Emergence of Quantum Phases in Novel Materials

Mott physics II

E. Bascones

Teoría y Simulación de Materiales
Instituto de Ciencia de Materiales de Madrid
Mott physics in multi-orbital systems. Outline

- Multi-orbital systems. Hund’s coupling a new interaction parameter

- The Mott transition in multi-orbital systems. Equivalent bands
  - Mott transition at half-filling and at other commensurate fillings
  - Effect of Hund’s coupling in the Mott transition and the quasiparticle weight. **Hund’s metal.**

- Non-equivalent bands. The orbital selective Mott transition

- Iron superconductors

- Spin-orbit Mott insulators
Mott physics in single-orbital systems. Outline

\[ \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} + U \sum_j n_j \uparrow n_j \downarrow \]

Fig: Pickett, RMP 61, 433 (1989)

La\textsubscript{2}CuO\textsubscript{4}

Half filling
Multi-orbital systems

$A_3C_{60}$

Alloul, EPJ Web of Conf. 23, 15 (2012)
Erwin & Pickett, Science 254, 842 (1991)

Oxides with cubic symmetry

Vildosola et al, PRB 78, 064518 (2008)
Kamihara et al, JACS, 130, 3296 (2008)

LaFeAsO

$Z(\text{As}) = 0.6507$
$d_x = 1.32 \text{ Å}$

E. Bascones leni@icmm.csic.es
Interactions in one orbital systems

$$\sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} + U \sum_j n_j \uparrow n_j \downarrow$$

Kinetic energy

Intra-orbital

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?

- Transition not only at half filling
- New energy scale: Hund’s coupling
Non hybridized & equivalent multi-orbital systems

\[ \sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_i^{\dagger,\gamma,\sigma} c_j,\beta,\sigma + h.c. \]

Assume \( t_{ij}^{\gamma\beta} = t_{ij} \delta_{\gamma\beta} \)

All bands are equivalent

An electron in an orbital can jump only to the same orbital in a neighbor electron
Simplified Hamiltonian for interactions in multi-orbital systems

Interactions restricted to electrons in the same atom. Only density-density interactions.

Intra-orbital repulsion

\[ U \sum_{m} \hat{n}_{m \uparrow} \hat{n}_{m \downarrow} \]

Inter-orbital repulsion (different spin)

\[ U' \sum_{m \neq m'} \hat{n}_{m \uparrow} \hat{n}_{m' \downarrow} \]

Inter-orbital repulsion (same spin)

\[ (U' - J) \sum_{\sigma, m < m', \sigma} \hat{n}_{m \sigma} \hat{n}_{m' \sigma} \]

Hund’s coupling

Reduces the repulsion between electrons with parallel spin

\[ U' = U - 2J \]

Two interaction parameters in the model $U, J_H$

Maximum $J_H = U/3$

with rotational invariance

E. Bascones leni@icmm.csic.es
Atomic gap: A hint for a Mott transition. Single orbital

Hopping saves energy $t$

Double occupancy costs energy $U$

Interaction energy cost involved in a hopping process.

Atomic gap for tunneling
Atomic gap: A hint for a Mott transition. Multi-orbital system

Energy cost for adding an electron to an atom with N orbitals which already has n electrons minus the energy for subtracting an electron from a neighbor atom with n electrons

\[ E(n+1) - E(n-1) - 2E(n) \]
Interaction energy in multi-orbital systems

\[ E(n+1) + E(n-1) - 2E(n) \]

- **Intra-orbital**
- **Inter-orbital** (different spin)
- **Inter-orbital** (same spin)

\[ U' = U - 2J_H \]

Cost in interaction energy due to hopping among two atoms with \( n \) electrons (an atom wins an electron and another atom loses it):

**Half-filling:**

\[ U + (N-1)J_H \]

\( N \) number of orbitals

**Away from half-filling but \( n \) integer:**

\[ U - 3J_H \]

Han et al. PRB 58, R4199 (1998)
Atomic gap for tunneling in multi-orbital systems

Cost in energy to add an electron to an atom containing n electrons:

Atomic gap $E(n+1)+E(n-1)-2E(n)$

Half-filling:
$U+(N-1)J_H$

Away from half-filling but n integer:
$U-3J_H$

Gap both at half-filling & away from half-filling:

In multi-orbital systems the Mott transition is not restricted to half-filling but it can happen when the average number of electrons per atom n is an integer, i.e. when $n/N$ is commensurate

E. Bascones  leni@icmm.csic.es
Atomic gap for tunneling in multi-orbital systems

Cost in energy to add an electron to an atom containing \( n \) electrons:

**Atomic gap** \( E(n+1) + E(n-1) - 2E(n) \)

- **Half-filling:** \( U + (N-1)J_H \)
- **Away from half-filling but \( n \) integer:** \( U - 3J_H \)

The gap depends not only on \( U \), but also on the Hund’s coupling \( J_H \), on the number of orbitals \( N \), and on the number of electrons \( n \) (half-filling or not)

**\( U_c \), the critical value of the interaction at which the Mott transition happens,**
will depend on \( J_H, N \) and \( n \)

- Decreases with \( J_H \) at half filling
- Increases with \( J_H \) away from half filling
Atomic gap for tunneling in multi-orbital systems

The gap depends not only on $U$, but also on the Hund’s coupling $J_H$, on the number of orbitals $N$, and on the number of electrons $n$ (half-filling or not).

**Half-filling:**

$U + (N-1)J_H$

**Away from half-filling but $n$ integer:**

$U - 3J_H$

Half-filling: the process blocked at the Mott transition involves double-occupying a given orbital.

Away from half-filling: the process blocked at the Mott transition involves occupying an empty orbital with spin parallel to that of the polarized atom.
Kinetic energy gain in single-orbital systems

Hopping saves energy $t$

Double occupancy costs energy $U$

W bandwidth

Interaction energy cost in a hopping process

Kinetic energy saved if electrons are not localized

Control parameter for the Mott transition $= \frac{U}{W}$

In single orbital system $U/W$
Kinetic energy gain in multi-orbital systems

Hopping saves kinetic energy

Atom with N=3 orbitals & n=2 electrons

Control parameter for the Mott transition

Interaction energy cost in a hopping process

Kinetic energy saved if electrons are not localized

= Gap \((U, J_H, N, n)\)

= \(W\) or something else?
Kinetic energy gain in multi-orbital systems

In multiorbital systems the kinetic energy gain when the system is metallic it is not just simply given by the bandwidth.

- In an N-orbital model with hopping restricted to the same orbital (intra-orbital hopping): N bands with bandwidth W. The kinetic energy lost in the Mott insulator is larger than W. This kinetic energy increases with the number of channels.

- The kinetic energy also depends on the number of electrons. For \( n < N \) the number of channels available for tunneling, and consequently the kinetic energy, increase with \( n \). For \( n > N \) they decrease.

- At zero Hund’s coupling all these channels are degenerate. For finite Hund they are not.
Mott transition in multi-orbital systems. Hund’s coupling

Away from half filling:
With $J_H$ the atomic gap decreases. $U_c$ increases

Degeneracy reduced by Hund’s coupling

Half filling: with $J_H$
Atomic gap increases $U_c$ decreases

Degeneracy (effective kinetic energy) and $U_c$ strongly reduced by Hund’s coupling

De’Medici PRB 83, 205112 (2011)
Mott transition in multi-orbital systems. Hund’s coupling

Away from half filling:
With $J_H$ the atomic gap decreases.
$U_c$ increases

Conflicting effect of Hund’s coupling

De’Medici PRB 83, 205112 (2011)
Quasiparticle weight in multi-orbital systems. Half-filling

3 electrons in 3 orbitals: half-filling

Mott insulator (zero Z)

Uc reduced by Hund’s coupling

At large $J_H$ the system becomes a Mott insulator for $U$ even below $U/W$

(remember maximum $J_H = U/3$)

Half filling

$J_H$ increases correlations & promotes insulating behavior

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

Calculations done with slave-spin technique
Quasiparticle weight in multi-orbital systems. Half-filling

3 electrons in 3 orbitals: half-filling

Mott insulator (zero Z)

