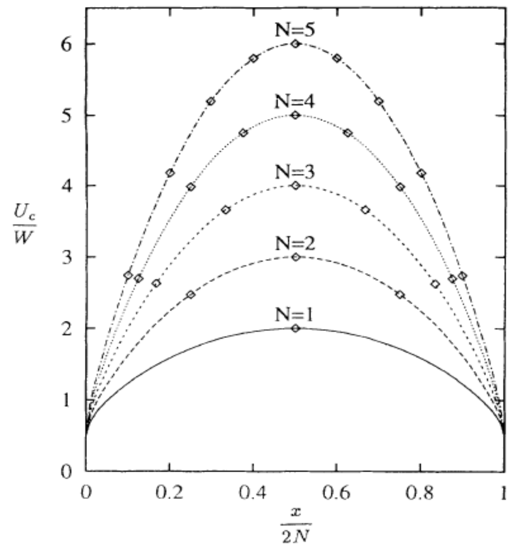
Summary: Equivalent orbitals. Zero Hund

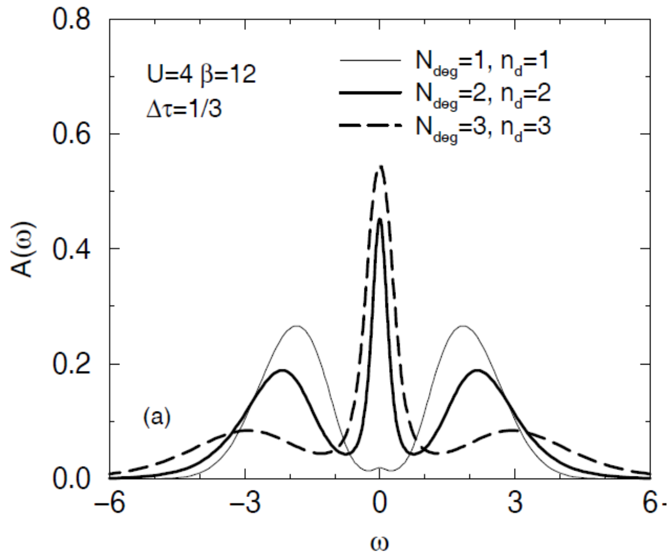
Half filling: Uc increases with degeneracy. Larger kinetic energy

Away from half filling: Mott transition at integer atomic filling.

The largest Uc is found for half filled systems

Hubbard bands become wider with degeneracy





Mott transicion at finite Hund. Degenerate orbitals

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

Intra-orbital

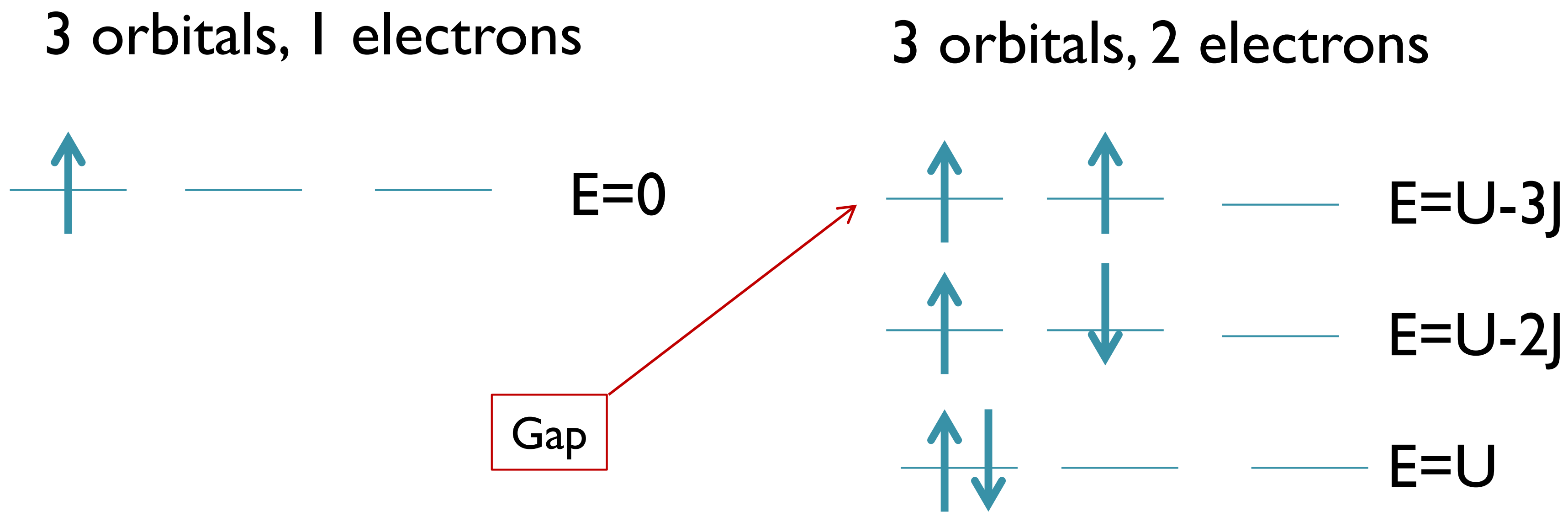
Inter-orbital (different spin)

Inter-orbital (same spin)

U’=U-2J

U-2J

U-3J



Mott transicion at finite Hund. Degenerate orbitals

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

Intra-orbital

Inter-orbital (different spin)

Inter-orbital (same spin)

U'=U-2J

U-2J

U-3J

3 orbitals, 3 electrons

3 orbitals, 4 electrons

$\Delta E = U+2J$

Gap

Mott transicion at finite Hund. Degenerate orbitals

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

Intra-orbital

Inter-orbital (different spin)

Inter-orbital (same spin)

U'=U-2J

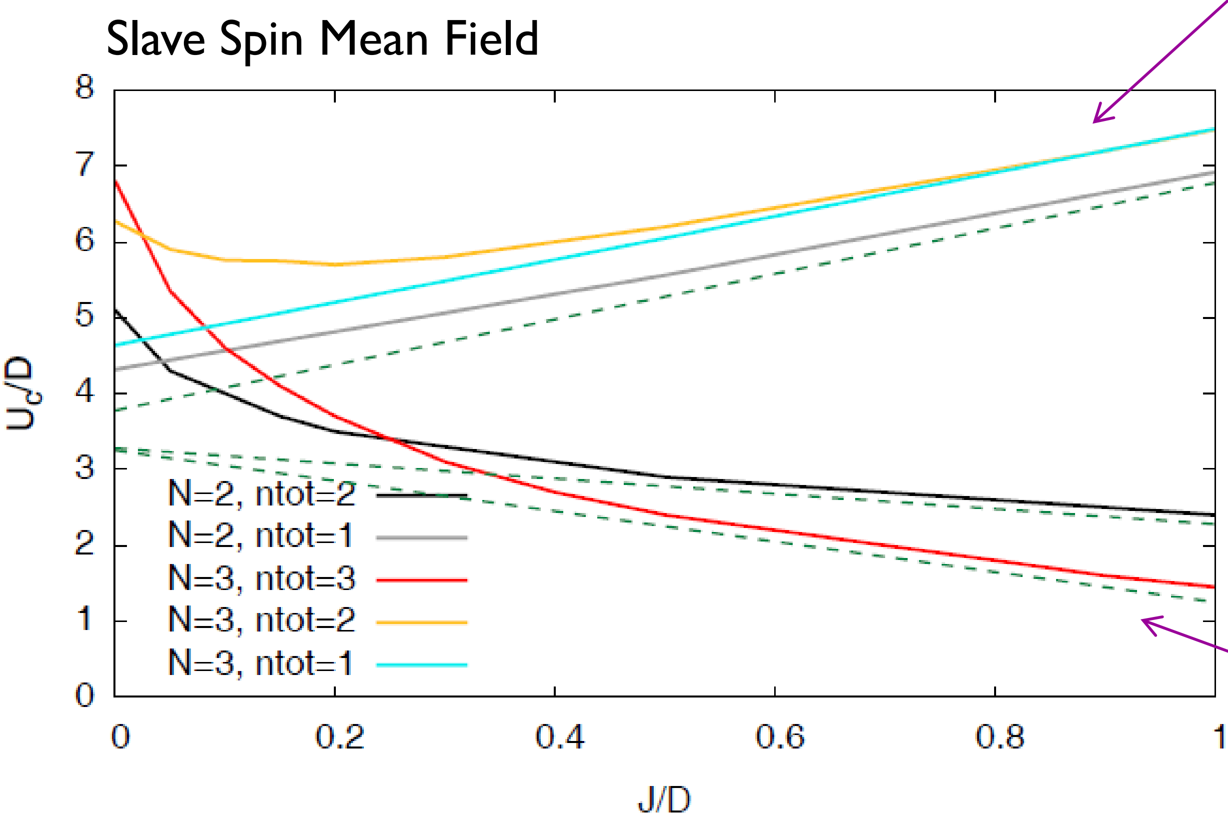
Atomic gap: E(N+1)+E(N-1)-2 E(N)

Half-filling: Gap:U+(N-1)J increases (Uc decreases)

Away from half-filling:Gap: U-3J decreases (Uc increases)

Han et al PRB 58, R4199 (1998)

Mott transicion at finite Hund



Away fom half filling:
With J the atomic gap decreases.
Uc increases

Gap:U-3J

Half filling : with J
Atomic gap increases
Uc decreases

Gap: U+(N-1)J

De'Medici PRB 83, 205112 (2011)

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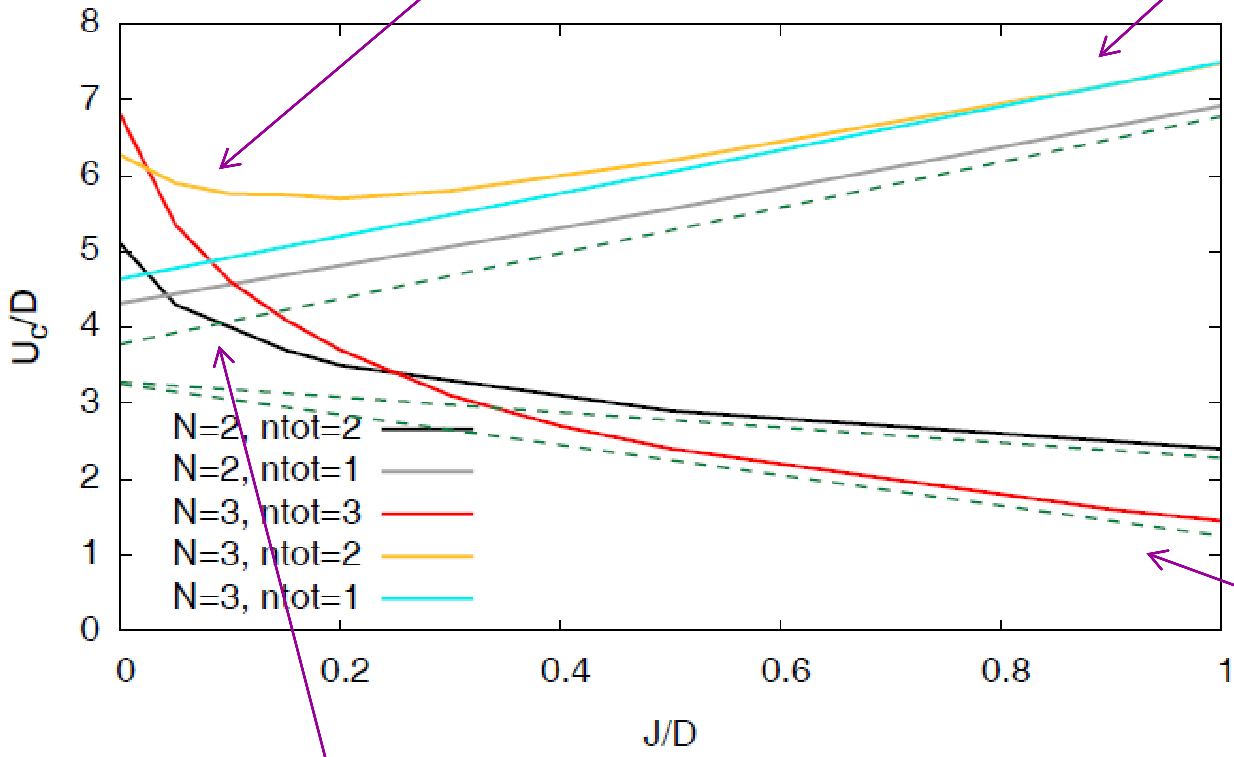
Mott transicion at finite Hund

Degeneracy
reduced by Hund's coupling

Away fom half filling:
With J the atomic
gap decreases.
Uc increases



Half filling : with J
Atomic gap increases
Uc decreases

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

De'Medici PRB 83, 205112 (2011)

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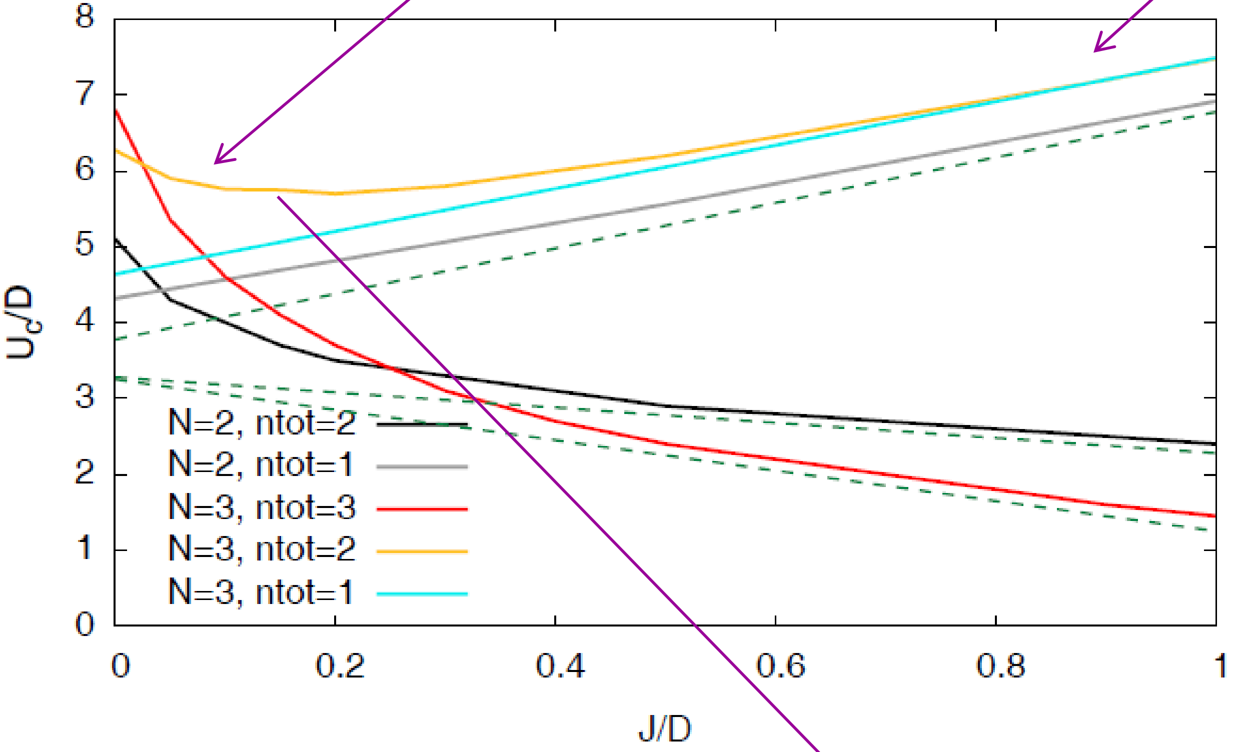
Mott transicion at finite Hund

N=3 n=2 Degeneracy
reduced by Hund's coupling

Away fom half filling:
With J the atomic
gap decreases.
Uc increases

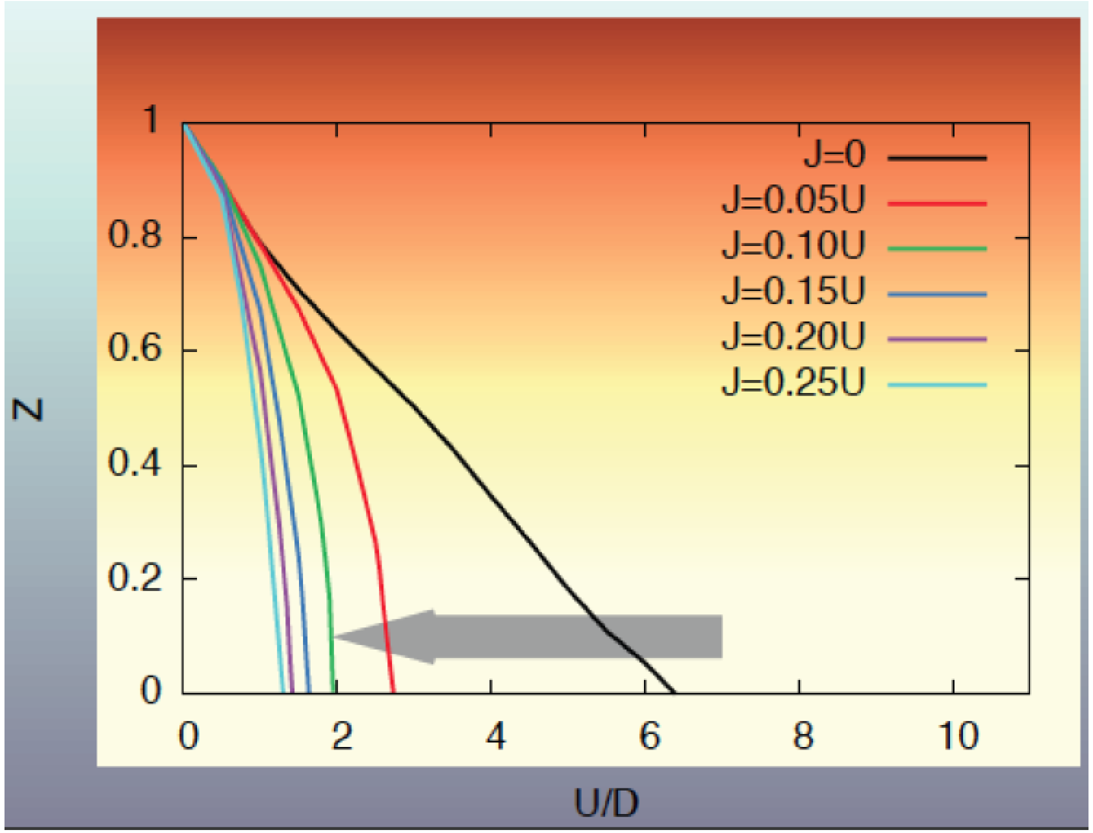


Conflicting effect of Hund's coupling

De'Medici PRB 83, 205112 (2011)

Correlated metal at finite Hund

Half filling



DMFT
N=3 n=3

Uc reduced by Hund's coupling

Gap: U+(N-1)J

Quasiparticle weight reduced by Hund's coupling (effective mass enhanced)

