``Enseigner la recherche en train de se faire"

COLLÈGE DE FRANCE
1530

Chaire de
Physique de la Matière Condensée

CORRELATIONS ELECTRONIQUES ET TRANSPORT DANS LES OXYDES 4d ET COMPOSES SUPRACONDUCTEURS DU FER : HUND PLUTOT QUE MOTT, DRUDE PLUTOT QUE LANDAU

Les mercredis dans l'amphithéâtre Maurice Halbwachs
11, place Marcelin Berthelot 75005 Paris
Cours à 14h30 - Séminaire à 15h45

Antoine Georges

Cycle 2011-2012
2/05/2012 – 13/06/2012
(Pas de séance le 23/05)

Main themes of this year's lectures:

- Part I (May 2 – May 30) :
- `*Hundness'* : Intra-atomic exchange (Hund's rule coupling) is responsible for strong correlations in materials which are not close to a Mott insulating state
- → Relevance to transition-metal oxides
- → Relevance to iron-based superconductors
- Part II (June 6, 13) – *time permitting (or 2012-2013 ?)*
- *Transport (electrical and thermal) in correlated materials: incoherent regimes (beyond Landau Fermi Liquid Theory)*

Séminaires – Partie I

2 mai	
Cours (2)	Corrélations loin de la transition de Mott : rôle du couplage de Hund (cours 1 et 2)
9 mai	
Cours	Matériaux fortement corrélés en raison du couplage de Hund.
Séminaire	**Felix BAUMBERGER** *(St Andrews) - The electronic structure of layered ruthenates from Angular-Resolved Photoemission Spectroscopy.*
16 mai	
Cours	Transport électronique dans les systèmes corrélés : introduction et bases théoriques.
Séminaires (2)	**Silke BIERMANN** *(Ecole Polytechnique) - Hubbard and Hund: incoherent metallic behavior in iron pnictide compounds*
	Luca 'de Medici (LPS Orsay) – *Orbital selectivity and Hund's rule coupling in iron-based superconductors*
23 mai	*- Pas de séance -*
30 mai	
Cours	Transport électronique et corrélations : bases théoriques (suite), phénoménologie.
Séminaire	***Orateur annoncé ultérieurement***

Séminaires – Partie II

6 juin	
Cours	Transport électronique: quand les quasiparticules de Landau n'existent plus.
Séminaire	**Nigel HUSSEY** *(Bristol) - High-temperature superconductivity and the Catch-22 conundrum (overdoped cuprates and their transport properties).*
13 juin	
Cours	Transport : propriétés thermoélectriques et corrélations fortes. Conclusion du cours.
Séminaires (2)	**Sriram SHASTRY** *(UC Santa Cruz) – 1-Simple insights into the thermopower of correlated matter. 2-Extremely correlated Fermi liquids*

Website of lectures and seminars:

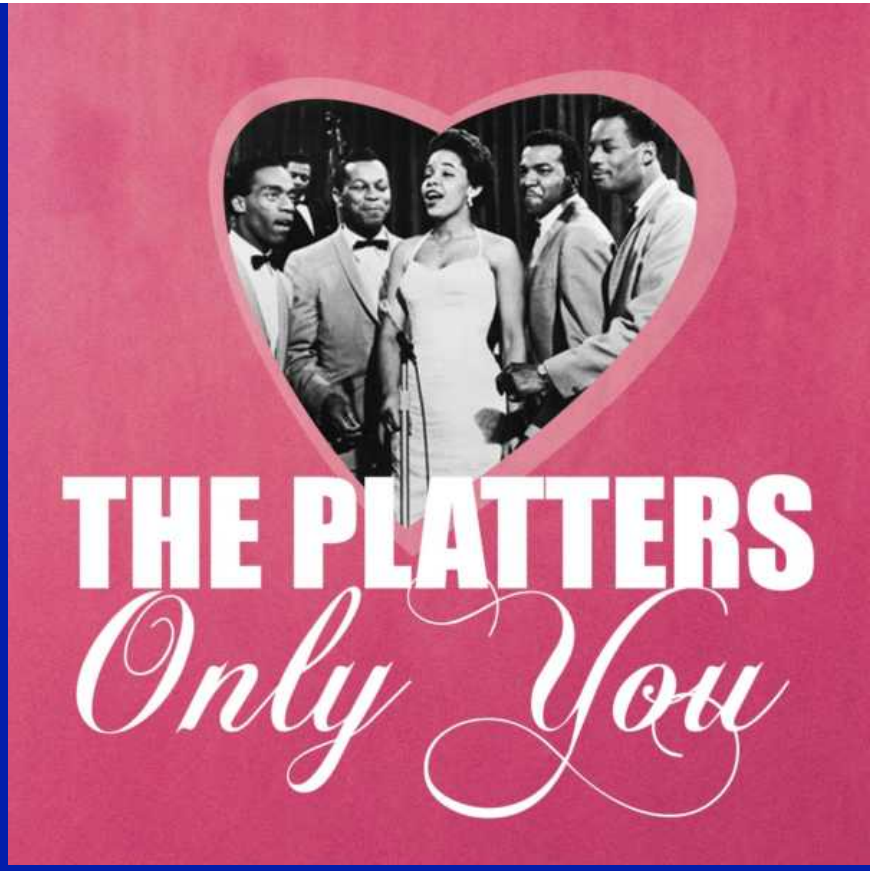
http://www.college-de-france.fr/site/antoine-georges/index.htm