Quasiparticle weight reduced by Hund’s coupling
Effective mass enhanced

Half filling
$J_H$ increases correlations & promotes insulating behavior

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

Calculations done with slave-spin technique
Quasiparticle weight in multi-orbital systems. Single electron or hole

1 electrons in 3 orbitals (same for 5 electrons=1 hole)

Mott insulator (zero Z)

Uc increased by Hund’s coupling

The system is metallic even at very large U if $J_H$ is large

1 electron or 1 hole

$J_H$ decreases correlations & promotes metallic behavior

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

Calculations done with slave-spin technique
Quasiparticle weight in multi-orbital systems. Single electron or hole

1 electrons in 3 orbitals (same for 5 electrons=1 hole)

Mott insulator (zero $Z$)

Uc increased by Hund’s coupling

Quasiparticle weight increased by Hund’s coupling (effective mass reduced)

1 electron or 1 hole

$J_H$ decreases correlations & promotes metallic behavior

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

Calculations done with slave-spin technique

$D=W/2$
Quasiparticle weight in multi-orbital systems. Hund metals

2 electrons in 3 orbitals
(same for 4 electrons)

Mott insulator (zero Z)

$U_c$ non-monotonous with Hund’s coupling

Strongly correlated metal
**Hund metal**

De’Medici et al PRL 107, 255701 (2011)
Fanfarillo & E.B. PRB 92, 075136 (2015)

Calculations done with slave-spin technique

$W$: bandwidth

$D = W/2$
Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

Colour plots: Quasiparticle weight $Z$

**Hund metal small $Z**

(strongly correlated, even for small U/W)

$n=6$ Mott insulator

Boundary (crossover):

different dependence on interaction parameters

than the Mott transition

Slave spin. Only density-density terms included

Fanfarillo & EB, PRB 92,075136 (2015)
Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

Hund metal small Z

 Colour plots: **Quasiparticle weight Z**

Away from half-filling the process blocked at the Mott transition does not involve increasing the double occupancy

Slave spin. Only density-density terms included

At the Hund metal crossover the hopping processes which increase the double occupancy are blocked

Fanfarillo & EB, PRB 92,075136 (2015)

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

Suppression of $Z$ associated to the atomic spin polarization

Enhancement of Spin fluctuations

Loss of kinetic energy to satisfy Hund’s rule

Slave spin. Only density-density terms included

Fanfarillo & EB, PRB 92,075136 (2015)
Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

Hund metal

Z(J_H) and C_{n_T}(J_H)

Charge fluctuations

Quasiparticle weight

Different behavior of charge and quasiparticle weight

Fanfarillo & EB, PRB 92,075136 (2015)

Slave spin.

Only density-density terms included
Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

Colour plots: Quasiparticle weight $Z$

**Hund metal**: correlated metallic state.
The atoms are locally polarized (Hund’s rule)
Itinerancy is only partially suppressed.
The strong correlations are not a measurement of the localization of the electrons

Slave spin.
Only density-density terms included

Fanfarillo & EB,
PRB 92,075136 (2015)

E. Bascones leni@icmm.csic.es
Hund metals: Doping dependence

6 electrons in 5 orbitals

 Colour plots: **Quasiparticle weight Z**

Hund metal

Half-filling Mott insulator

Strong correlations linked to avoiding intraorbital double occupancy

To some extent resembles a doped half-filled Mott insulator

Electron-hole asymmetry around n=6

---

Correlations in multi-orbital systems: Not half-filling, not single hole/electron

**Weak correlations**
(properties, origin of magnetism and of superconductivity described in terms of **itinerant electrons. Fermi surface physics**)

**Localized electrons**
(properties, origin of magnetism and of superconductivity described in terms of **localized electrons. Spin models**)

**Hund metal**
(spin polarized atoms & itinerancy)

6 electrons in 5 orbitals
Average doping \( n=1.2 \)
Like doped Mott insulators
(note differences with single orbital doped Mott insulator)

Increase of correlations towards half-filling
Summary: Mott physics in multi-orbital systems. Equivalent bands

- In multi-orbital systems the Mott transition is not restricted to half-filling \( n = N \), but it also happens for commensurate fillings: \( 2N/n \) integer (\( n \): number of electrons per atom, \( N \), number of orbitals)

- Hubbard bands wider with increasing degeneracy

- **Hund’s coupling** \( J_H \): a new interaction parameter in the problem

- \( U_c \) the critical interaction at which the Mott transition happens depends on \( n \), \( N \), & on Hund’s coupling \( J_H \).