Half filling

J increases correlations & promotes insulating behavior

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

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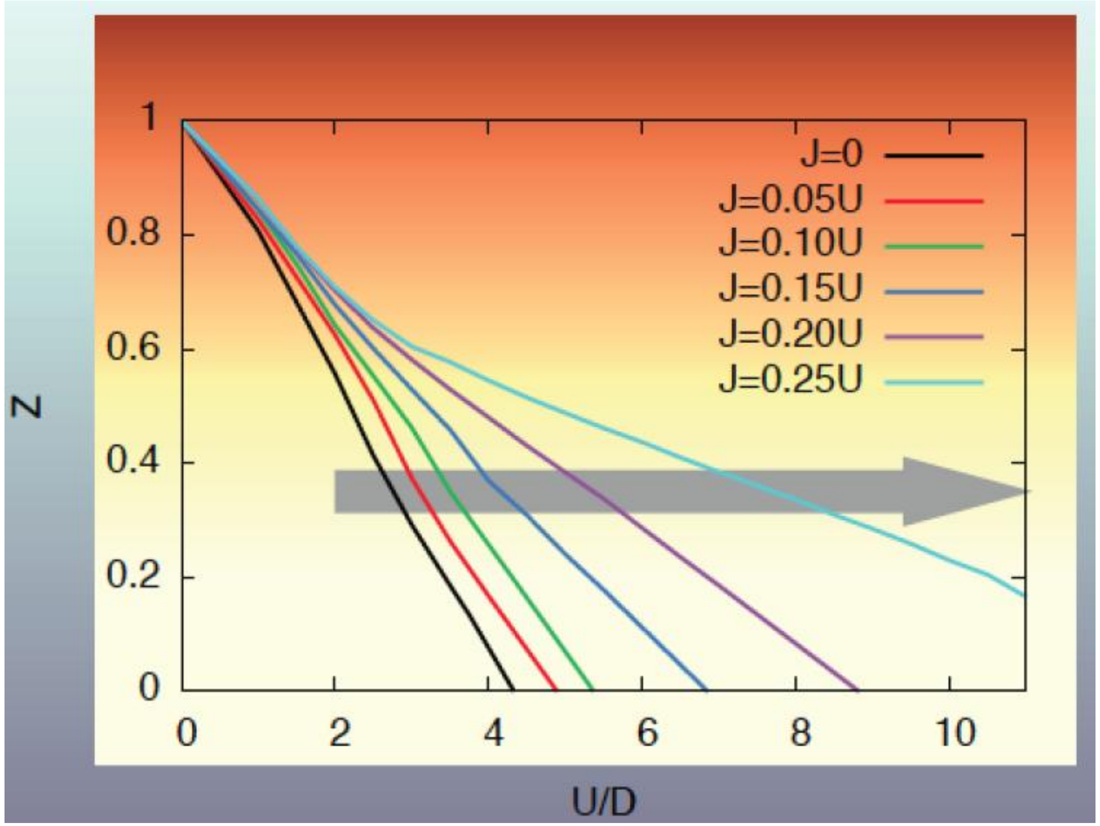
Correlated metal at finite Hund

Single electron or single hole



DMFT
N=3 n=1

Uc increased by Hund's coupling   Gap:U-3J

Quasiparticle weight increased by Hund's coupling (effective mass decreased)

Single electron or single hole

J decreases correlations & promotes metallic behavior

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

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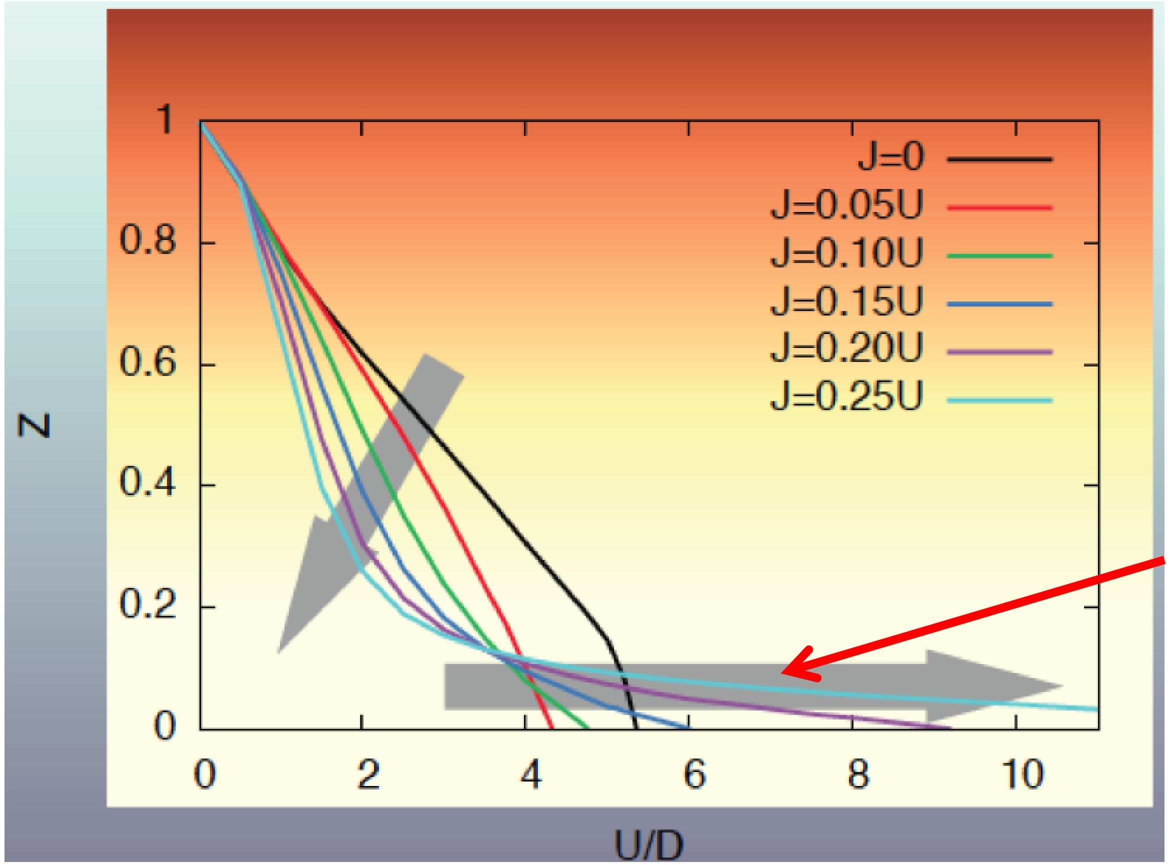
Correlated metal at finite Hund



DMFT
N=3 n=2

Hund metals:
U far from Uc &
correlations due to
Hund's coupling

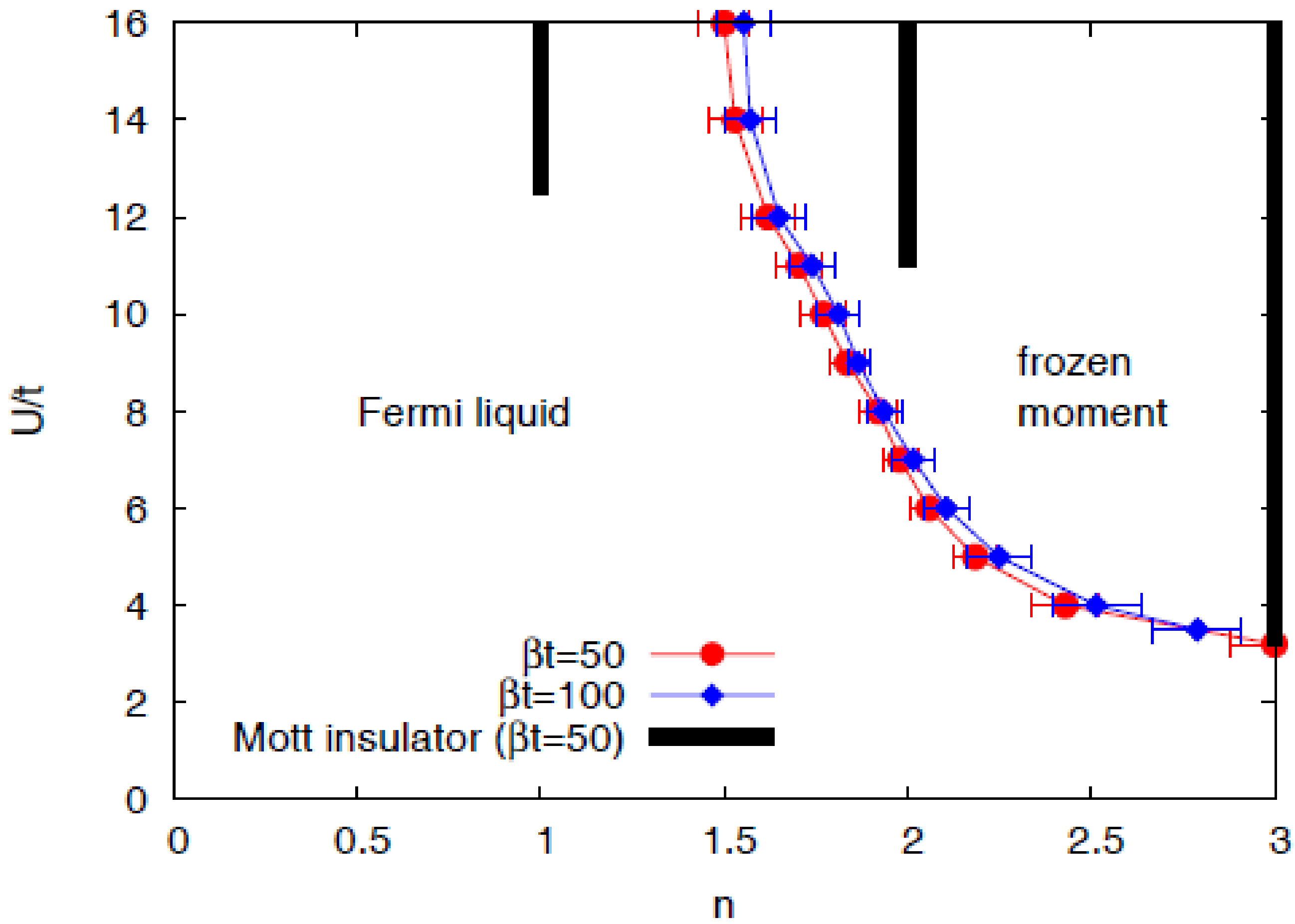
$n \neq N, 1, N\text{-}1$

J has a conflicting effect and promotes bad metallic behavior

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

ICMM CSIC

Correlated metal at finite Hund



DMFT N=3
J/U=1/6

Spin freezing due to Hund's coupling

Werner et al PRL 101, 166405 (2008)

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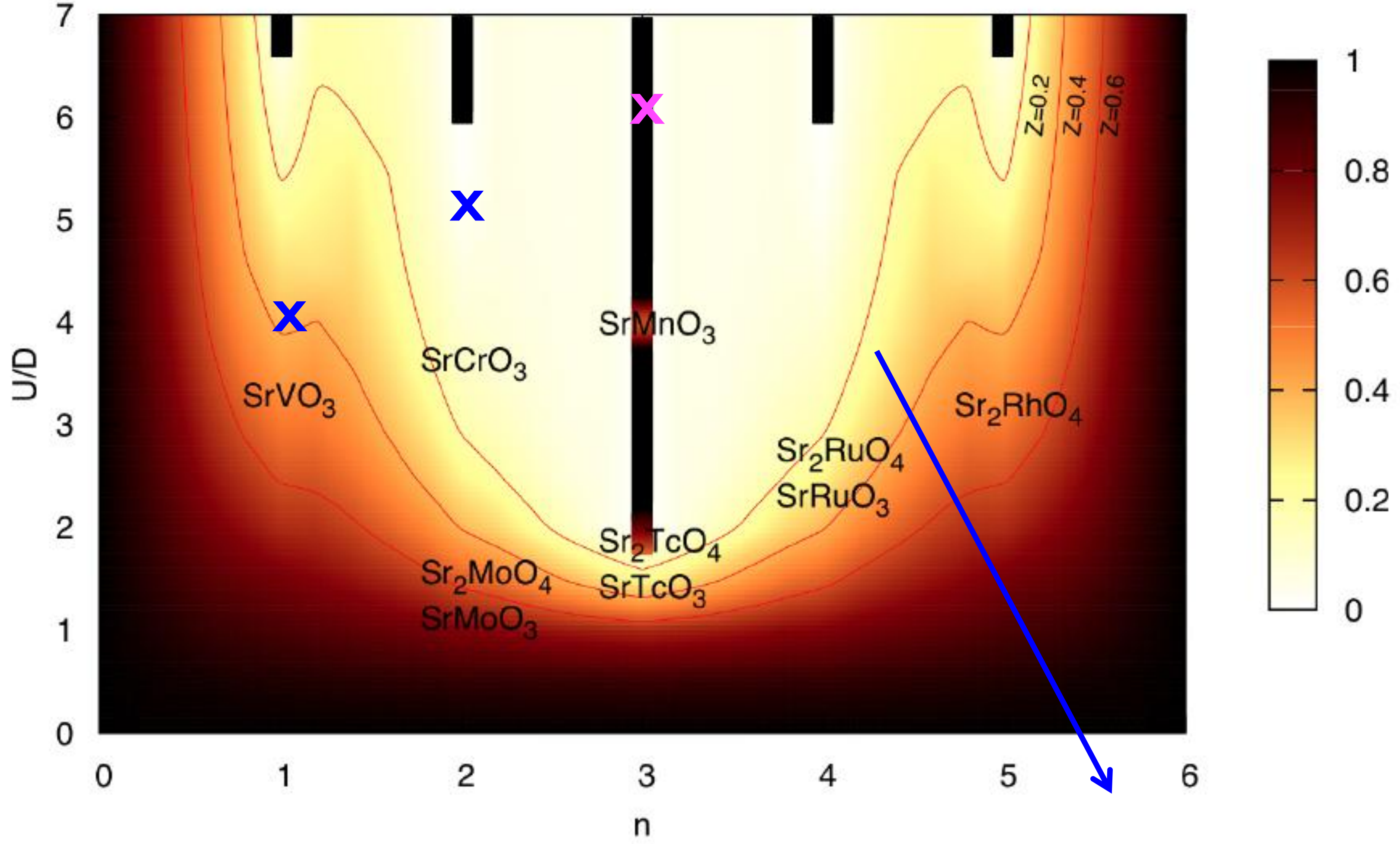
Correlated metal at finite Hund

Color scale:
Quasiparticle weight Z



DMFT N=3
J/U=0.15

Bad metal

Low coherence temperature

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

Hund metal

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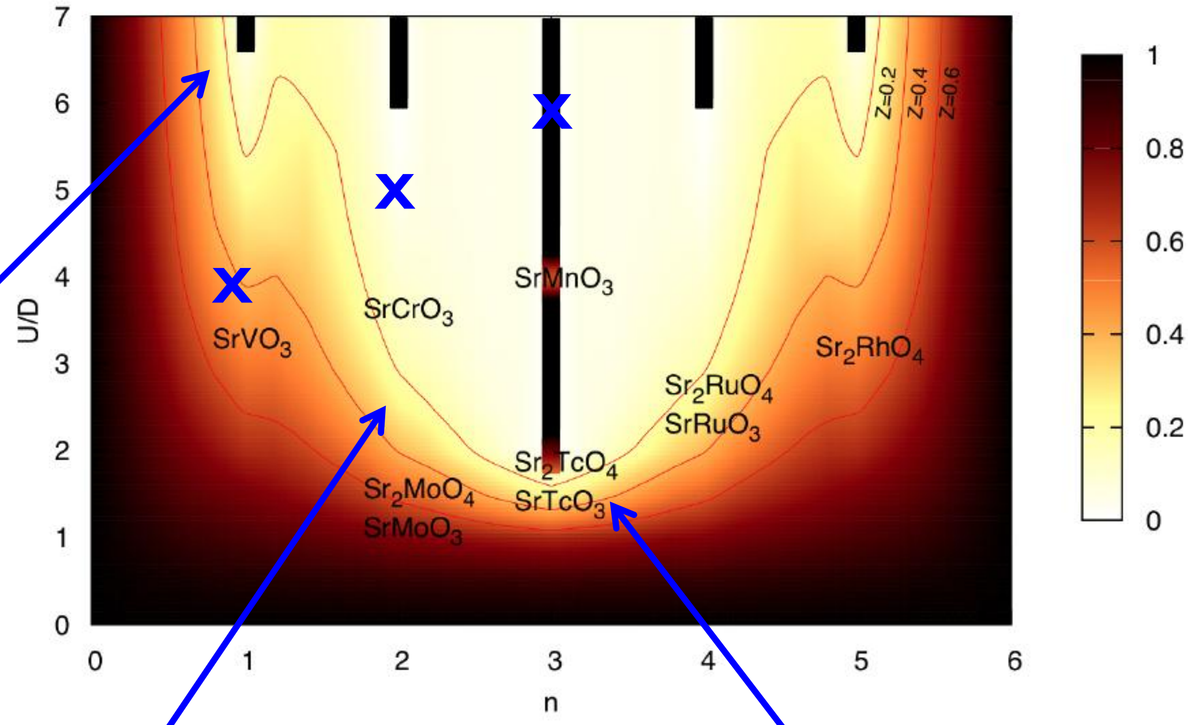
Summary: Hund in degenerate multi-orbital systems



single
electron or hole
Uc increases
J promotes
metallic behavior

other cases:
bad metallic behavior.
Hund metal &
spin freezing

Half filling :
Uc decreases
J promotes
insulating behavior

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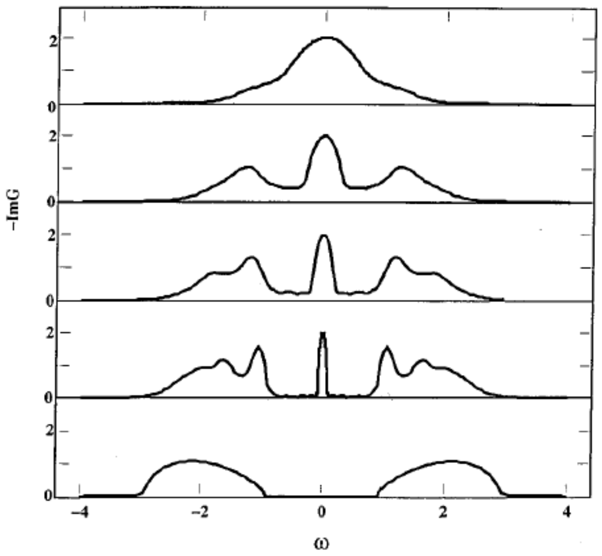
Summary



MIT as a function of interactions

Single-orbital: Mott transition at half-filling

Multi-orbital: Mott transition at commensurate filling.
Also away from half-filling.

Uc $\propto$ W.