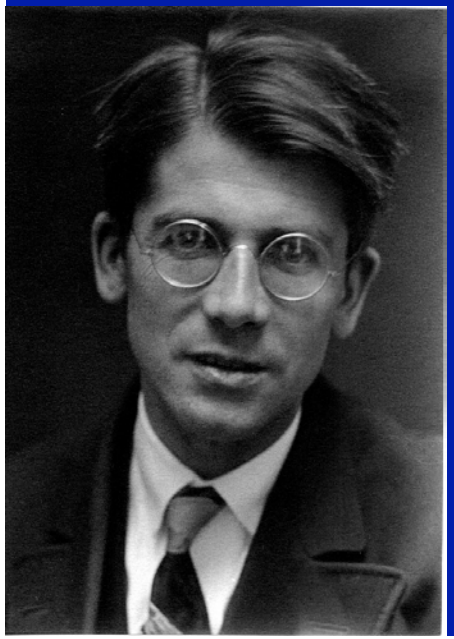
In order to receive weekly email-announcements,
pls send me a mail: antoine.georges@college-de-france.fr

PART I :
``HUNDNESS''
Hund's rule correlated materials

The Platters said:

« Only U can do
make all this world
seem right… »





… Take-home message of these lectures:

« Not only U, also J_H » !

Friedrich Hund
1896-1997

Main message :

A large class of materials

(including: transition-metal oxides of the 4d series and iron pnictides)

are best characterized as

`Hund's metals'