- Single electron or hole per atom: Hund’s coupling promotes metallicity

- Half-filling: Hund’s coupling promotes insulating behavior

- Intermediate filling: Conflicting behavior. Hund’s metal: correlations due to Hund’s rule
  Different behavior of charge correlations and Quasiparticle weight

**Hund’s metal**
Strongly correlated metal: small quasiparticle weight \( Z \) due to Hund’s rule
Mott physics in multi-orbital systems. Non-equivalent bands

Assume orbitals do not mix $t_{ij}^\gamma t_{ij}^\beta = t_{ij}^\gamma \delta_{\gamma \beta}$ (hopping different in different bands)

Orbitals are coupled via interorbital interaction and Hund’s coupling

When isolated Mott transition at $U=U_{c1}$

When isolated Mott transition at $U=U_{c2}$

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

De’Medici et al PRB 72, 205124 (2005)
Ferrero et al, PRB 72, 205126 (2005)
Mott physics in multi-orbital systems. Non-equivalent bands

Assume orbitals do not mix $t^{\gamma\beta}_{ij}=t^{\gamma\beta}_{ij} \delta_{\gamma\beta}$ (hopping different in different bands)

Orbitals are coupled via interorbital interaction and Hund’s coupling

When isolated Mott transition at $U=U_{c1}$

When isolated Mott transition at $U=U_{c2}$

Two degenerate orbitals.
Unequal bandwidths
$n=2$ Half-filling

OSMT: Orbital Selective Mott transition
One band metallic, one insulating

De’Medici et al PRB 72, 205124 (2005)
Ferrero et al, PRB 72, 205126 (2005)
Mott physics with non-equivalent bands. OSMT. Hund’s coupling

2 bands, unequal bandwidth. Half-filling

Hund’s coupling enhances the tendency towards an Orbital Selective Mott Transition (OSMT)

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

Coloured region: OSMT

$J_H = 0$

$J_H / U = 0.01$

$J_H / U = 0.1$

De’Medici et al PRB 72, 205124 (2005)
Ferrero et al, PRB 72, 205126 (2005)
Mott physics with non-equivalent bands. OSMT. Hund’s coupling

2 bands, unequal bandwidth. Half-filling

Hund’s coupling enhances the tendency towards an Orbital Selective Mott Transition (OSMT)

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

Hund’s coupling decouples the electrons

Coloured region: OSMT

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

\[
U \sum_m \hat{n}_m^{\uparrow} \hat{n}_m^{\downarrow} + U' \sum_{m \neq m'} \hat{n}_m^{\uparrow} \hat{n}_{m'}^{\downarrow} + (U' - J) \sum_{m < m', \sigma} \hat{n}_m^{\sigma} \hat{n}_{m'}^{\sigma} +
\]

Intraorbital interaction

Interorbital Interaction (different spin)

Interorbital Interaction (same spin)
OSMT. Quasiparticle weight

Ferrero et al, PRB 72, 205126 (2005)

\[ \frac{D_2}{D_1} = 0.15 \]

J=0

\[ \frac{U}{D_1} \]

3 bands 4 electrons
Crystal field.
Unequal occupancy
n=(1,1.5,1.5)

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

J/U=0.25

Correlated metal
Low coherence temperature

Itinerant and localized electrons coupled via Hund

Ferromagnetic Kondo lattice

Biermann et al, PRL 95, 206401 (2005)

E. Bascones leni@icmm.csic.es
High Temperature superconductivity in iron materials

Layered materials (FeAs/Se planes)

pnictides (As/P, pnictogen atom)
chalcogenides (Se/Te, chalcogen atom)