Increases with degeneracy in multi-orbital systems

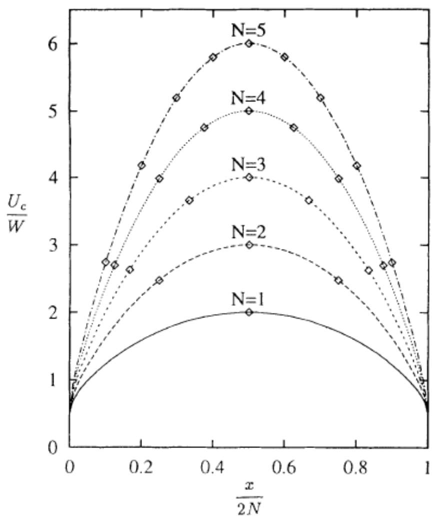
Uc larger at half-filling if Hund's coupling is zero

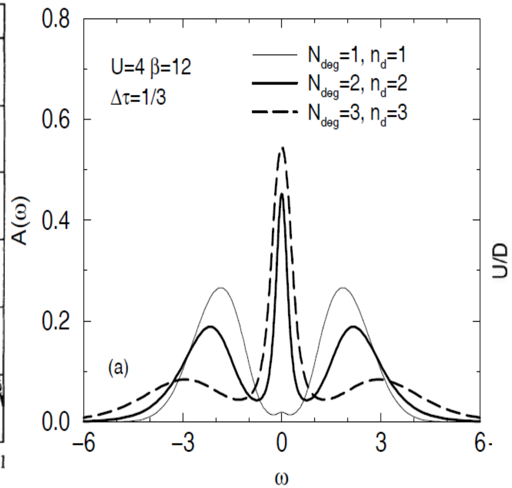
Hubbard bands & renormalized quasiparticle

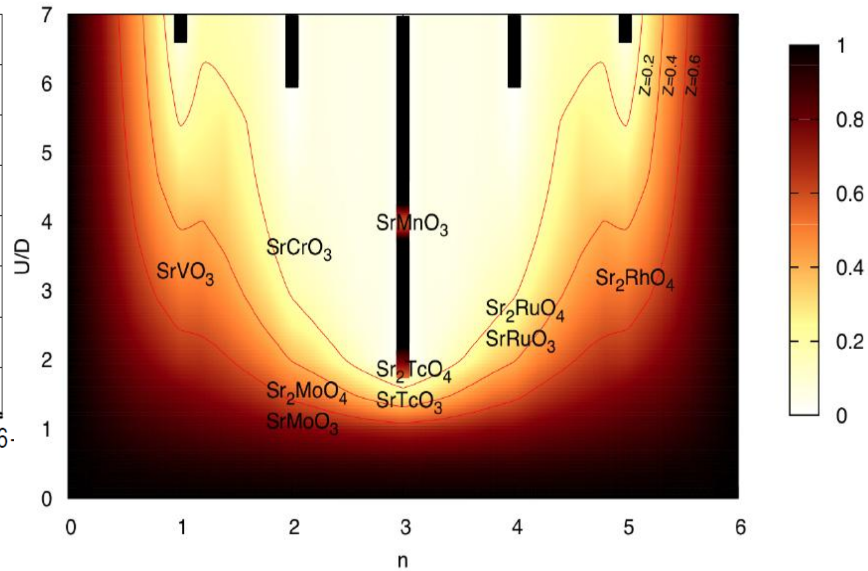
Wider Hubbard bands with increasing degeneracy

Effect of Hund's coupling on Mott physics

depends on filling. Hund metals







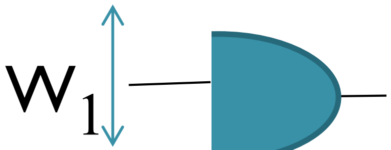
Non-equivalent bands

$$\sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_{i,\gamma,\sigma}^{\dagger} c_{j,\beta,\sigma} + h.c. \ +$$

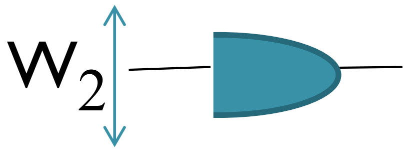
Assume

$t^{\gamma\beta}_{ij} = \delta^{\gamma\beta}_{ij}$

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



When isolated Mott transition at $U=Uc_1$

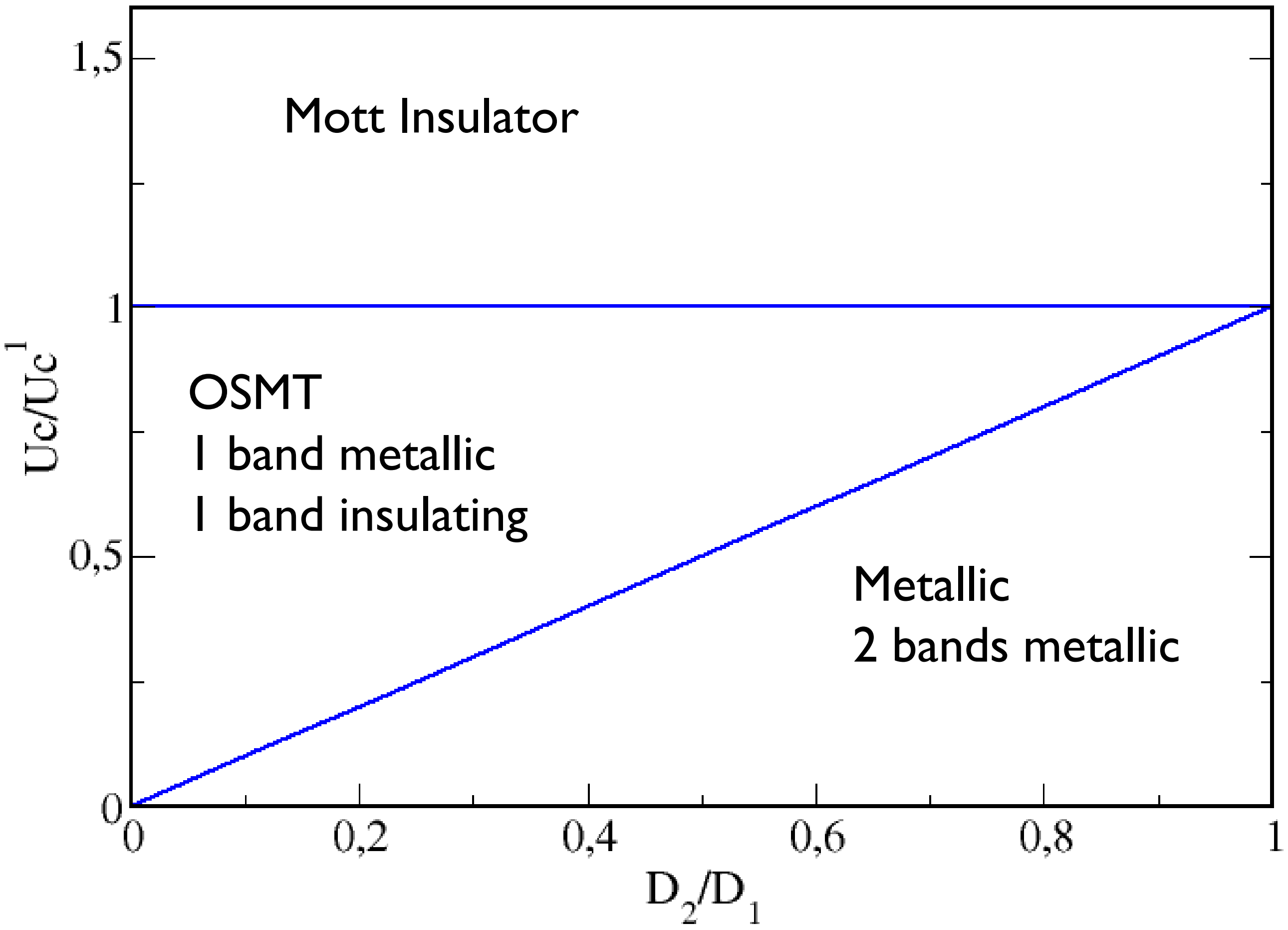


When isolated Mott transition at $U=Uc_2$

Orbital selective Mott transition. Zero Hund

J=0

2 degenerate orbitals.
Unequal bandwidths
N=2 Half-filling

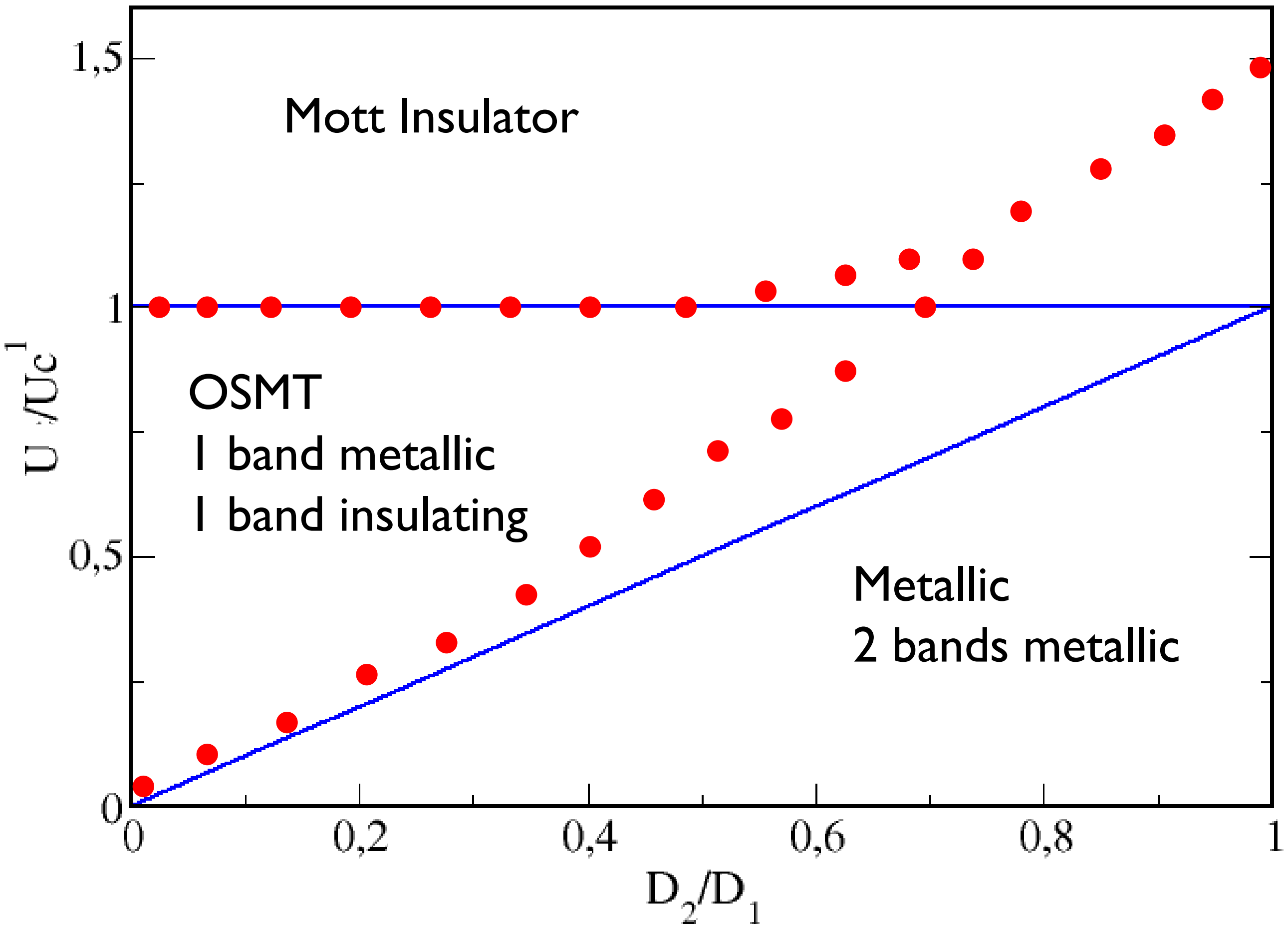


Phase diagram assuming uncorrelated metallic state

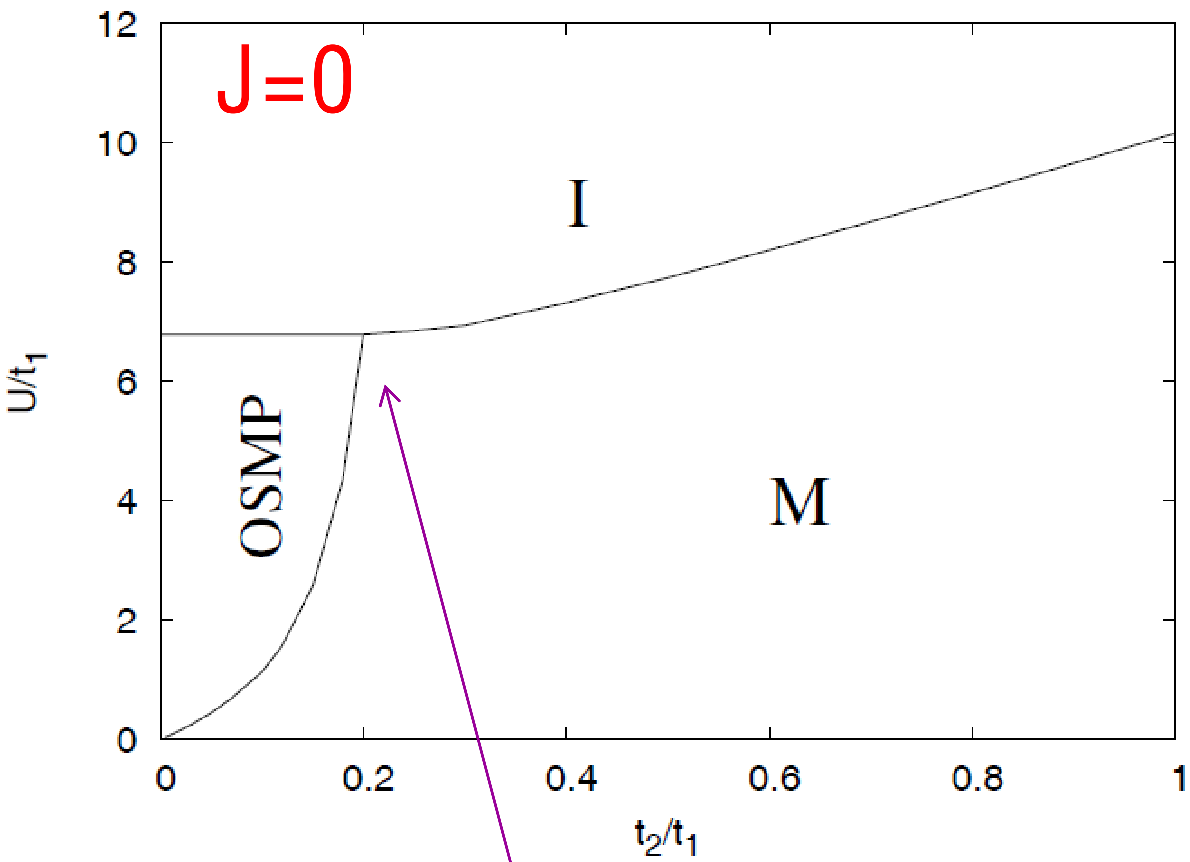
Orbital selective Mott transition. Zero Hund

J=0

2 degenerate orbitals.
Unequal bandwidths
N=2 Half-filling



Orbital selective Mott transition. Zero Hund

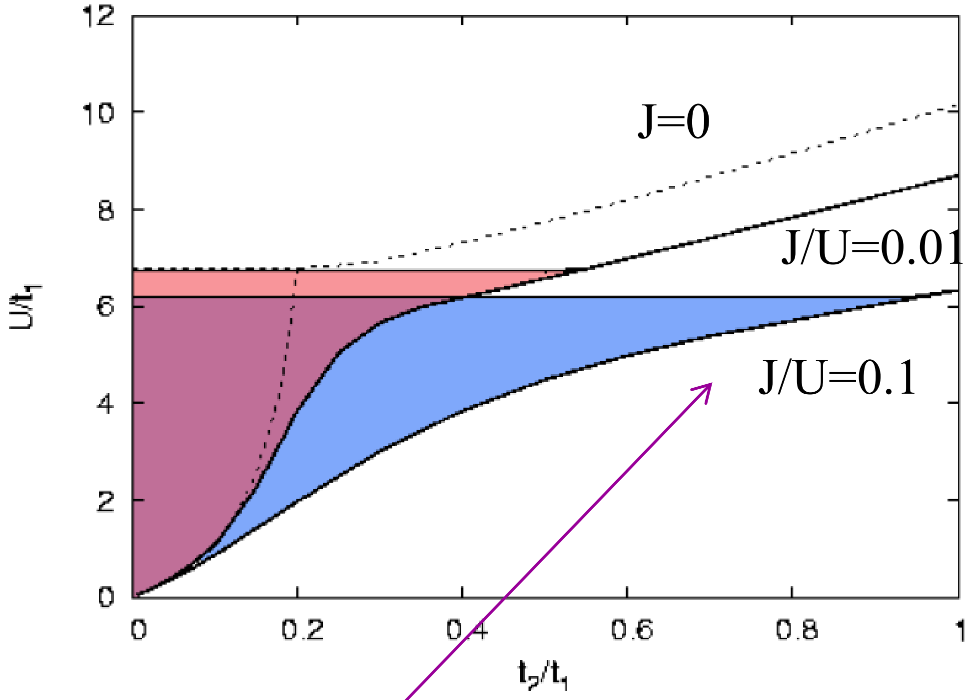


2 degenerate orbitals.
Unequal bandwidths
N=2 Half-filling

A large difference between both bands required for OSMT

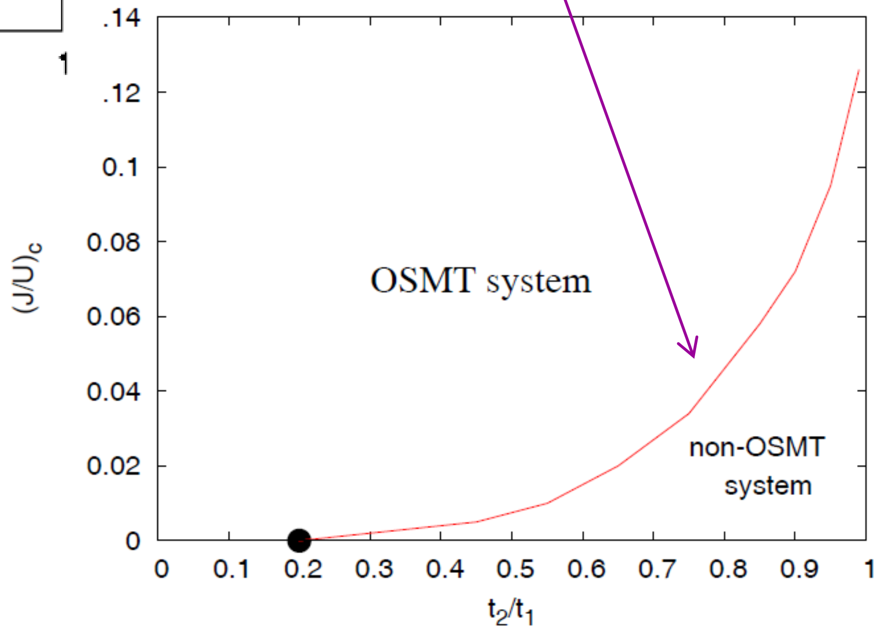
De'Medici et al PRB 72, 205124 (2005) Ferrero et al, PRB 72, 205126 (2005)

Orbital selective Mott transition. Hund's coupling



2 degenerate orbitals.
Unequal bandwidths
N=2 Half-filling

Minimum J/U required for OSMT



With finite Hund's coupling the metallic system does not benefit from degeneracy

De'Medici et al PRB 72, 205124 (2005)
Ferrero et al, PRB 72, 2051 26 (2005)

Slave Spin Mean Field
Spin flip & pair hopping included

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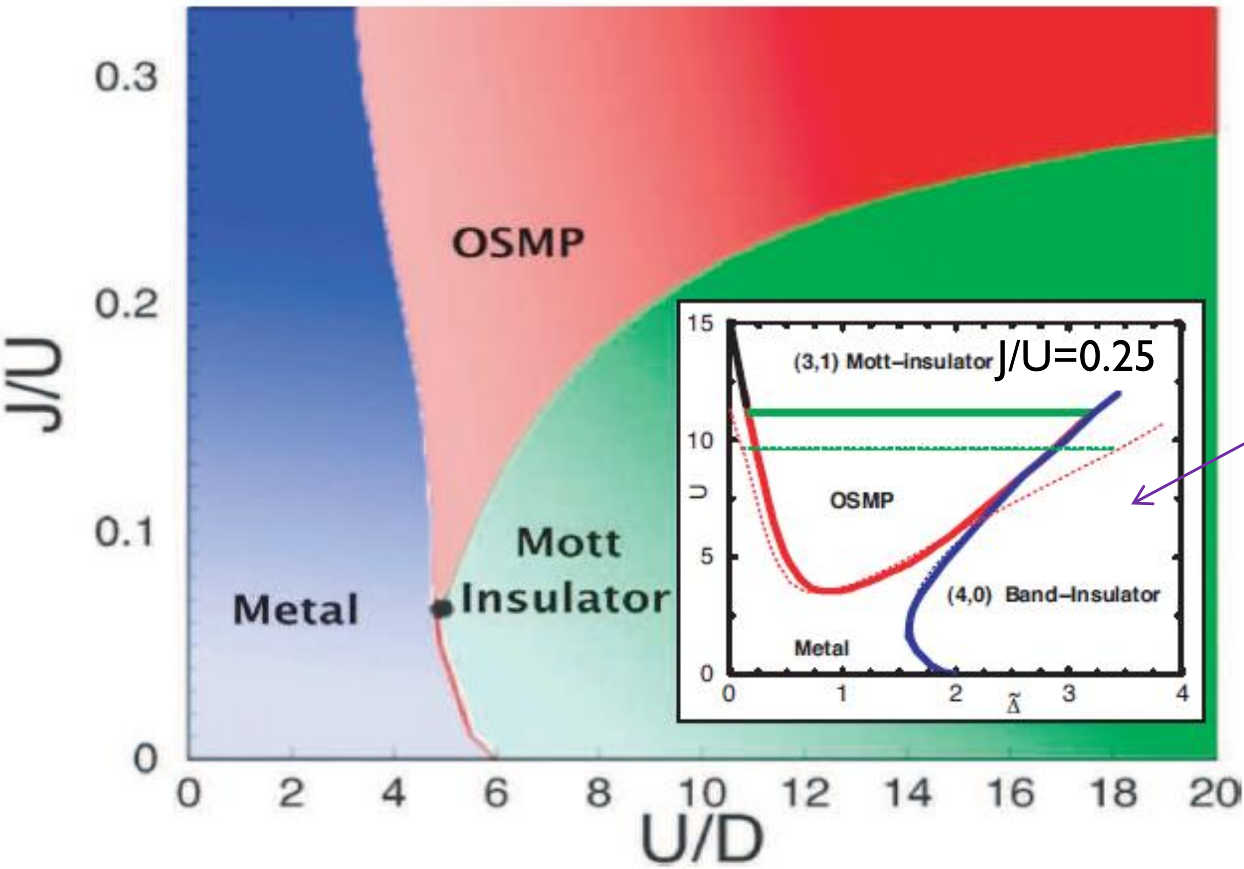
OSMT. Crystal field & Different degeneracy