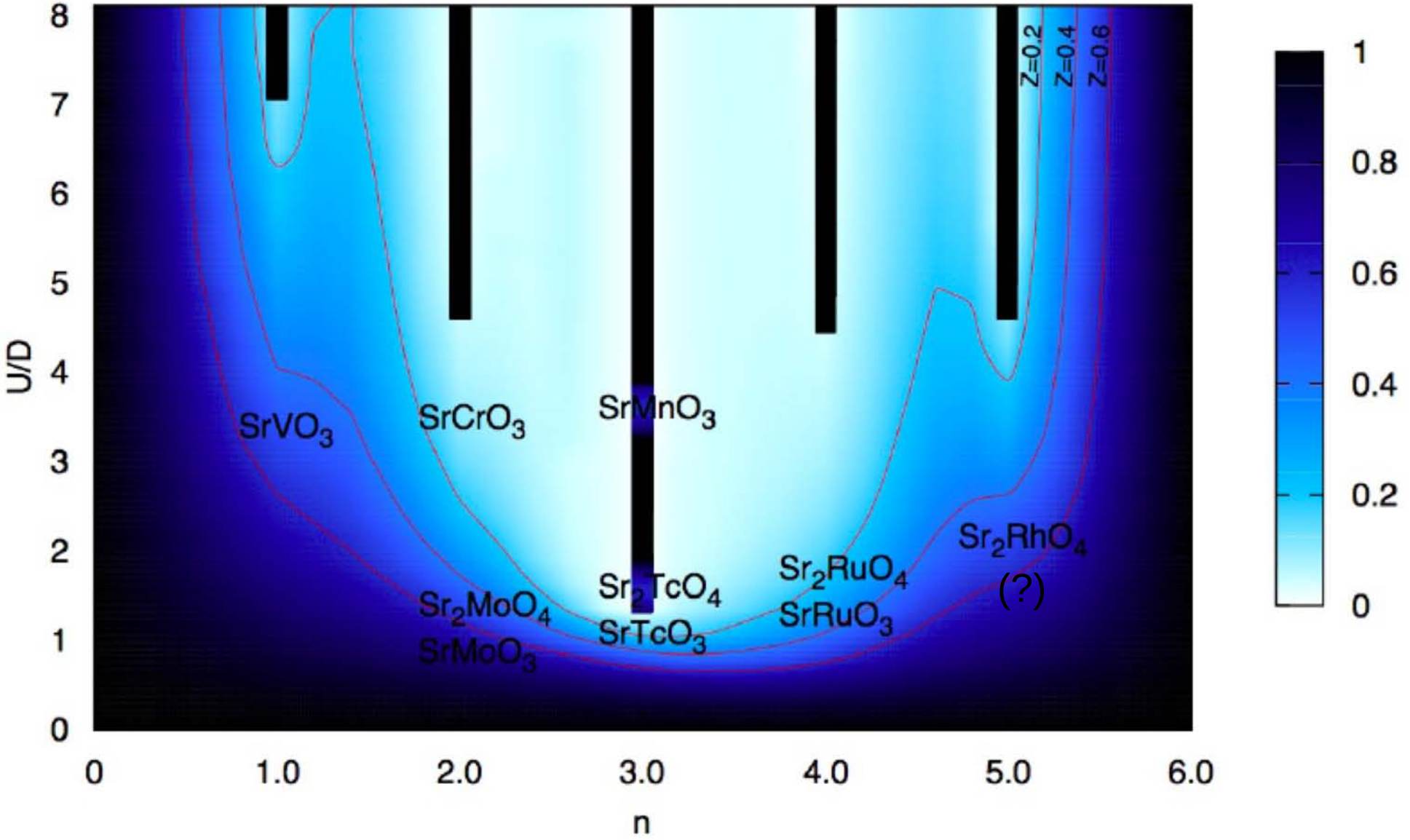
They are not close to a Mott transition

but still display strong correlations

because of the Hund's rule coupling

Hundness: overview

(plot to be discussed in details in lecture 3 or 4)



Two key players/collaborators:

Jernej Mravlje
(Collège de France,
& École Polytechnique
and Joszef Stefan Institute
Ljubljana, Slovenia)

Luca de' Medici
(Laboratoire de Physique
des Solides, Université
Paris-Sud, Orsay)

→ ***Review article in preparation***
(Annual Reviews)

Thanks also to :

S.Biermann, X.Deng, M.Ferrero,

L.Pourovskii, L. Vaugier

O.Parcollet (CEA-Saclay)

K.Haule, G.Kotliar (Rutgers)

A.J. Millis (Columbia & École Polytechnique)

D. van der Marel (Genève)

J. Kunes (Praha)

For collaborations and discussions

Two key recent papers:

Coherence–incoherence crossover in the normal state of iron oxypnictides and importance of Hund's rule coupling

K Haule[1] and G Kotliar
Department of Physics, Rutgers University, Piscataway, NJ 08854, USA
E-mail: haule@physics.rutgers.edu

New Journal of Physics **11** (2009) 025021 (13pp)
Received 16 December 2008
Published 27 February 2009

PRL **101**, 166405 (2008) PHYSICAL REVIEW LETTERS week ending 17 OCTOBER 2008

Spin Freezing Transition and Non-Fermi-Liquid Self-Energy in a Three-Orbital Model

Philipp Werner,[1] Emanuel Gull,[2] Matthias Troyer,[2] and Andrew J. Millis[1]
[1]*Columbia University, 538 West, 120th Street, New York, New York 10027, USA*
[2]*Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*
(Received 16 June 2008; published 16 October 2008)

And in the Paris area…

PHYSICAL REVIEW B 83, 205112 (2011)

Hund's coupling and its key role in tuning multiorbital correlations

Luca de' Medici
Laboratoire de Physique des Solides, UMR8502 CNRS-Universite Paris-Sud, Orsay, France

PRL 106, 096401 (2011) PHYSICAL REVIEW LETTERS week ending 4 MARCH 2011

Coherence-Incoherence Crossover and the Mass-Renormalization Puzzles in Sr_2RuO_4