Fe square lattice

Kamihara et al, JACS 130, 3296 (2008)
Phase diagram of iron superconductors

Undoped: 6 e- per Fe

Doping with electrons

Doping with holes

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


Undoped iron pnictides/chalcogenides are (not always) AF. The magnetic order ((\(\pi,0\)), double stripe, block, ...) depends on the material. As in cuprates superconductivity appears when doping with electrons or holes.
Phase diagram of iron superconductors

In iron pnictides/chalcogenides AF can be suppressed & Superconductivity induced by pressure or isovalent chemical substitution

The role of doping is less clear than in cuprates

Metallicity in iron superconductors

Contrary to cuprates, undoped iron pnictides are **NOT** Mott insulators

Chen et al, PRL 100, 247002 (2008)

Zhao et al, Nat. Mat. 7, 953 (2008)
Metallicity in iron superconductors

Contrary to cuprates undoped iron pnictides are NOT Mott insulators

Does this mean that iron superconductors are not correlated?

Iron electrons as itinerant weakly correlated electrons
Iron electrons as almost localized strongly correlated electrons
Correlations in iron based superconductors


Bands can be observed: there are quasiparticles
Bandwidth reduced compared to LDA calculations
Mass enhancement in undoped arsenides $m^*/m \sim 3$

Iron superconductors are correlated metals
Correlations in iron based superconductors

Weak correlations
(properties, origin of magnetism and of superconductivity described in terms of itinerant electrons. Fermi surface physics)

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)

Localized electrons
(properties, origin of magnetism and of superconductivity described in terms of localized electrons. Spin models)

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

Iron superconductors are multi-orbital systems
Iron superconductors are multiorbital systems

LDA: Fe bands at the Fermi level. Several orbitals involved

In cuprates a single band crosses the Fermi level

Fig: Pickett, RMP 61, 433 (1989)
Correlations in iron based superconductors

**Weak correlations**
(proPERTIES, ORIGIN OF MAGNETISM AND OF SUPERCONDUCTIVITY DESCRIBED IN TERMS OF ITINERANT ELECTRONS. FERMI SURFACE PHYSICS)

**Hund metal**
(CORRECTIONS DUE TO HUND’S COUPLING)

- Shorikov et al, arXiv:0804.3283
- Haule & Kotliar NJP 11, 025021 (2009)
- de Medici et al, PRL 107, 255701 (2011)
- Yu & Si, PRB 86, 085104 (2012)

**Localized electrons**
(PROPERTIES, ORIGIN OF MAGNETISM AND OF SUPERCONDUCTIVITY DESCRIBED IN TERMS OF LOCALIZED ELECTRONS. SPIN MODELS)

- de Medici et al, arXiv 1212.3966

Correlations can be different for different orbitals leading even to a description in terms of the coexistence of localized and itinerant electrons (OSMT)

6 electrons in 5 orbitals
Average doping n=1.2
Like doped Mott insulators

Liebsch, PRB 82, 1551006 (2010)
Werner et al, Nature Phys. 8, 331 (2012)

Multiorbital character may play an important role
Correlations in iron based superconductors

5 band model for iron superconductors

6 electrons (undoped)

5 band model (Equivalent orbitals)

6 electrons

Yu & Si, PRB 86, 085104 (2012), Ishida & Liebsch PRB 81, 054513 (2010)

Correlations enhanced towards half-filling (hole-doping)

Review: EB et al, CRAS 17, 36 (2016)
Correlations in iron superconductors

5 band model for iron superconductors

6 electrons (undoped)

Drop of quasiparticle weight (crossover)

Orbital differentiation (some orbitals more correlated than other)

Correlations enhanced
Towards half-filling (hole-doping)

Yu & Si, PRB 86, 085104 (2012), Ishida & Liebsch PRB 81, 054513 (2010)
Calderon, de Medici, Valenzuela, EB, PRB 90, 115128(2014)

Review: EB et al, CRAS 17, 36 (2016)
Correlations in iron based superconductors

FeAs compounds

FeP compounds

K_{x}Fe_{y-x}Se_{2}

FeSe, FeTe

Low spin

Metal moderate correlations
Z≥0.5

High-spin

Strongly correlated Hund metal

Mott Insulator

Review: Bascones, Valenzuela, Calderón, Comptes Rendus Physique 17, 36 (2016)
Correlations in iron based superconductors

Multiorbital character seems to play an important role in the analysis of correlations in iron superconductors

- The so-called undoped iron superconductors (n=6 in 5 orbitals) are metallic, not Mott insulators.