Unequal orbital occupancy n=(1,1.5,1.5)

3 bands. 4 electrons



Hund's coupling decouples the orbitals

De'Medici et al PRL 102, 162401 (2009)

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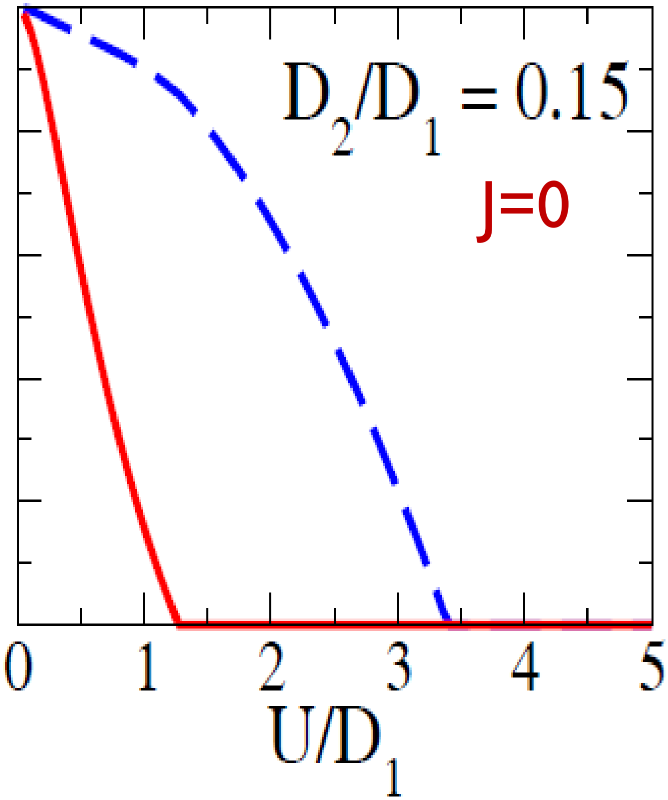
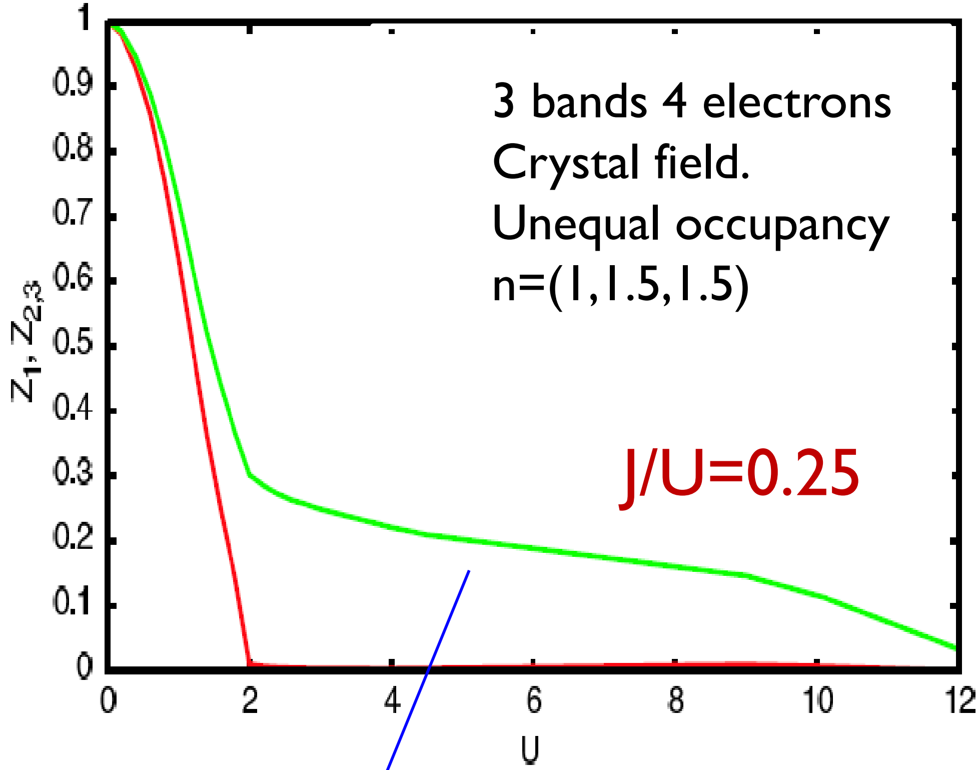
OSMT. Quasiparticle weight

Ferrero et al, PRB 72, 205126 (2005)





De'Medici et al
PRL 102, 162401 (2009)

Bad metal Low coherence temperature

Itinerant and localized electrons coupled via Hund

Biermann et al , PRL 95, 206401 (2005)

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Outline

- ❑ Mott physics: Basic concepts (single orbital & half filling)
  - Mott transition & breakdown of independent electron picture
  - Insulating state (Hubbard bands)
  - Correlated metallic state (renormalized quasiparticles)
  - Magnetic exchange & metallicity away from half-filling

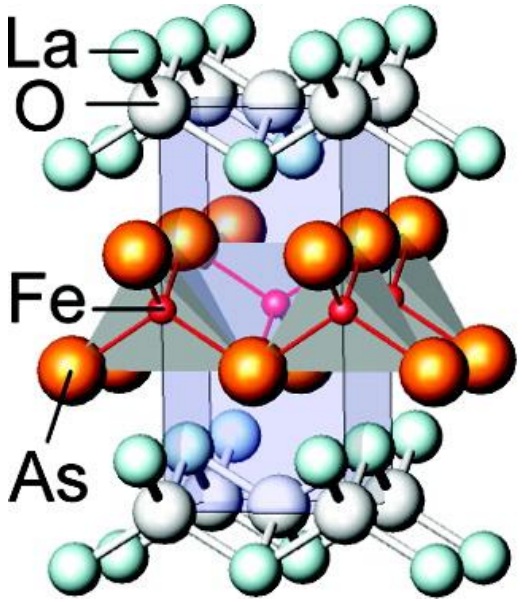
- ❑ Mott physics in Multi-orbital systems (at & away half filling)
  - Degenerate bands
  - Non degenerate bands (OSMT)

  Hund's coupling

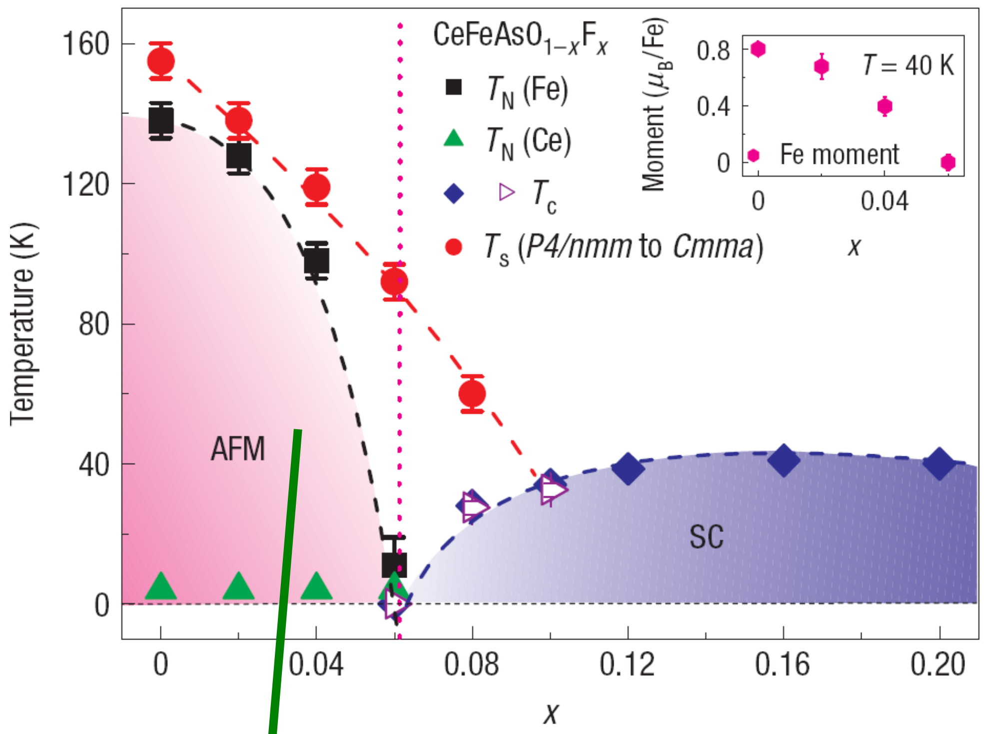
- ❑Mott physics in iron superconductors. Magnetic &non-magnetic

Iron based superconductors

Zhao et al, Nat. Mat. 7, 953 (2008),



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

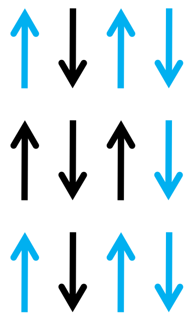


Since then many other superconductors with FeAs/FeSe layers have been discovered

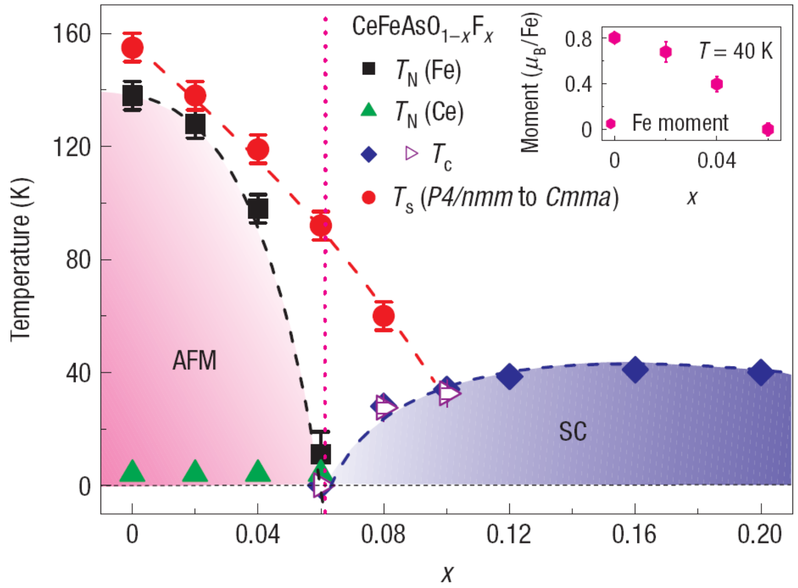
Metallic

Antiferromagnetism

(π,0) stripe order



Correlations in iron based superconductors



Metallic Antiferromagnetism

Contrary to cuprates iron parent compounds are NOT Mott insulators

Does this mean that iron superconductors are not correlated?

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Correlations in iron based superconductors

Weak correlations

(Fermi surface instabilities, Renormalized Fermi liquid)

Raghu et al, PRB 77, 220503 (2008),
Mazin et al, PRB 78, 085104 (2008),
Chubukov et al, PRB 78, 134512 (2008),
Cvetkovic & Tesanovic,EPL85, 37002 (2008)

Localized electrons

(J_1-J_2 model, spins interact to first & second nearest neighbors)

Yildirim, PRL 101, 057010 (2008),
Si and Abrahams, PRL 101, 057010 (2008)

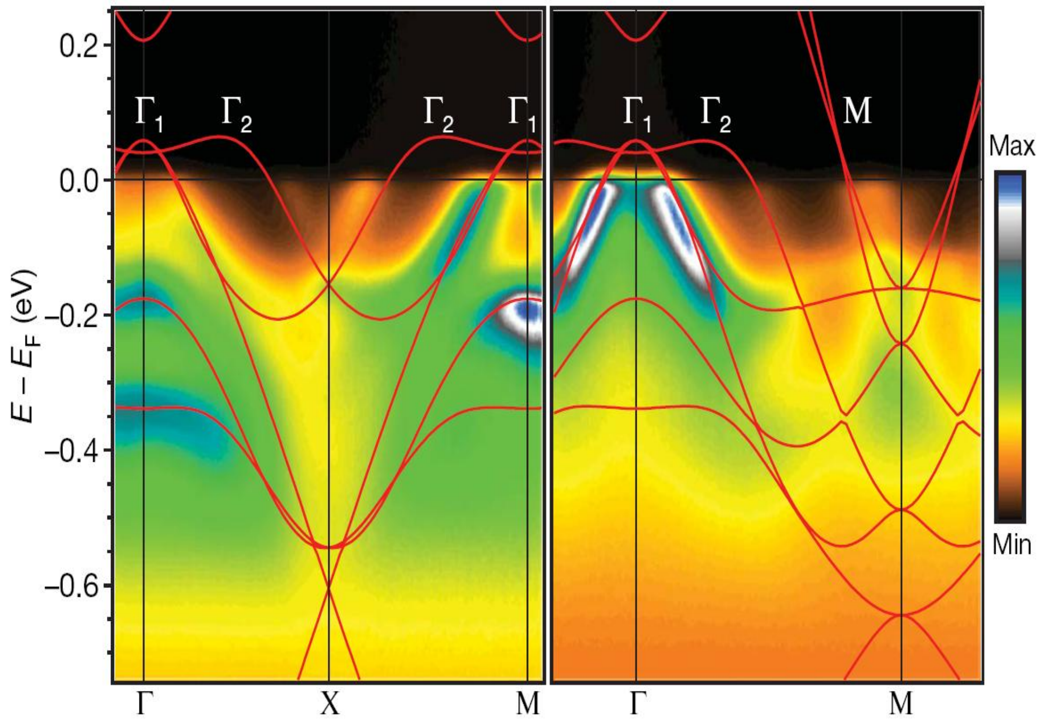
Correlations in iron based superconductors

Weak correlations

(Fermi surface instabilities, Renormalized Fermi liquid)

Localized electrons

(J_1-J_2 model, spins interact to first & second nearest neighbors)



Lu et al, Nature 455, 81 (2008)

Strength of interactions somewhere in between (mass enhancement ~ 3)

Correlated metal

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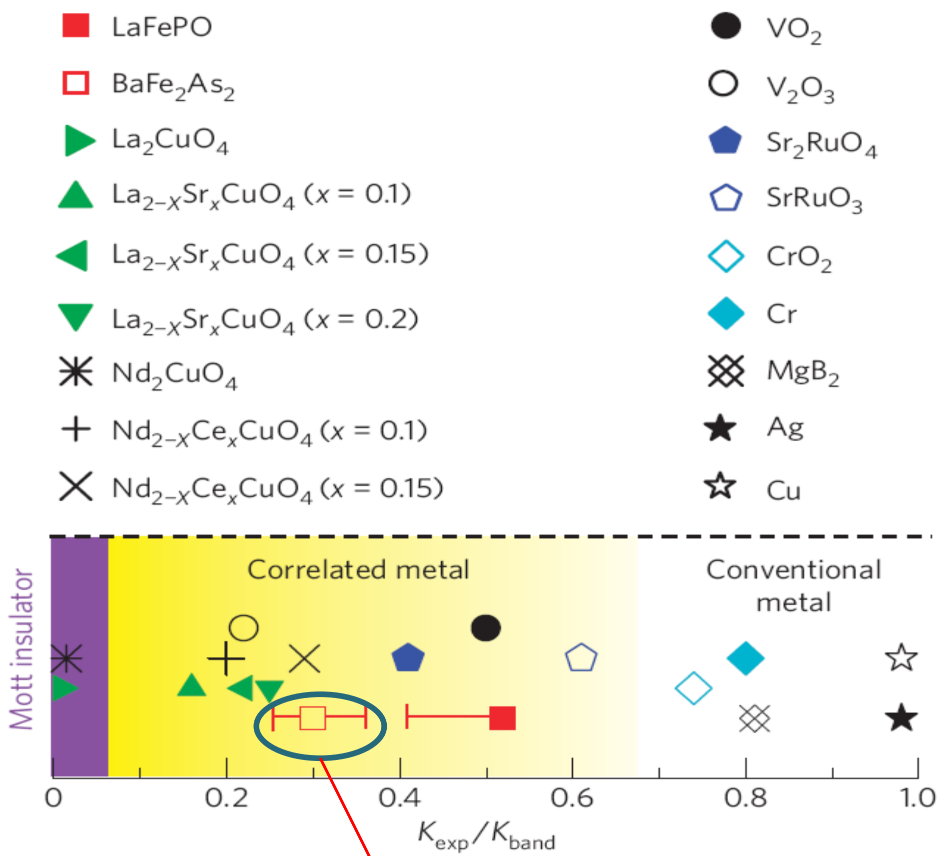
Correlations in iron based superconductors

Weak correlations

(Fermi surface instabilities, Renormalized Fermi liquid)

Localized electrons

(J_1-J_2 model, spins interact to first & second nearest neighbors)



We are here

From optics:

Correlated metal (similar to x ~0.15-0.20 doped cuprates)

Qazilbash et al, Nature Physics 5, 647 (2009)

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Correlations in iron based superconductors

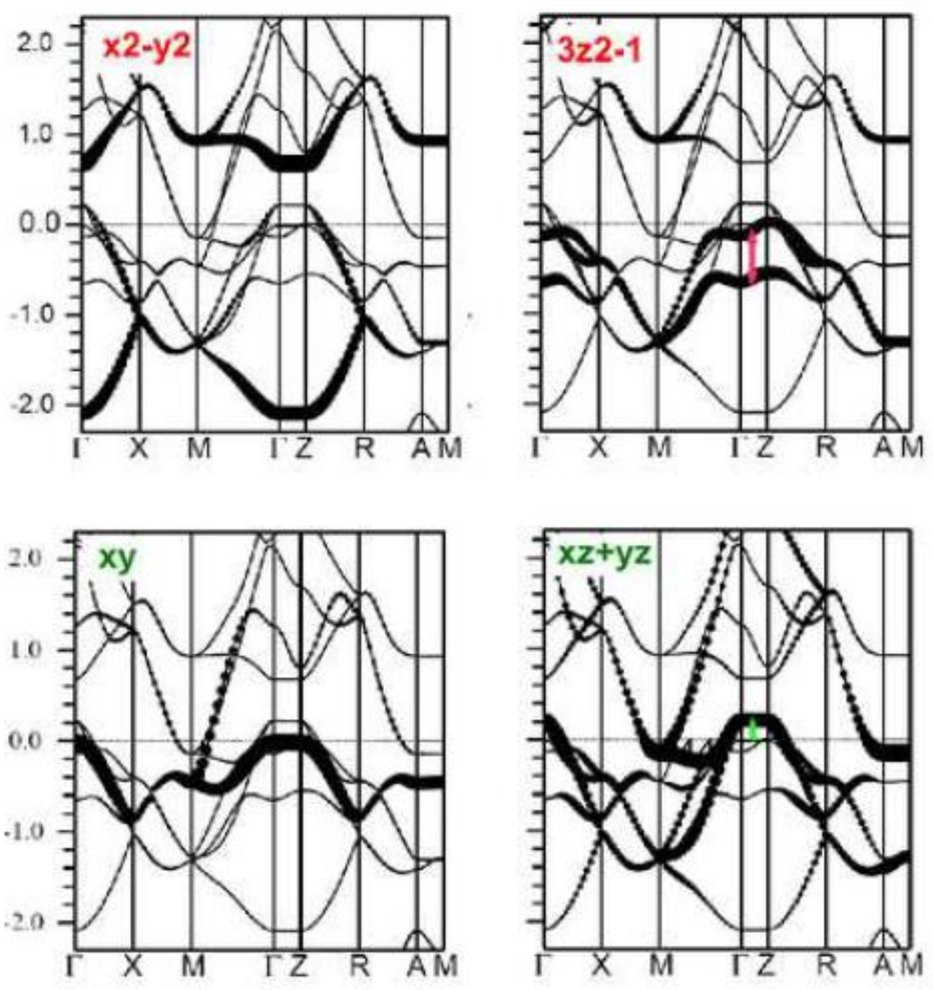
Weak correlations

(Fermi surface instabilities, Renormalized Fermi liquid)