Jernej Mravlje,[1,2] Markus Aichhorn,[3,1] Takashi Miyake,[4,5] Kristjan Haule,[6] Gabriel Kotliar,[6] and Antoine Georges[1,7,5]

PRL 107, 256401 (2011) PHYSICAL REVIEW LETTERS week ending 16 DECEMBER 2011

Janus-Faced Influence of Hund's Rule Coupling in Strongly Correlated Materials

Luca de' Medici,[1] Jernej Mravlje,[2,3,4] and Antoine Georges[2,4,5,6]

nature physics

ARTICLES

PUBLISHED ONLINE: 4 MARCH 2012 | DOI:10.1038/NPHYS2250

Satellites and large doping and temperature dependence of electronic properties in hole-doped $BaFe_2As_2$

Philipp Werner[1,2]*, Michele Casula[3], Takashi Miyake[4,5,6], Ferdi Aryasetiawan[7,8], Andrew J. Millis[9] and Silke Biermann[5,10]

PHYSICAL REVIEW LETTERS

arxiv.:1108.1168

Origin of the High Néel Temperature in $SrTcO_3$

Jernej Mravlje,[1,2,3] Markus Aichhorn,[4] and Antoine Georges[2,1,5]

OUTLINE of lectures (Part I)

- Intra-atomic exchange and Hund's rule coupling
- Multi-orbital Hamiltonians
- Effective atomic U and energetic of the Mott gap
- Hund - impeded Kondo screening
- The `Janus-faced' influence of Hund's coupling
- Global view on 3d and especially 4d oxides
- Ruthenates [→ seminar Baumberger]
- Crystal-field effects, HS/LS transitions
- Hund's coupling as a band decoupler, OSMTs
- Are iron-based superconductors`Hund's metals' ?

[→ Seminars Biermann, de'Medici]

1. Hund's rules

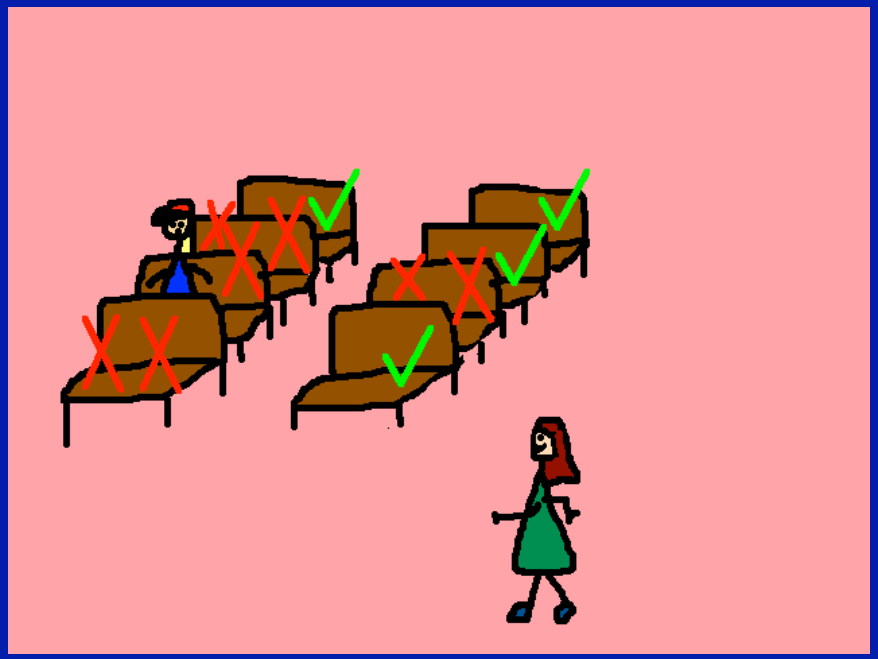
(1925 – Z.Phys on atomic spectra of transition metals)

N electrons in a M=2l+1-fold degenerate shell

- Maximize S [= N/2 N<M ; = M-N/2 N>M]
- Given S, maximize L
- Given (S,L) lowest J=|L-S| if N<M (less than ½ filling) , highest J=L+S if N>M

``The bus-seat rule”

For example a d-shell with 3 electrons (less than half-filling corresponding to 5 electrons) will have $\uparrow, \uparrow, \uparrow, 0, 0$ and with 7 electrons $\uparrow\downarrow, \uparrow\downarrow, \uparrow, \uparrow, \uparrow$. These rules are sometimes referred to as the ‘bus-seat’ rule: singly-occupied spots are filled first, then double occupancies are created when singly-occupied spots are no longer available.