- Strong controversy regarding the strength of correlations: Fermi liquid description, local moment, Hund metal?

- Iron superconductors could be Hund’s metals: small quasiparticle weight due to Hund’s coupling. In this case correlations are expected to be linked to the half-filled (n=5) Mott insulator.

- Correlations seem to be more important when the system is doped with holes (n <6 in 5 orbitals approaching half-filling) than when the system is doped with electrons (n>6, getting away from half-filling).

- Some orbitals seems to be more affected by correlations than other. This is related to their particular filling and it is enhanced when doping with holes.
Spin-orbit Mott insulators

\[ \text{Sr}_2\text{IrO}_4 \]

Canted Antiferromagnetic Insulator (5d electrons)

IrO\(_2\) planes which resemble the CuO\(_2\) planes in cuprates

**Fig:** Kim et al, Science, 323, 1331 (2009)
Spin-orbital Mott insulators

Fig: Kim et al, PRL 101, 076402(2009)

Ir: 5d$^5$

1 hole in 3-degenerate t2g orbitals
Small U in 5d orbitals but large Uc (even more with $J_H$)

Correlations are not expected to be very important
Or is there something else?
Spin-orbit Mott insulators

3d: competition between kinetic energy & interaction

Interaction strength decreases in 4d & overall in 5d

New Energy Scale

Spin-orbit increases with atomic number Z. Large in 5d

Note: The subgroup numbers 1-15 were adopted in 1984 by the International Union of Pure and Applied Chemistry. The names of elements 112-118 are the Latin equivalents of these numbers.
Spin-orbit Mott insulators

5d

\[ t_{2g} \]

\[ e_g \]

\[ L_{\text{eff}} = 1 \]

\[ 10Dq \]

\[ J_{\text{eff}} = 1/2 \]

\[ \zeta_{SO} \]

\[ J_{\text{eff}} = 3/2 \]

Crystal Field SO coupling

Fig: Kim et al, PRL 101, 076402(2009)
Spin-orbit Mott insulators

Ir: $5d^5$

$5d$

$e_g$

$L_{eff} = 1$

$t_{2g}$

$10Dq$

$J_{eff} = 1/2$

$\xi_{SO}$

$J_{eff} = 3/2$

Crystal Field SO coupling

Fig: Kim et al,
PRL 101, 076402(2009)
Spin-orbit Mott insulators

$5d$  
$e_g$  
$t_{2g}$  
$J_{eff} = 1$  
$10Dq$  
$\zeta_{SO}$  
$J_{eff} = 1/2$  
$J_{eff} = 3/2$  
$+ U$

Crystal Field - SO coupling

$\mu$  
$t_{2g}$ band  
wide $t_{2g}$-band Metal  
$J_{eff} = 1/2$ band  
$J_{eff} = 3/2$ band  
$J_{eff} = 1/2$ band split due to SO

Fig: Kim et al,  
PRL 101, 076402(2009)

Not $S=1/2$ Mott, but $J_{eff}=1/2$ Mott
Summary

- **Mott transition in degenerate multi-orbital systems.**
  - Mott transition also from half filling: Mott transition at integer filling.
  - $U_c$ depends on Hund’s coupling

- **Hund’s coupling promotes**
  - correlations and insulating behavior at half filling
  - metallicity for single electron or hole
  - other cases: strongly correlated metal. Hund metal.
    - Hund metals as “doped Mott insulators”

- **Non-equivalent multi-orbital systems. Orbital selective Mott transition (OSMT)**
  - Metallic & insulating bands
  - Hund stabilizes the OSMT & promotes bad metallic behavior

- **Iron superconductors.** Multiorbital systems (6 electrons in 5 orbitals).
  - Correlated metals. Hund’s physics. Different correlation strength in different orbitals

- **Spin-orbital Mott insulators.** $J_{\text{eff}} = 1/2$ a new playground for physics.