Localized electrons

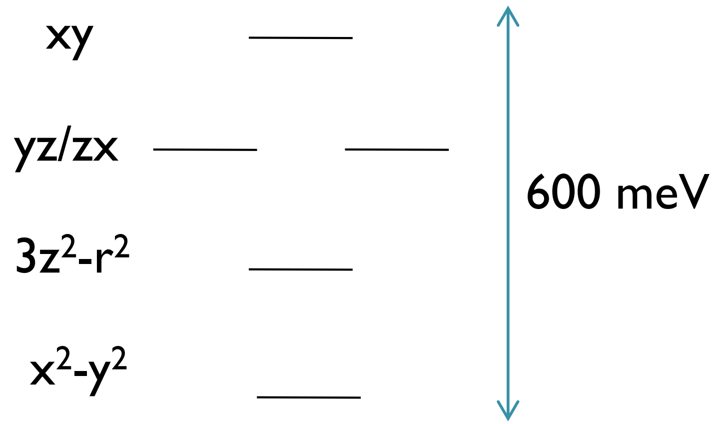
(J_1-J_2 model, spins interact to first & second nearest neighbors)

Iron superconductors are multi-orbital systems



Boeri et al, PRL 101, 026403 (2008),

The five 3d orbitals
highly entangled



The five 3d orbitals have to be included in the effective models

6 electrons in 5 orbitals
in undoped compounds

Iron superconductors are multi-orbital systems

Weak correlations
(Renormalized Fermi liquid)

Localized electrons
(Localized spins)

Hund metal/Doped Mott insulator
(6 e in 5 orbitals)

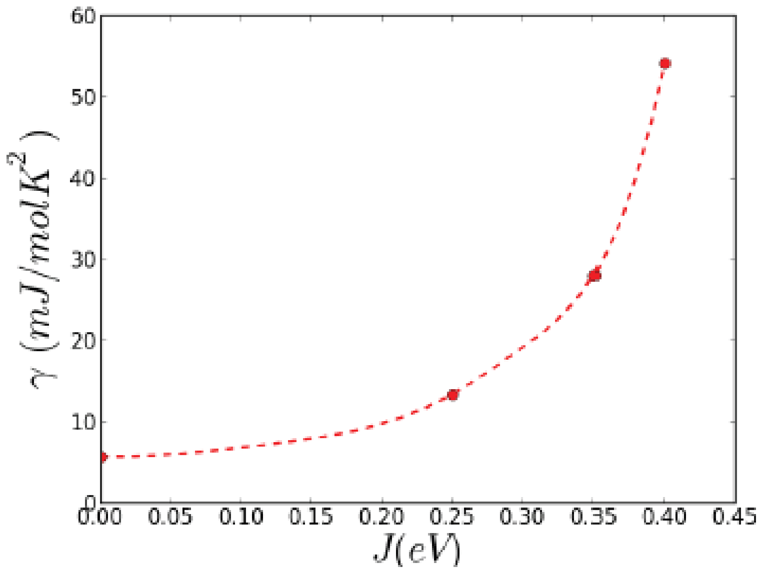
Coexistence of localized
and itinerant electrons (OSMT)

Multiorbital character may play an important role

Iron superconductors as Hund metals

Correlations due to Hund coupling from LDA+DMFT **Z(J=0) =0.8**

Shorikov et al, arXiv:0804.3283

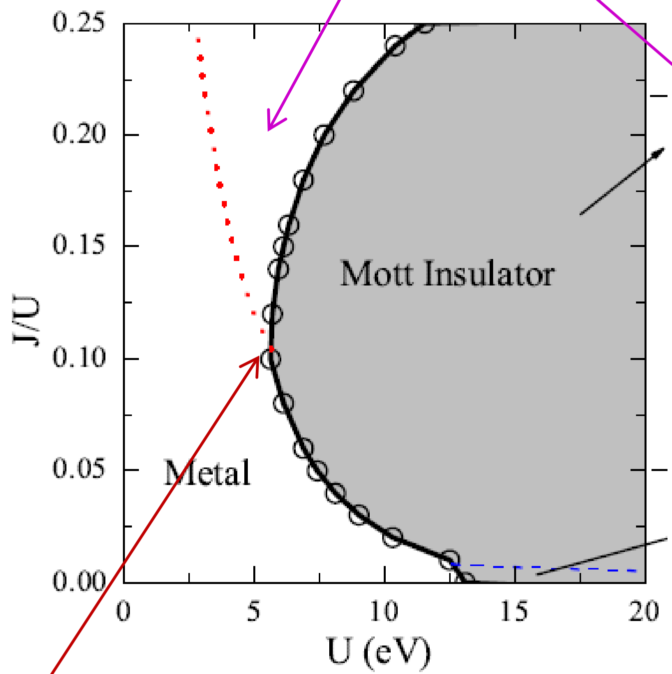


Haule & Kotliar NJP 11,025021 (2009)

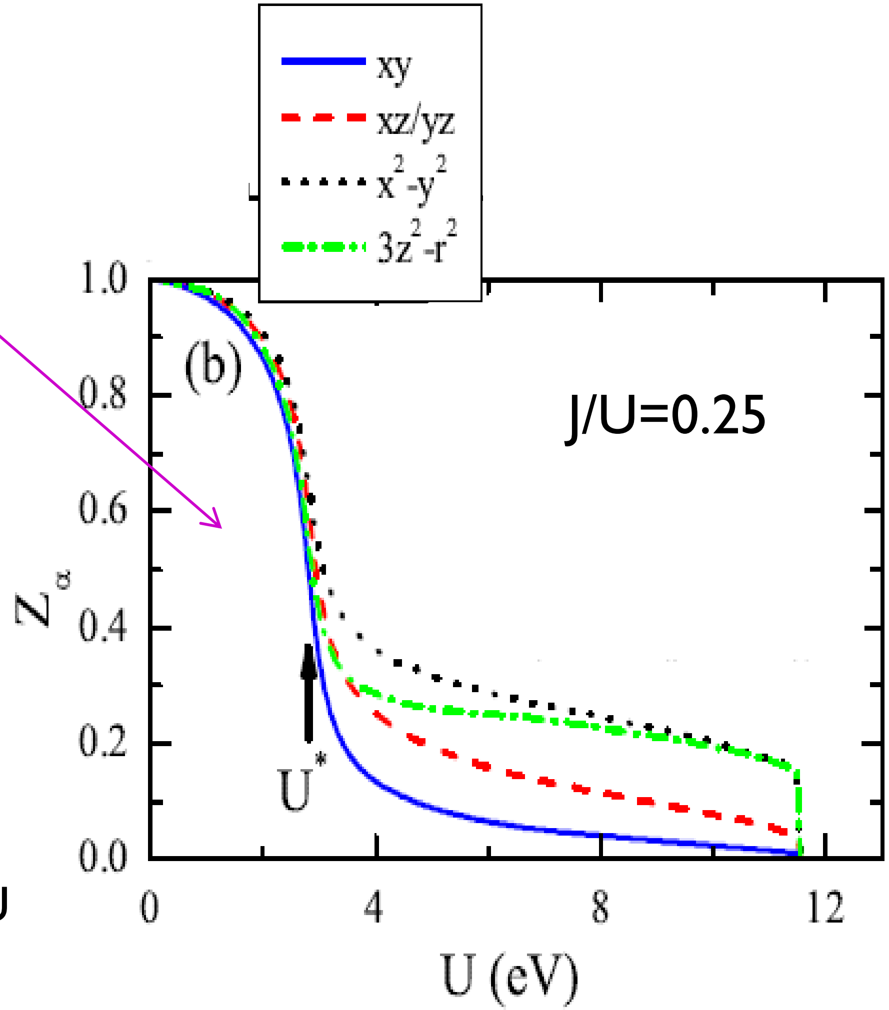
The concept of **Hund metals** coined withing iron superconductors context

Iron superconductors as Hund metals

Strongly correlated metallic phase at finite Hund



From metal to Mott insulator at small J/U



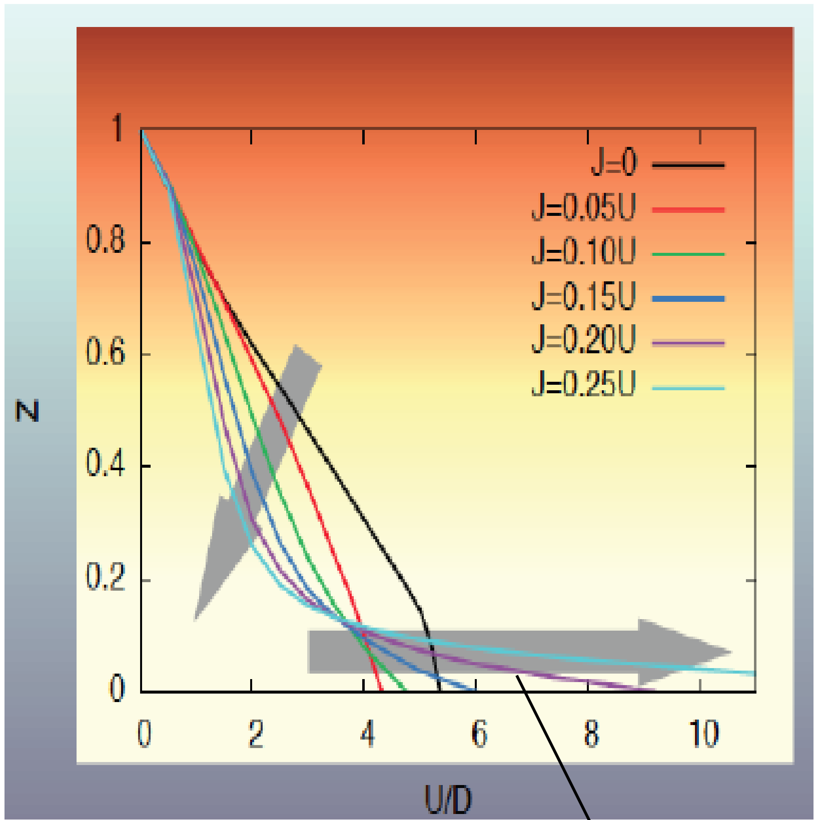
Paramagnetic phase diagram for an interacting for five orbital model for iron superconductors

U(1) slave spin representation

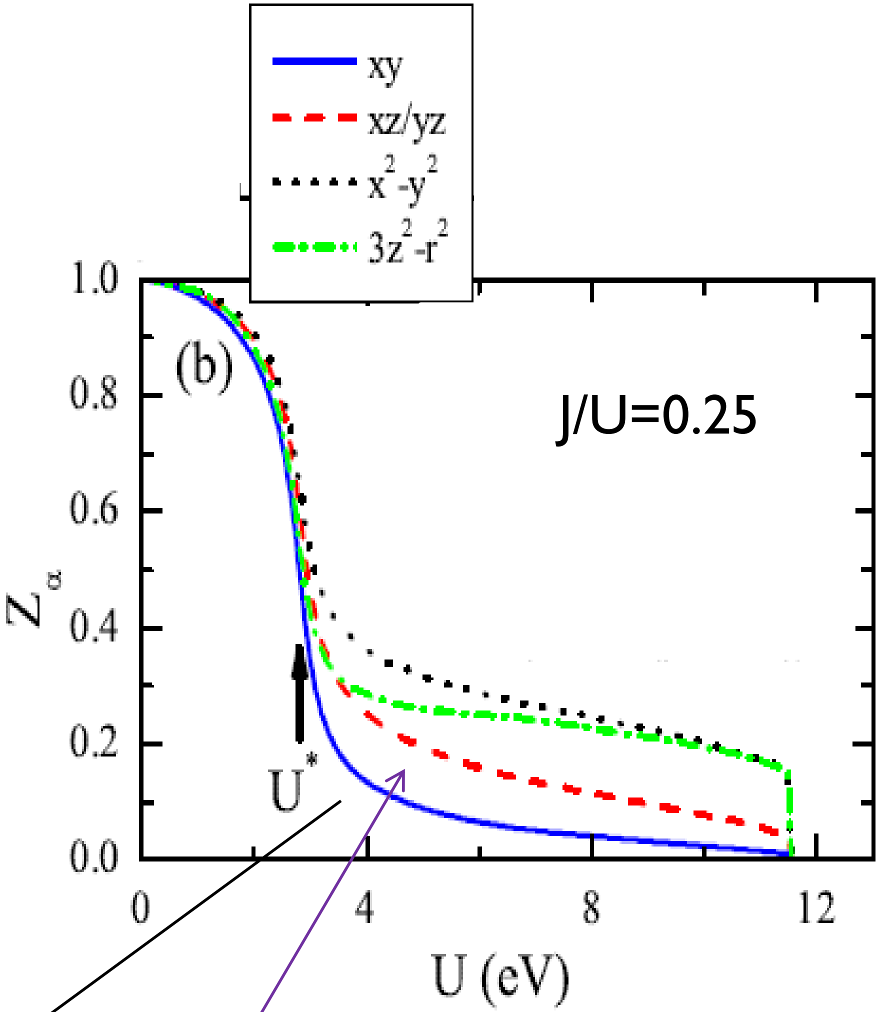
Yu & Si, arXiv: 1202.6115

Iron superconductors as Hund metals

3 bands   2 electrons



De Medici, PRB 83, 205112 (2011)

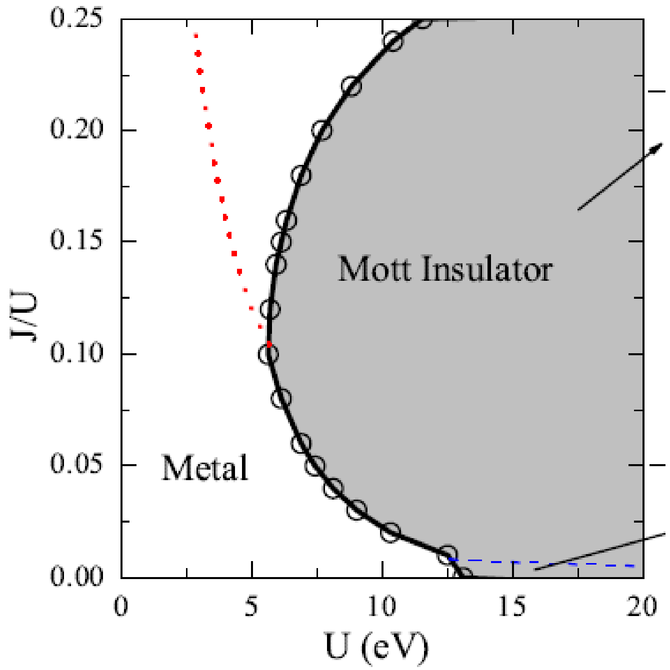


Low coherence temperature

Similar dependence

Yu & Si, arXiv: 1202.6115

Correlations in multi-orbital iron superconductors

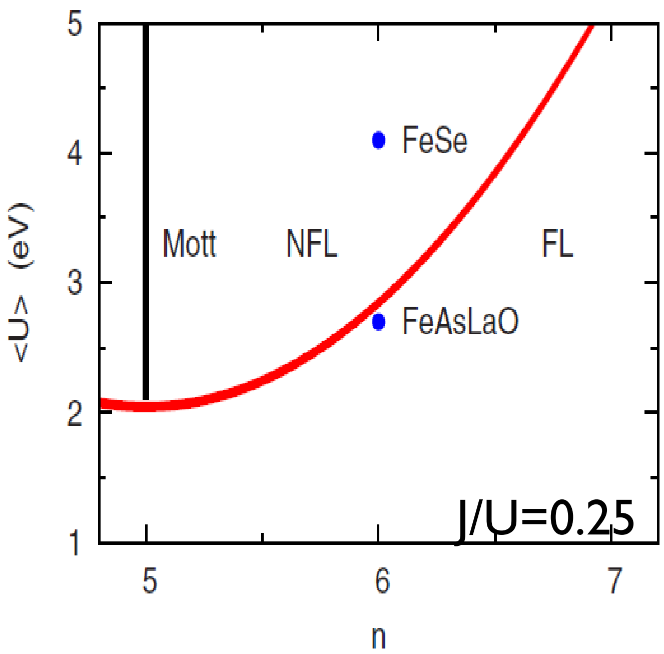


Yu & Si, arXiv: 1202.6115

Are iron superconductors in the strongly or in the weakly correlated region ?