Physical origin: exchange (QM)

- Minimize cost of inter-electron Coulomb repulsion
- Ex: For 2 electrons, S=1 forces an antisymmetric orbital wave-function (`electrons further apart'), in contrast to S=0
- Actually, screening of nucleus-electron interaction (smaller in singly occupied orbitals) actually plays a key role (cf. Levine, Quantum Chemistry) in lowering the energy of singly-occupied states
- 3rd rule due to spin-orbit

Examples: isolated atoms/ions

- Mn^{2+} (as in MnO) half-filled shell $[Ar]3d^5$

→ Largest spin S=5/2

→ Quenched angular momentum L=0

→ J=S=5/2 magnetism entirely spin

n	$l_z = 2$	1	0	-1	-2	S	L	J
1	↑					1/2	2	3/2
2	↑	↑				1	3	2
3	↑	↑	↑			3/2	3	3/2
4	↑	↑	↑	↑		2	2	0
5	↑	↑	↑	↑	↑	5/2	0	5/2
6	↑↓	↑	↑	↑	↑	2	2	4
7	↑↓	↑↓	↑	↑	↑	3/2	3	9/2
8	↑↓	↑↓	↑↓	↑	↑	1	3	4
9	↑↓	↑↓	↑↓	↑↓	↑	1/2	2	5/2
10	↑↓	↑↓	↑↓	↑↓	↑↓	0	0	0

Atomic config.
Transition elements

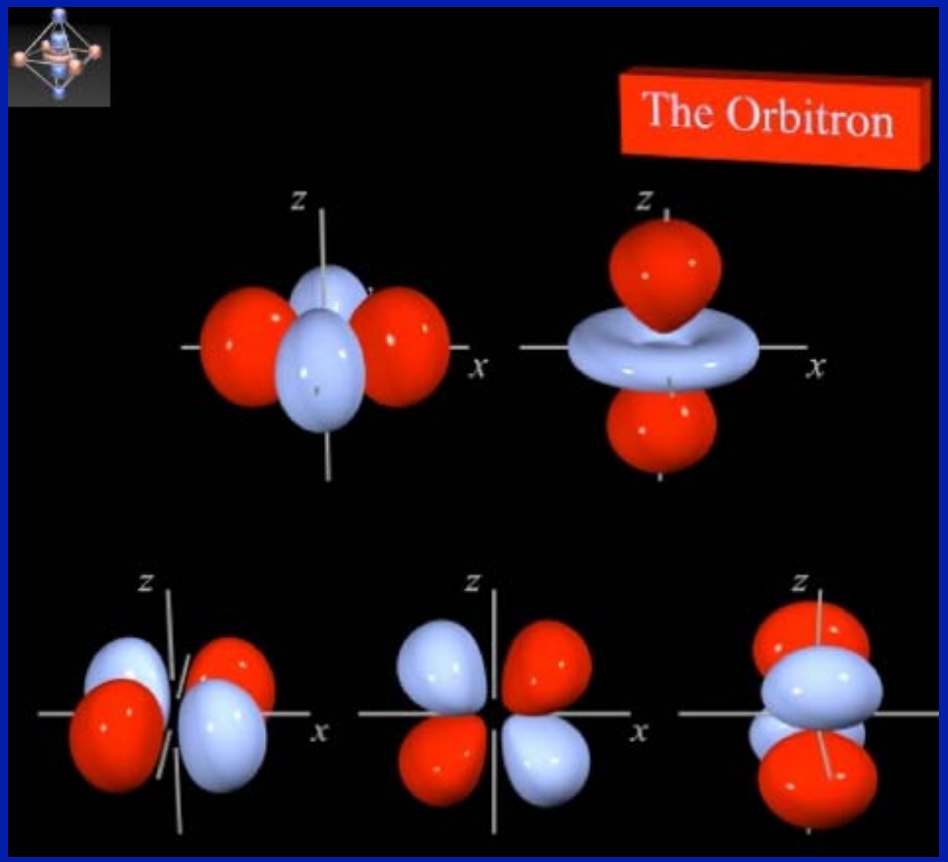
2. In the solid-state: hamiltonian of a multi-orbital shell