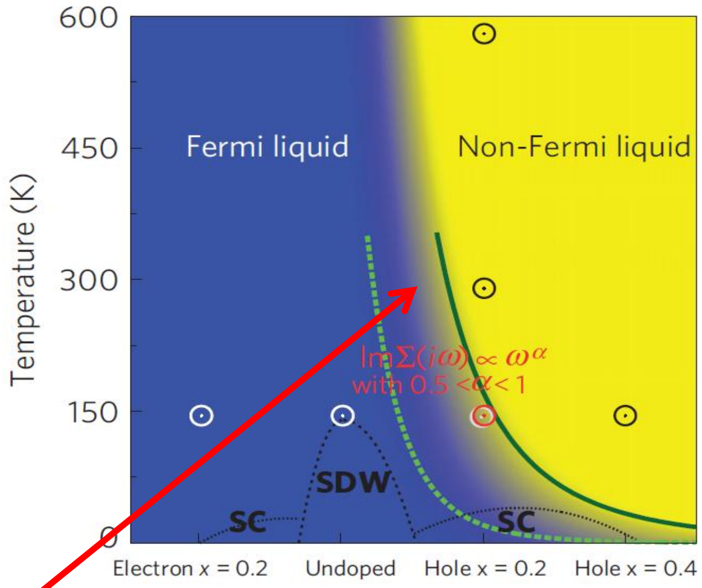
Correlations in multi-orbital iron superconductors

Undoped: 5 orbitals, 6 electrons



Liebsch, PRB 82, 1551006 (2010)

$BaFe_2As_2$



Crossover temperature (strongly sensitive to Hund coupling

Haule & Kotliar
NJP 11,025021 (2009)

Towards half-filling

Werner et al,
Nature Phys. 8, 331 (2012)

Hole-doping increases correlations

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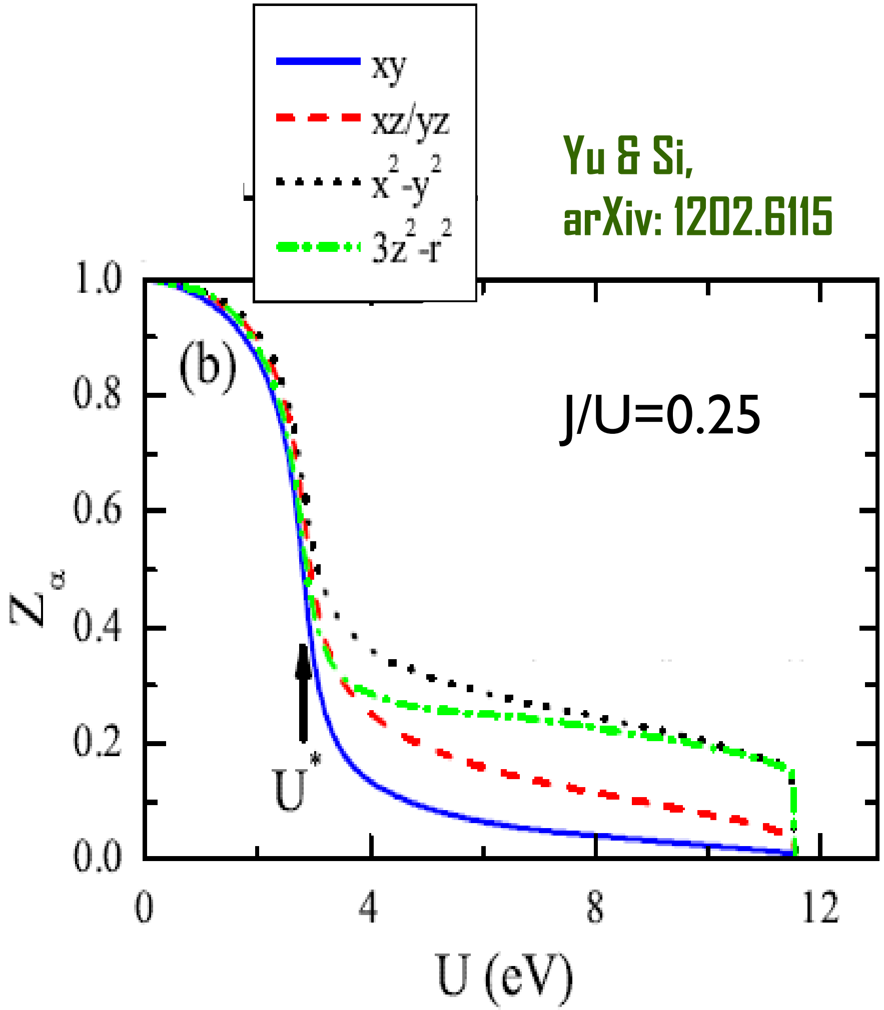
Orbital differentiation in iron superconductors



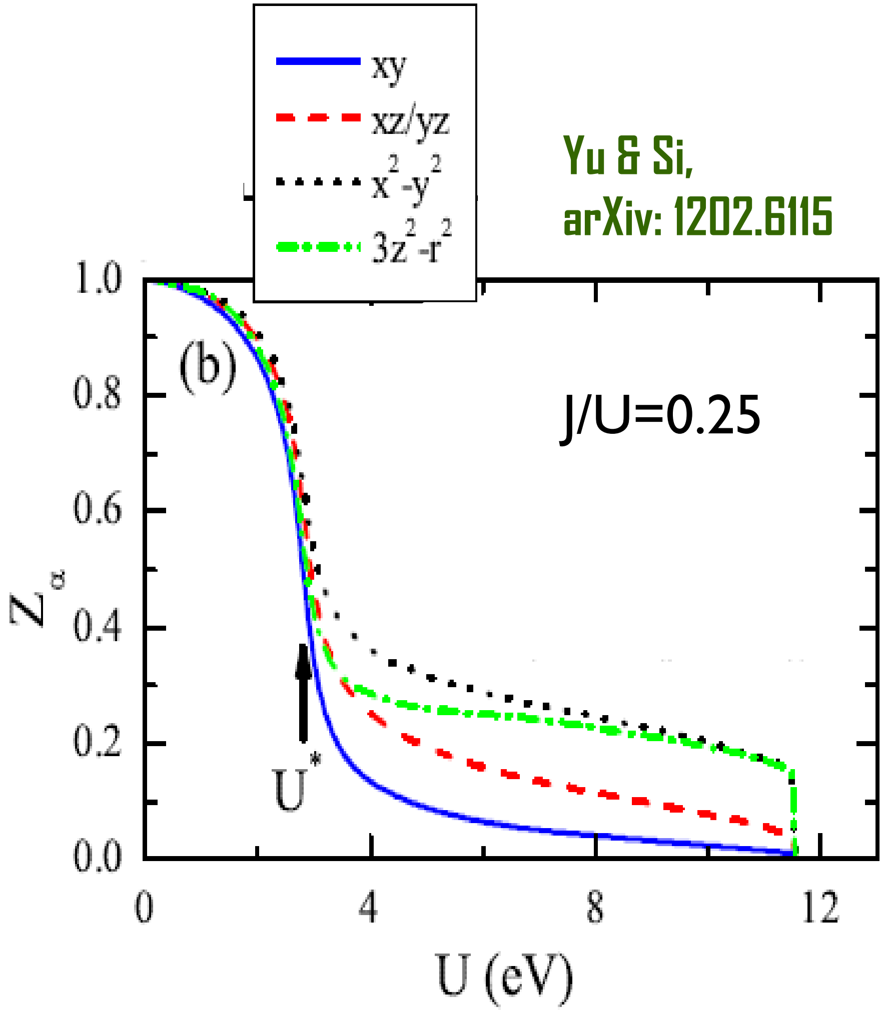
Degree of correlations is orbital dependent

xy
yz/zx
x^2-y^2/$3z^2$-r^2

Increasing correlations

Already discussed in Shorikov et al, arXiv:0804.3283

Orbital differentiation in iron superconductors



Degree of correlations is orbital dependent

xy

yz/zx

x^2-y^2/$3z^2$-r^2

Increasing correlations

Do we expect an Orbital Selective Mott transition?

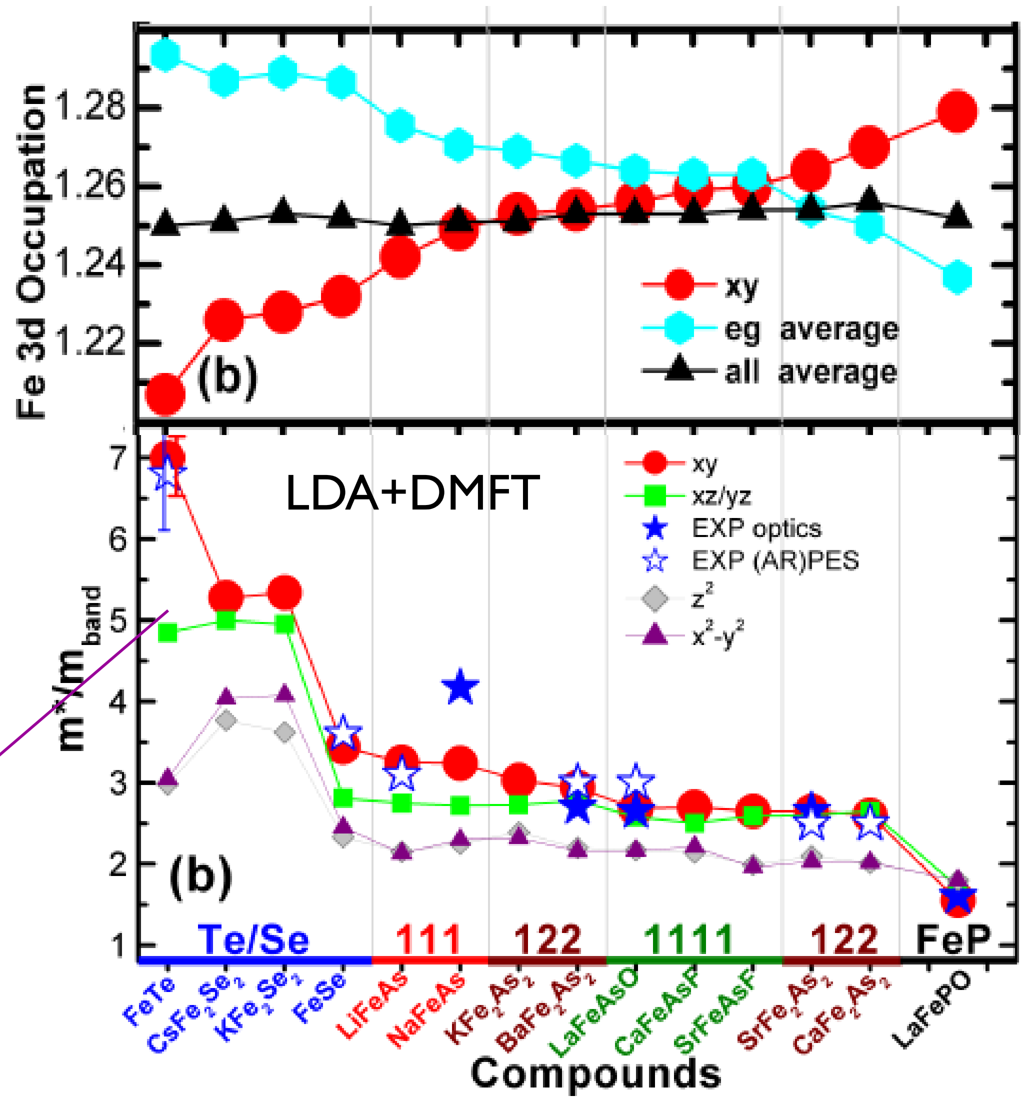
Orbital differentiation in iron superconductors

Larger correlations in orbitals closer to half filling

xy
yz/zx
x^2-y^2/$3z^2$-r^2

Increasing correlations

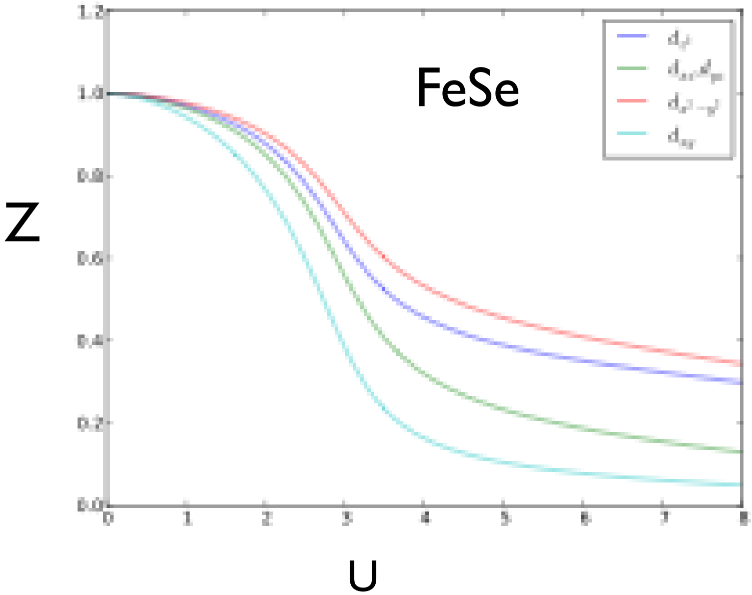
Some materials at the verge of an OSMT



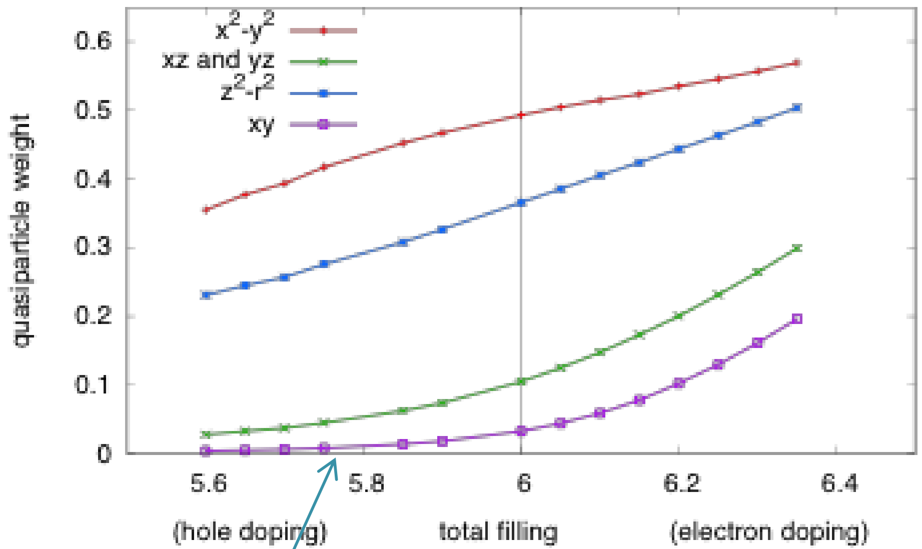
Yin et al, Nature Materials 10, 932 (2011)

Orbital differentiation in iron superconductors

DMFT



FeSe



N. Lanatà, G. Giovannetti,
L. de' Medici, M. Capone, unpublished

L. de' Medici, G. Giovannetti
and M. Capone, unpublished

Orbital selective Mott transition
induced by hole-doping

De Medici, S.R. Hassan and M. Capone,
JSNM 22, 535 (2009)

Courtesy M. Capone

Summary: Iron superconductors in non-magnetic state

Weak correlations
(Renormalized Fermi liquid)

Localized electrons
(Localized spins)

Hund metal
Doped Mott insulators
(6 e in 5 orbitals)

Coexistence of localized and itinerant electrons (OSMT)

xy
yz/zx
x^2-y^2/$3z^2$-r^2

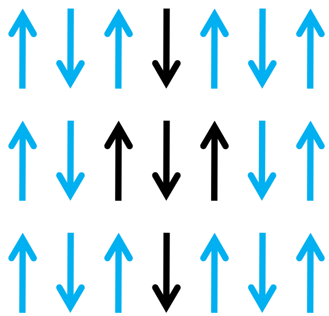
Increasing correlations

Hole doping increases correlations

How correlated are the electrons? Which is the nature of magnetism?

Weak correlations
(Fermi surface instabilities,
Renormalized Fermi liquid)

Localized electrons
(J1-J2 model)



Columnar state

$(\pi,0)$ ordering

Raghu et al, PRB 77, 220503 (2008),
Mazin et al, PRB 78, 085104 (2008),
Chubukov et al, PRB 78, 134512 (2008),
Cvetkovic & Tesanovic, EPL 85, 37002 , (2008)

Yildirim, PRL 101, 057010 (2008),
Si and Abrahams, PRL 101, 057010 (2008)

How correlated are the electrons? Which is the nature of magnetism?

Weak correlations
(Fermi surface instabilities,
Renormalized Fermi liquid)

Localized electrons
(J1-J2 model)

Antiparallel
orbital moments

Does orbital ordering
play any role?

Correlations due to
Hund's coupling/
Doped Mott insulators
(6 e in 5 orbitals. Filling 1.2)

Coexistence of localized
and itinerant electrons
Which ones?

Multiorbital character may play an important role

Haule & Kotliar, NJP 11, 025021 (2009)
Liebsch, PRB 82, 1551006 (2010)
Yin et al, Nature Phys 7, 294 (2011)
Werner et al, Nature Phys. 8, 331 (2012)

Yu & Si, arXiv: 1202.6115
Yin et al, PRL 105, 107004 (2010),
Lv et al, PRB 82, 045125 (2010)
De Medici et al, JSNM 22, 535 (2009)

EB, et al, PRL 104, 227201 (2010)
Cricchio et al, PRB 81, 140403 (2009),

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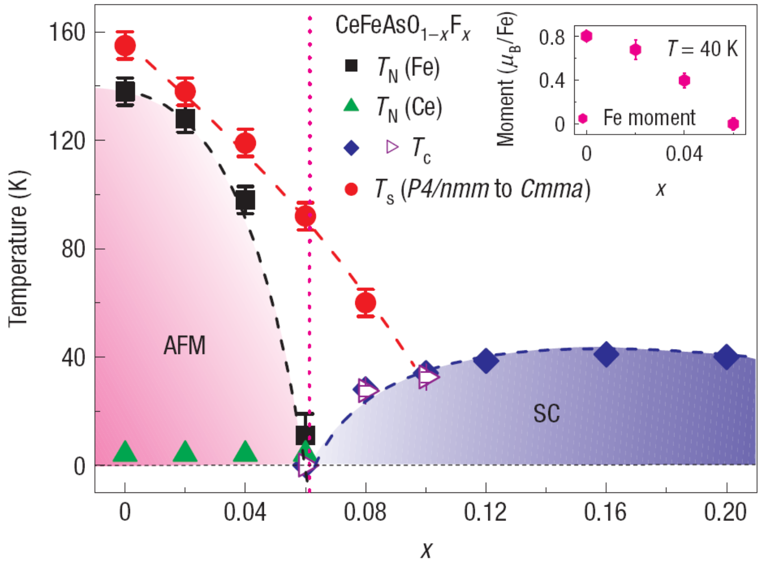
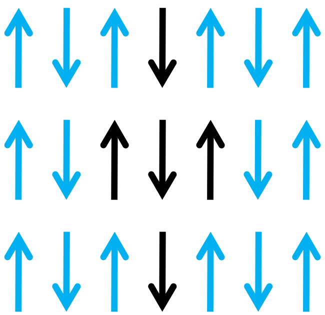
Metallic antiferromagnetic state

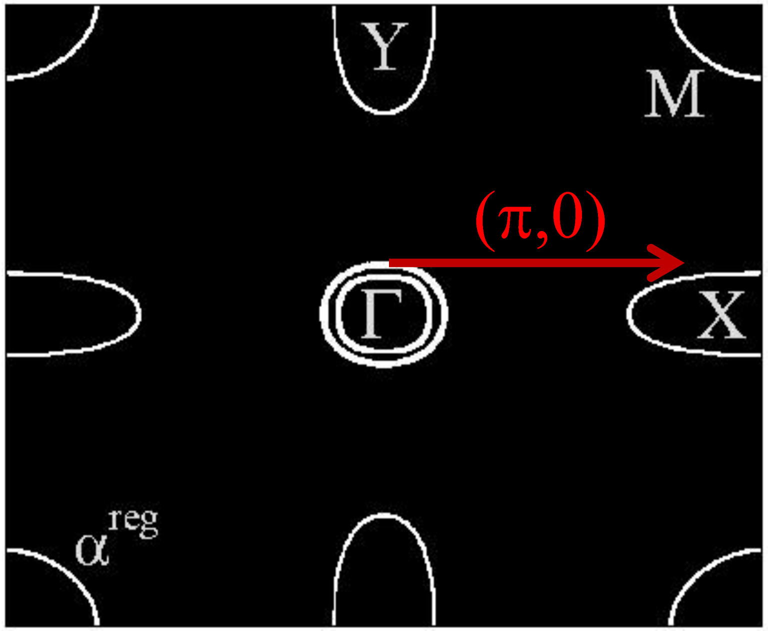


Zhao et al, Nat. Mat. 7, 953 (2008),



Columnar state

(π,0) ordering



Raghu et al, PRB 77, 220503 (2008), Mazin et al, PRB 78, 085104 (2008),
Chubukov et al, PRB 78, 134512 (2008), Cvetkovic & Tesanovic, EPL 85, 37002 , (2008)

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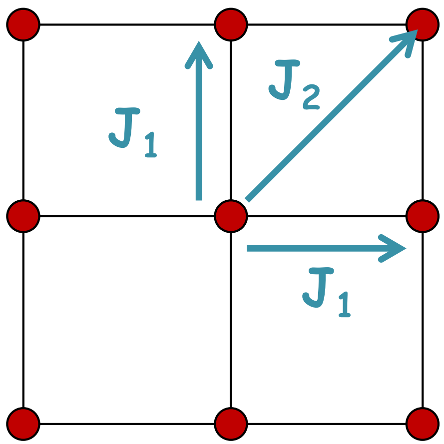
Local moment description of AF state

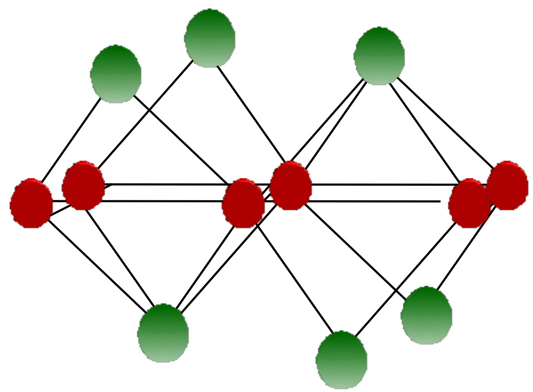
Heisenberg model with large second nearest neighbor interaction

$$H = J_1 \Sigma_{ij} (S_{ij} S_{ij+1} + S_{ij} S_{i+1j}) + J_2 \Sigma_{ij} (S_{ij} S_{i+1j+1} + S_{ij} S_{i+1j-1})$$

J_1 -J_2 model

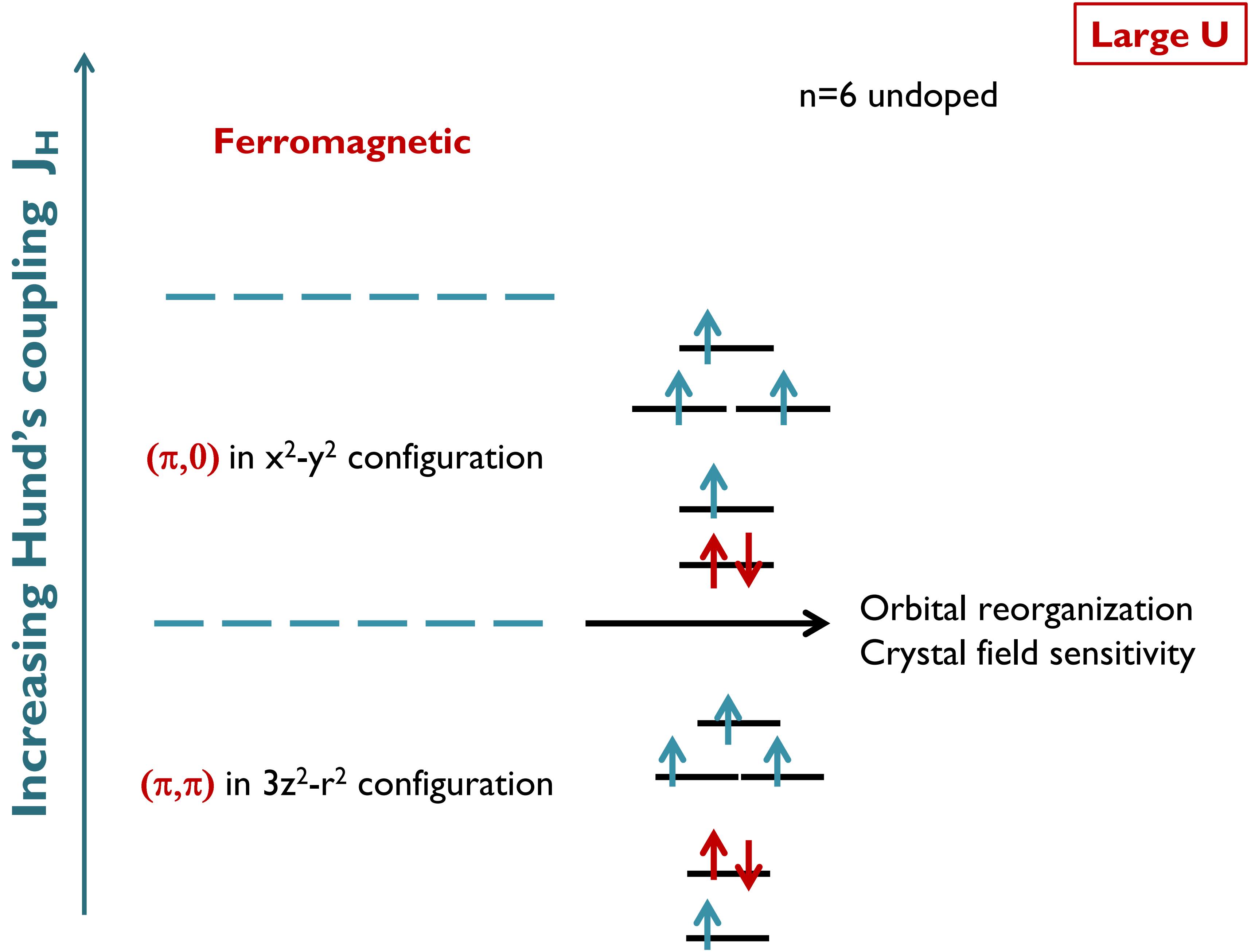


Columnar order for $J_2 > J_1/2$



Yildirim, PRL 101, 057010 (2008), Si and Abrahams, PRL 101, 057010 (2008)

Mapping to Heisenberg model. Hund's coupling



M.J. Calderón et al , arXiv: 1107.2279 (2011)

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Mapping to Heisenberg model. Doping

Strong coupling (Heisenberg)

$n = 5$ | $n = 6$ | $n = 7$ → *doping*

$n = 5$	$n = 6$	$n = 7$
(π,π)	$(\pi,0)$ (π,π) FM	$(\pi,0)$ / FM Enhanced tendency towards FM compared to $n = 6$

Electron-hole doping asymmetry (large hole doping) in the magnetic interactions

M.J. Calderón et al , arXiv: 1107.2279 (2011)

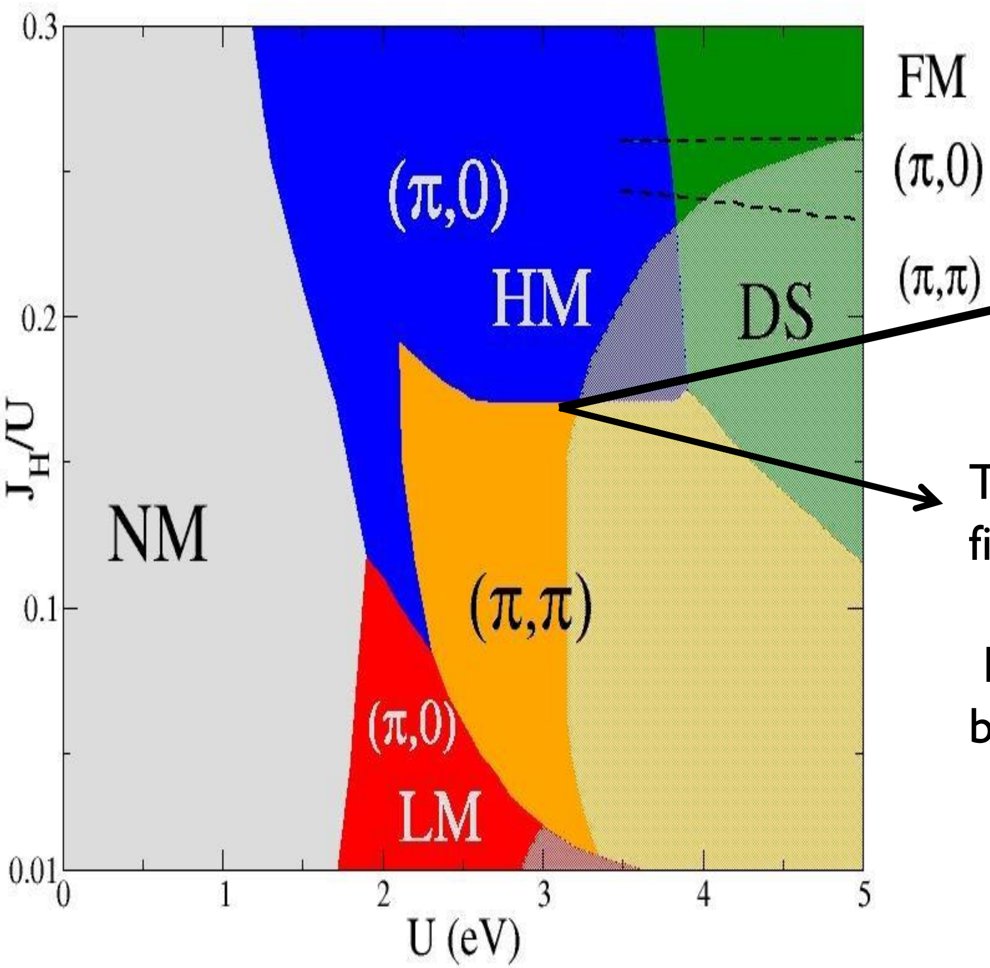
Mapping to Heisenberg model. Doping

Strong coupling (Heisenberg)

$n = 5$	$n = 6$	$n = 7$
		doping
(π,π)	$(\pi,0)$ (π,π) FM	$(\pi,0)$ / FM Enhanced tendency towards FM compared to $n = 6$
$BaMn_2As_2$	$BaFe_2As_2$	LaOCoAs
(π,π)	$(\pi,0)$	FM

M.J. Calderón et al , arXiv: 1107.2279 (2011)

Hartree-Fock phase diagram



(π,π) –$(\pi,0)$ transition with increasing Hund's coupling J_H

Transition very sensitive to crystal field changes.

It involves charge reorganization between x^2-y^2 and $3z^2$-r^2 orbitals.

Localized Physics

EB, M.J. Calderón, B. Valenzuela, PRL, 104, 227201 (2010)

M.J. Calderón, G. León , B. Valenzuela, EB, arXiv: 1107.2279

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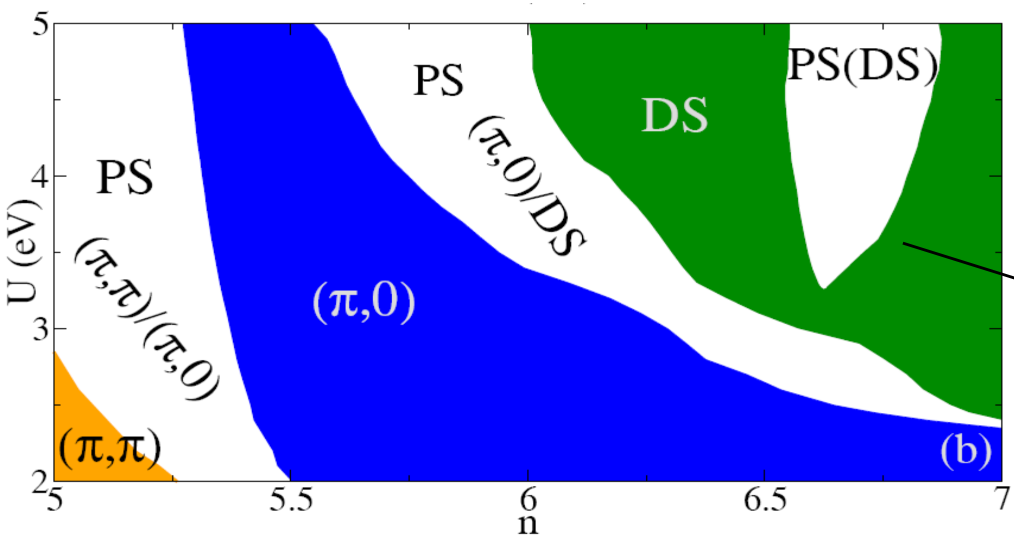
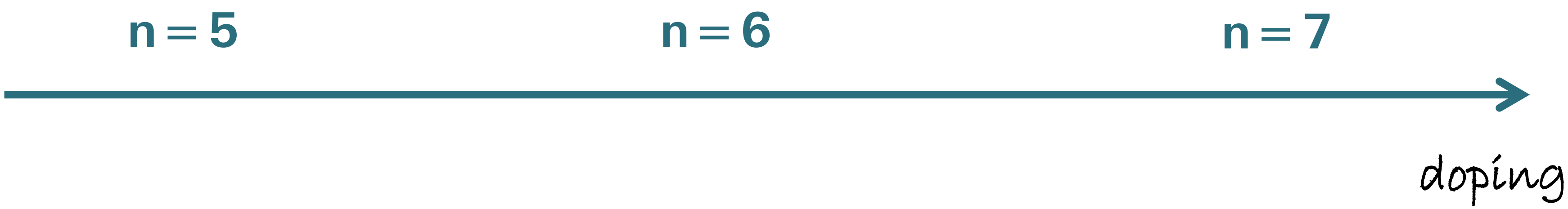
Hartree-Fock phase diagram. Doping

J_H=0.22 U



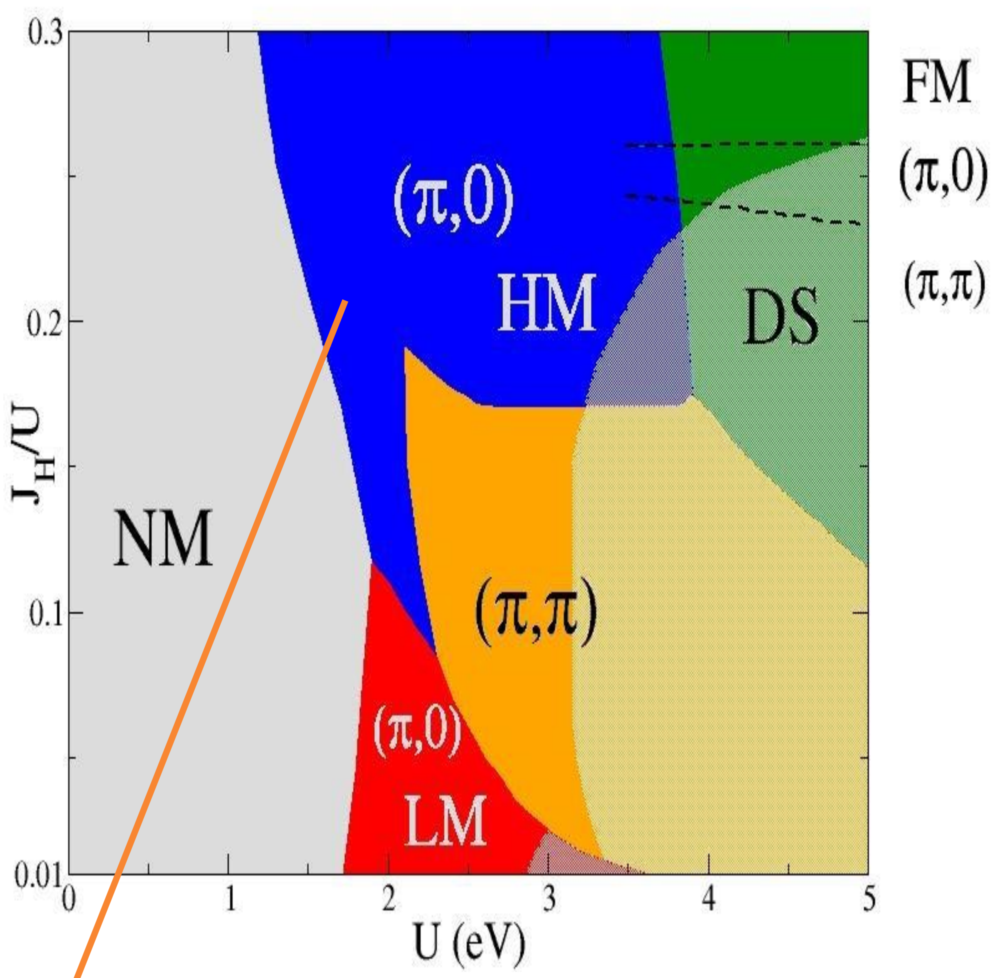
Double stripe instead of Ferromagnetism

Strong coupling (Heisenberg)



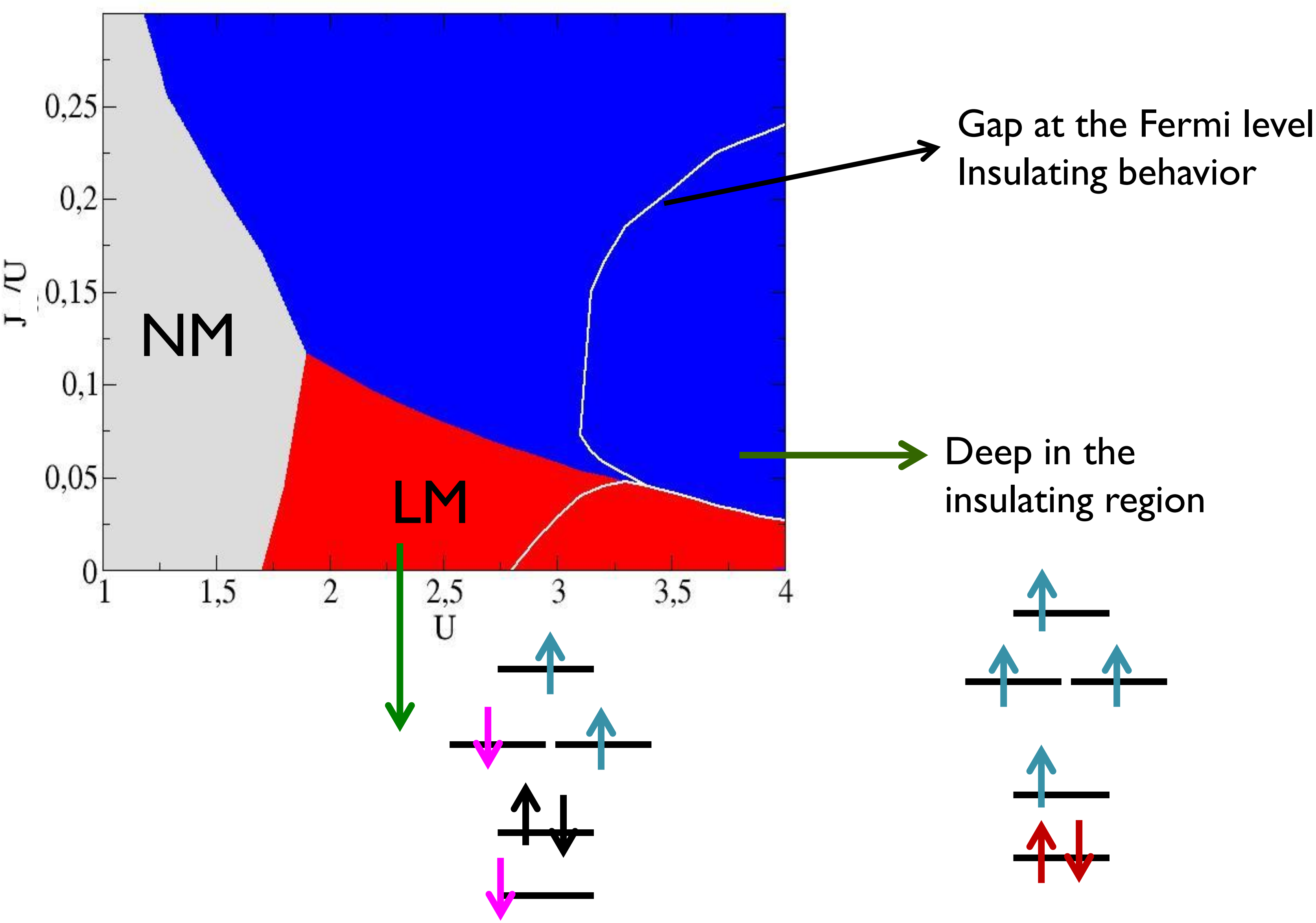
(π,π) **$(\pi,0)$** **$(\pi,0)$ / FM**

Hartree-Fock phase diagram



What is the nature of this metallic (π,0) state?

(π,0) magnetic state of iron superconductors.