Simple case first:
well-isolated degenerate t2g triplet
in a cubic oxide
with octahedral environment of the TM atom

Cf. Lecture 5, 2009-2010 (slides on website)

Orbitals: from the isolated atom to the solid - crystal-field splitting – (Bethe, van Vleck)

Cubic-symmetry adapted 3d-orbitals:



3d orbitals are quite localized:
- No nodes in radial part
- Large centrifugal barrier $l(l+1)/r^2$

$$d_{x^2-y^2}\ ,\ d_{3z^2-r^2}$$

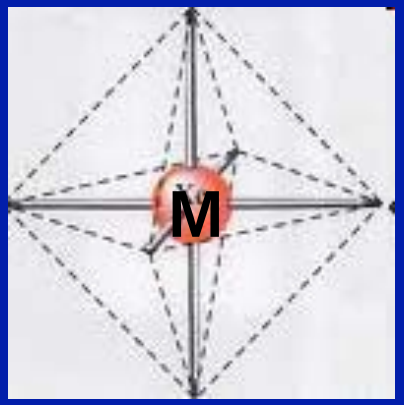
→ The e_g doublet

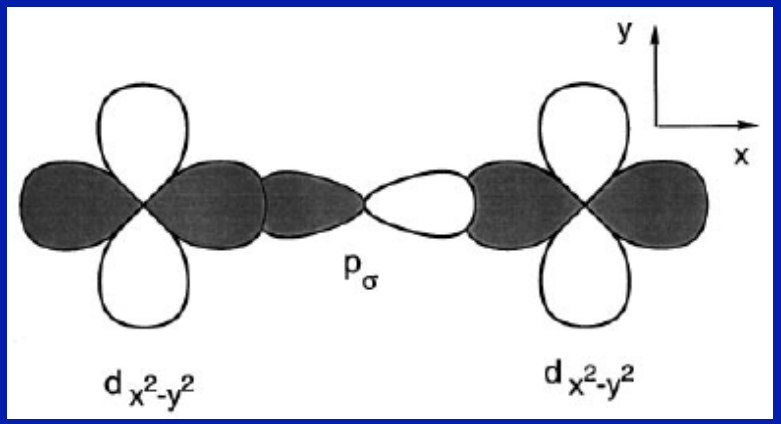
$$d_{xy}\ ,\ d_{xz}\ ,\ d_{yz}$$

→ The t_{2g} triplet

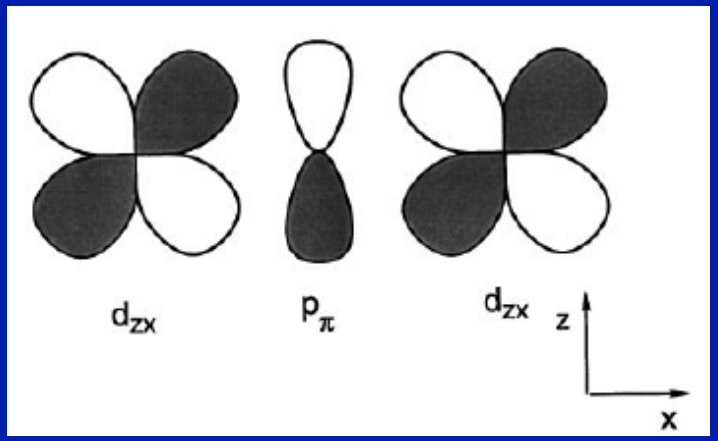
http://winter.group.shef.ac.uk/orbitron

Crystal-field splitting in octahedral environment :





eg orbitals point towards oxygen atoms(sigma-bonding)
→feel larger Coulomb potential
→ pushed to higher energy



t2g orbitals point away from oxygen atoms(pi-bonding)
→feel smaller Coulomb potential
→ lower energy than eg

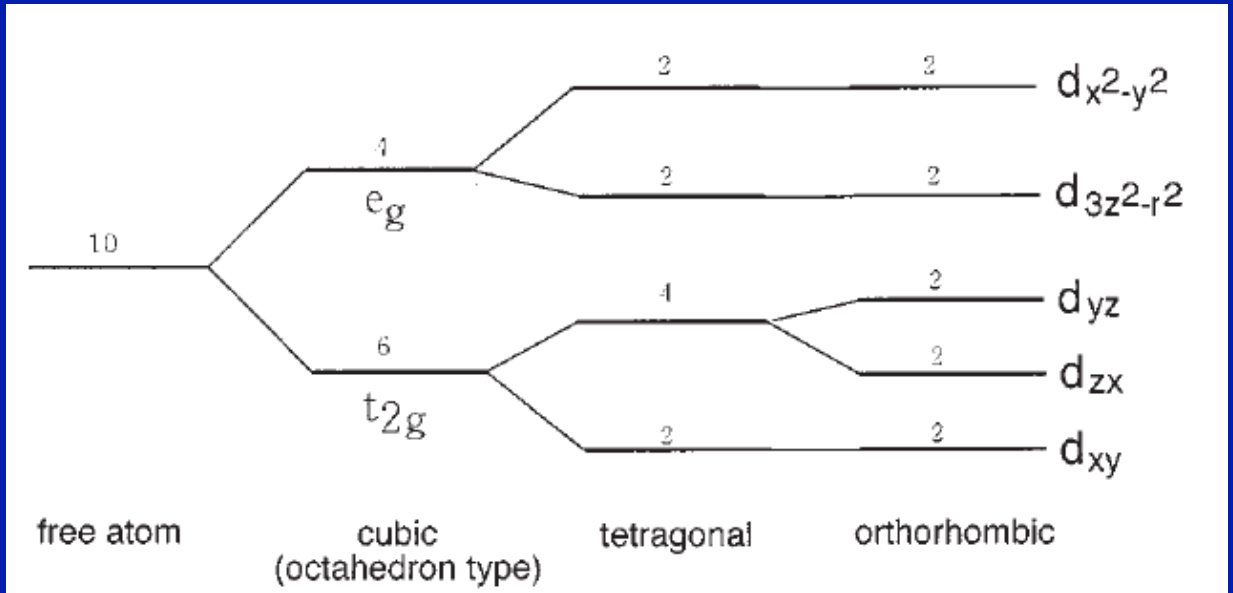


FIG. 2. Crystal-field splitting of $3d$ orbitals under cubic, tetragonal, and orthorhombic symmetries. The numbers cited near the levels are the degeneracy including spins.

Lowering further the crystal symmetry (distort from cubic)
Induces additional lifting of degeneracy

Tetrahedral environment (MO_4):
eg has lower energy, t2g higher

For a t_{2g} triplet, only 3 independent Coulomb integrals:

$$U = \int d\mathbf{r}d\mathbf{r}' \, |\phi_m(\mathbf{r})|^2 \, V_c(\mathbf{r},\mathbf{r}') \, |\phi_m(\mathbf{r}')|^2$$

$$U' = \int d\mathbf{r}d\mathbf{r}' \, |\phi_m(\mathbf{r})|^2 \, V_c(\mathbf{r},\mathbf{r}') \, |\phi_{m'}(\mathbf{r}')|^2$$

$$J = \int d\mathbf{r}d\mathbf{r}' \, \phi_m(\mathbf{r})\phi_{m'}(\mathbf{r}) \, V_c(\mathbf{r},\mathbf{r}') \, \phi_m(\mathbf{r}')\phi_{m'}(\mathbf{r}')$$

Indeed:
J=J' (real wave-functions)
$U_{m'mmm}$=0 by symmetry

Vc: SCREENED Coulomb interaction in the solid

Hence, Kanamori hamiltonian:

[J.Kanamori, Prog. Theor. Phys. 30 (1963) 275]

$$H_{\mathrm{K}} = U \sum_{m} \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U' \sum_{m\neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U'-J) \sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma} +$$
$$-J \sum_{m\neq m'} d^{+}_{m\uparrow} d_{m\downarrow}\, d^{+}_{m'\downarrow} d_{m'\uparrow} + J \sum_{m\neq m'} d^{+}_{m\uparrow} d^{+}_{m\downarrow}\, d_{m'\downarrow} d_{m'\uparrow}$$

is EXACT for a t_{2g} shell

Useful reference: Sugano, Tanabe & Kamimura,
Multiplets of transition-metal ions in crystals
Academic Press, 1970

Generalized Kanamori (3 orbitals)

$$H_{\rm GK} = U\sum_m \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U'\sum_{m\neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U'-J)\sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma} +$$
$$-J_X\sum_{m\neq m'} d^+_{m\uparrow}d_{m\downarrow}\,d^+_{m'\downarrow}d_{m'\uparrow} + J_P\sum_{m\neq m'} d^+_{m\uparrow}d^+_{m\downarrow}\,d_{m'\downarrow}d_{m'\uparrow}$$