EB, M.J. Calderón, B. Valenzuela, PRL 104, 227201 (2010)

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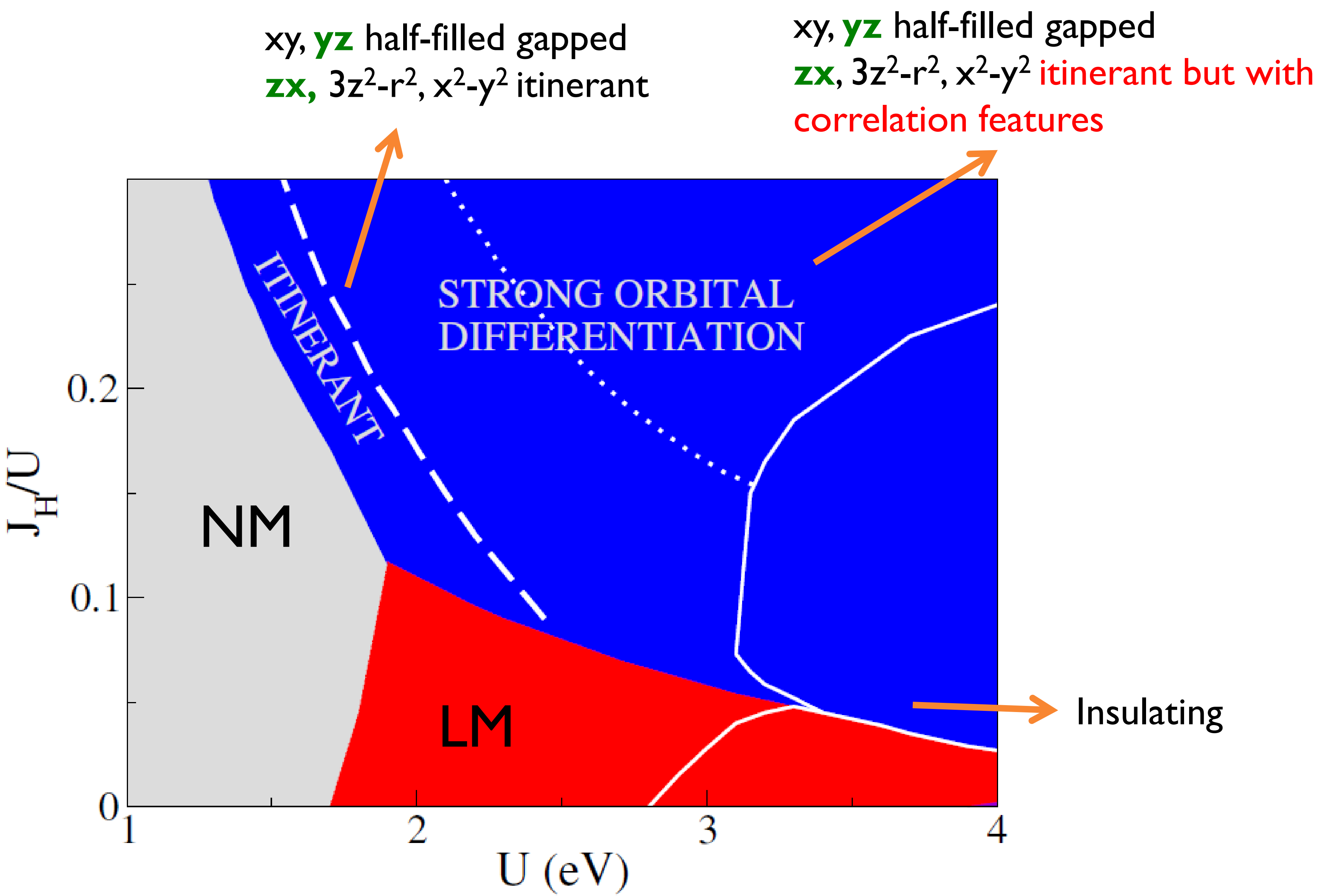
(π,0) magnetic state of iron superconductors.



EB, M.J. Calderón, B. Valenzuela (2012)

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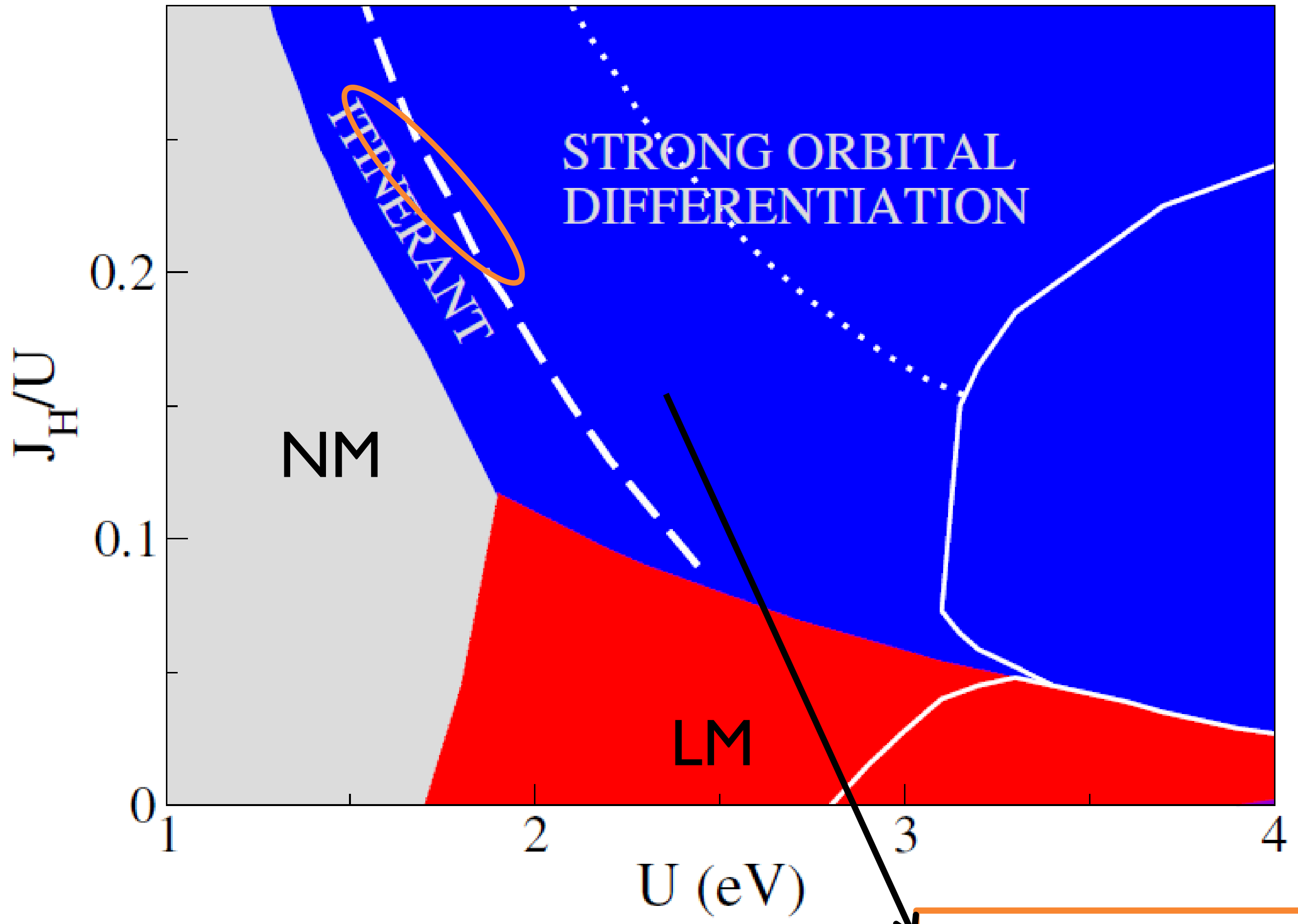
Pnictides in the (π,0) phase diagram. Undoped



xy, yz half-filled gapped

zx,$3z^2$-r^2,x^2-y^2 itinerant

EB, M.J. Calderón, B. Valenzuela (2012)

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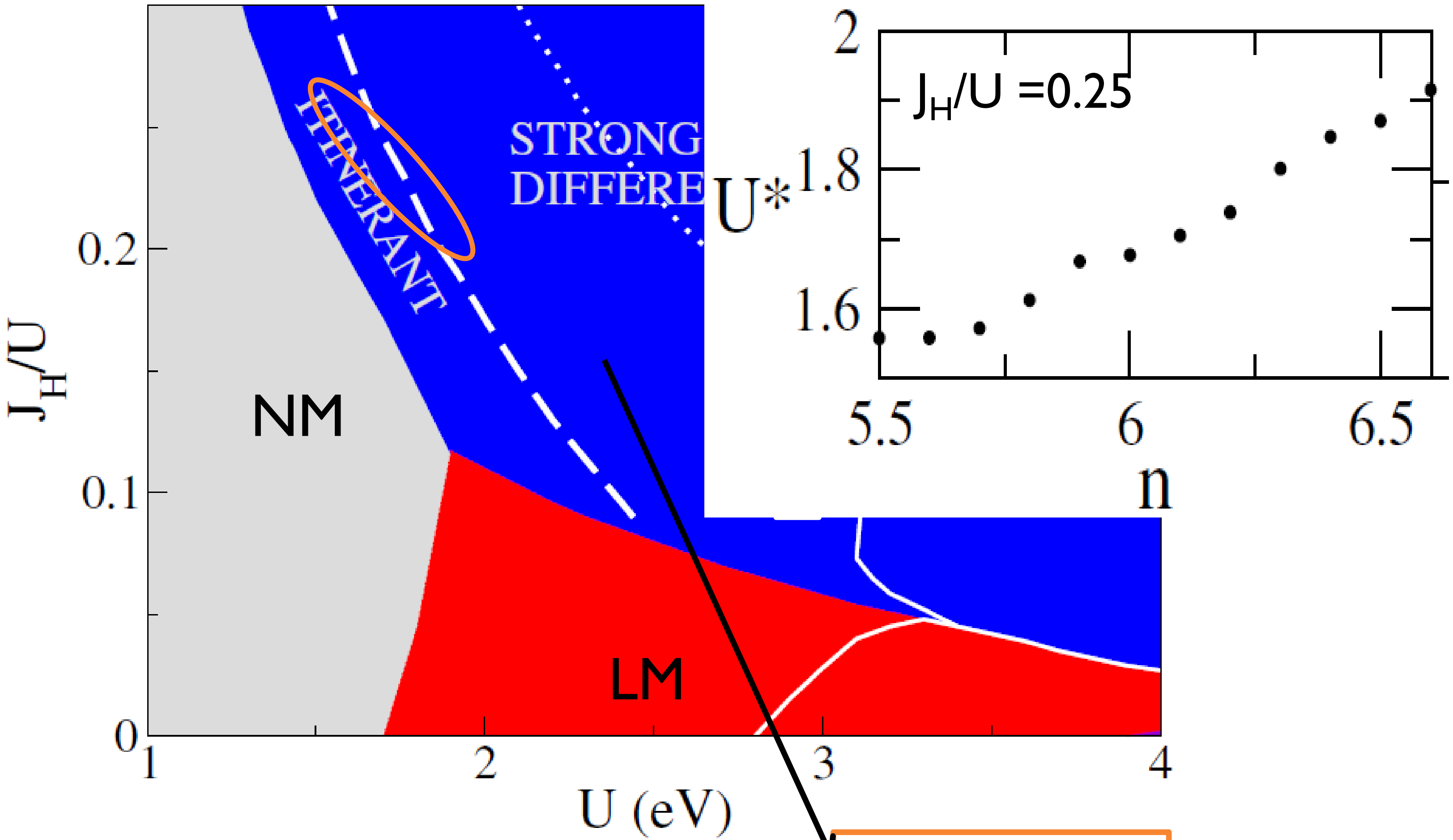
Pnictides in the (π,0) phase diagram.



xy, yz localized

$zx, 3z^2-r^2, x^2-y^2$
itinerant

EB, M.J. Calderón, B. Valenzuela (2012)

Summary: magnetic state of iron pnictides

Weak correlations
(Fermi surface instabilities,
Renormalized Fermi liquid)

Localized electrons
(J1-J2 model)

Antiparallel
orbital moments

Does orbital ordering
play any role?

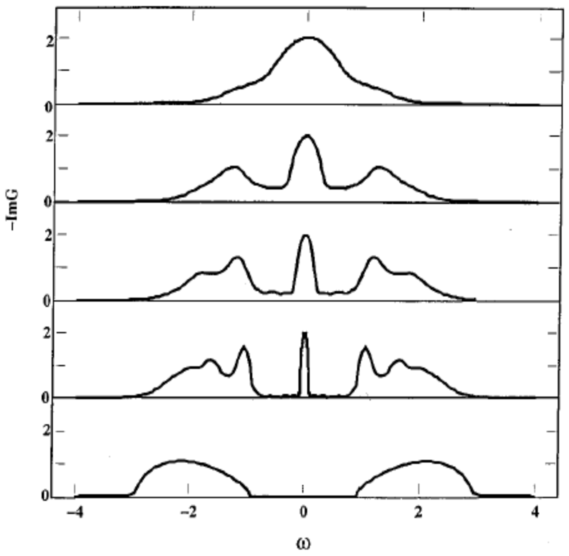
Correlations due to
Hund's coupling/
Doped Mott insulators
(6 e in 5 orbitals. Filling 1.2)

Orbital differentiation:
localized and itinerant electrons
xy,yz localized
zx, $3z^2$-r^2,x^2-y^2 itinerant

Posibility to cross the boundary between itinerant and orbital differentiated regimes with doping .Asymmetry electron-hole doping

Large doping also changes the nature of the magnetic interactions to (π,π) (hole-doping) or FM/double stripe (electron-doping)

Summary I



MIT as a function of interactions

Single-orbital: Mott transition at half-filling. AF correlations

Multi-orbital: Mott transition at commensurate filling, also away from half-filling.

$U_c \propto W$.

Increases with degeneracy in multi-orbital systems

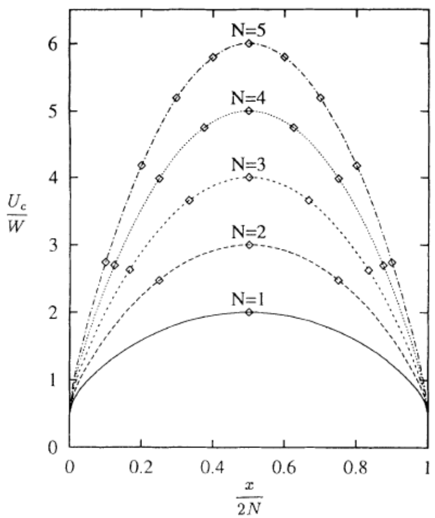
Uc larger at half-filling if Hund's coupling is zero

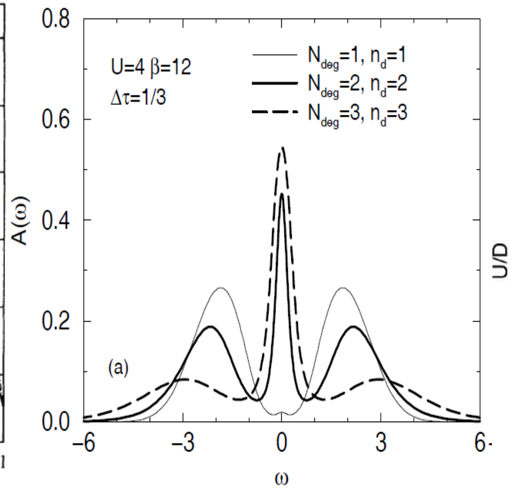
Hubbard bands & renormalized quasiparticle

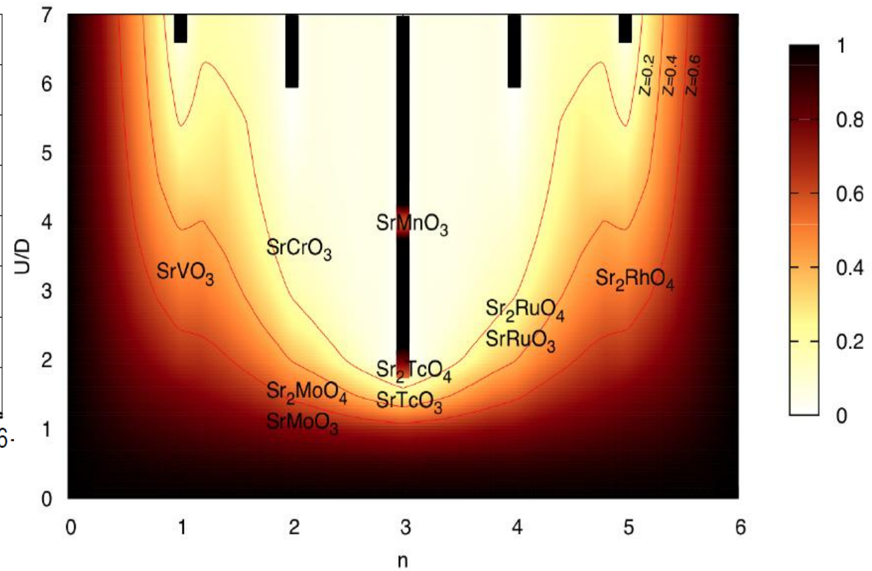
Wider Hubbard bands with increasing degeneracy

Effect of Hund's coupling on Mott physics

depends on filling. Hund metals



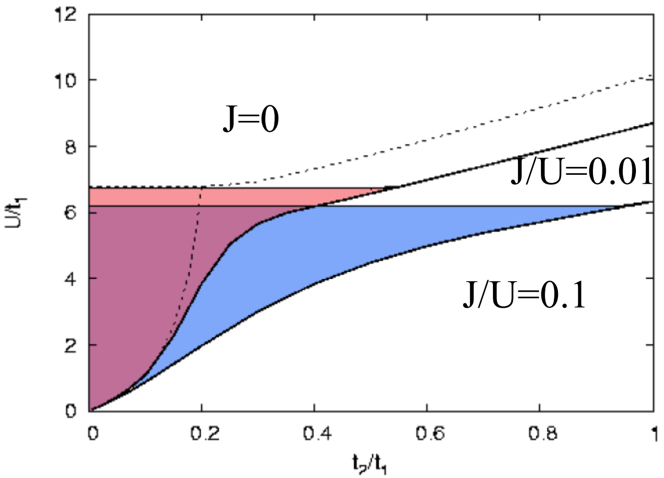


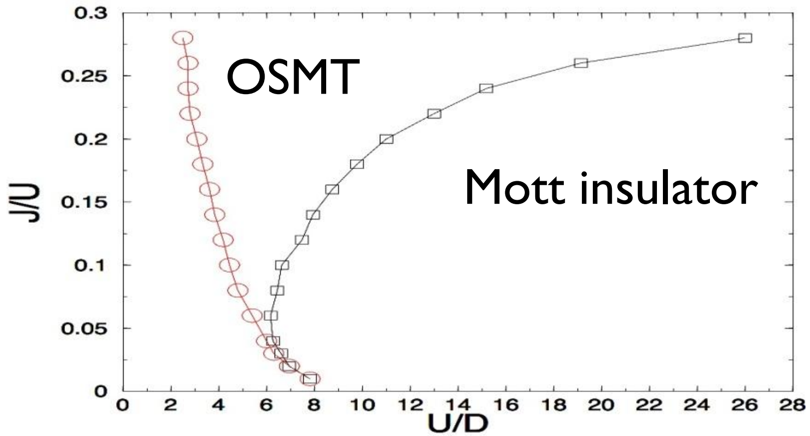


Summary II

Orbital selective Mott transitions (OSMT) possible for non-equivalent orbitals

Hund's coupling increases tendency towards an OSMT





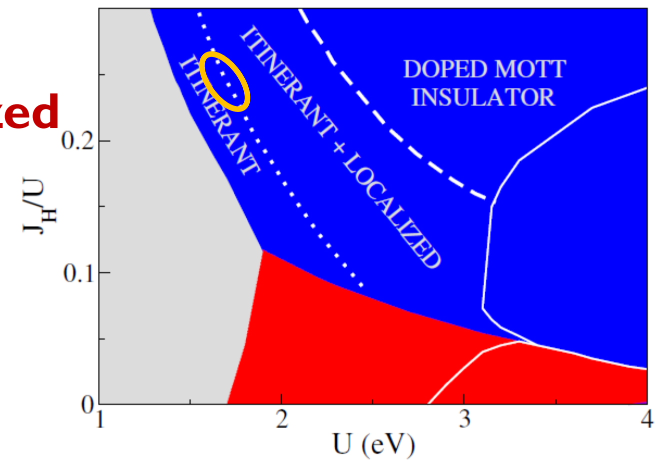
Iron SC are multiorbital systems with 6 electrons in 5 non-equivalent orbitals

Orbital differentiation

Iron SC close to itinerant/itinerant+localized boundary in both non-magnetic and magnetic states which **could be crossed with doping**

Large doping changes the nature of the magnetic interactions

Magnetic state



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