Defining the total charge, spin and orbital isospin generators ($\vec{\tau}$ are the Pauli matrices):

$$\hat{N} = \sum_{m\sigma}\hat{n}_{m\sigma}\ ,\ \ \vec{S} = \frac{1}{2}\sum_m\sum_{\sigma\sigma'} d^\dagger_{m\sigma}\vec{\tau}_{\sigma\sigma'}d_{m\sigma'}\ ,\ \ L_m = i\sum_{m'm''}\sum_\sigma \epsilon_{mm'm''}d^\dagger_{m'\sigma}d_{m''\sigma},$$

the t_{2g} Kanamori hamiltonian (2) can be rewritten as:

$$\tfrac{1}{4}(3U'-U)\hat{N}(\hat{N}-1) + (U'-U)\vec{S}^2 + \tfrac{1}{2}(U'-U+J)\vec{L}^2 + (\tfrac{7}{4}U - \tfrac{7}{4}U' - J)\hat{N}$$
$$+(U'-U+2J)\sum_{m\neq m'} d^+_{m\uparrow}d^+_{m\downarrow}\,d_{m'\downarrow}d_{m'\uparrow}$$

Rotationally invariant cases:

1) U' = U-2J ; J_X=J_P=J

$$H_{t_{2g}} = (U-3J)\frac{\hat{N}(\hat{N}-1)}{2} - 2J\,\vec{S}^2 - \frac{J}{2}\vec{L}^2 + \frac{5}{2}J\,\hat{N}$$

Appropriate for a t_{2g} shell, assuming furthermore spherical symmetry of the interactions. Angular momentum only Partially quenched from l=2 to l=1.

2) U' = U-J ; J_X=J ; J_P=0

A hamiltonian first introduced by Dworin and Narath [PRL 25, 1287 (1970)] In the context of (Kondo) magnetic impurities:

$$H_{\mathrm{DN}} = \left(U - \frac{3J}{2}\right)\frac{\hat{N}(\hat{N}-1)}{2} - J\,\vec{S}^2 + \mathrm{const.}$$

Spectrum of atomic t_{2g} hamiltonian with U'=U-2J

N	S	L	Degeneracy $= (2S+1)(2L+1)$	Energy
0,[6]	0	0	**1**	0
1,[5]	1/2	1	**6**	$-5J/2$,$[10\mathcal{U}-5J/2]$
2,[4]	1	1	**9**	$\mathcal{U}-5J$,$[6\mathcal{U}-5J]$
2,[4]	0	2	5	$\mathcal{U}-3J$,$[6\mathcal{U}-3J]$
2,[4]	0	0	1	$\mathcal{U}$,$[6\mathcal{U}]$
3	3/2	0	**4**	$3\mathcal{U}-15J/2$
3	1/2	2	10	$3\mathcal{U}-9J/2$
3	1/2	1	6	$3\mathcal{U}-5J/2$

Table 1: Eigenstates and eigenvalues of the t_{2g} Hamiltonian $\mathcal{U}\hat{N}(\hat{N}-1)/2 - 2J\vec{S}^2 - J\vec{T}^2/2$ in the atomic limit ($\mathcal{U} \equiv U - 3J$). The boxed numbers identifies the ground-state multiplet and its degeneracy, for $J > 0$.

- Hund's rule ground-state in each particle-number sector
- Symmetry broken by J from SU(6) to U(1)c×SU(2)s×SO(3)o
- → Degeneracies lifted by J

2-orbital case: e_g doublet

Again, Kanamori form is exact.
But this time U'=U-2J is dictated by cubic symmetry

Generators of orbital `isospin' (T=1/2)

$$\vec{T} = \frac{1}{2} \sum_{\sigma} d^{+}_{m\sigma} \vec{\tau}_{mm'} d_{m'\sigma}$$

THEN :

$$H_{e_g} = (U - J)\frac{\hat{N}(\hat{N}-1)}{2} + 2J(T_x^2 + T_z^2) - J\hat{N}$$

No symmetry left !
Indeed, angular momentum FULLY quenched !

2-orbitals: general case

$$\frac{1}{4}(U+U'-J+J_X)(\hat{N}-2)^2+J_X\vec{T}^2+$$

$$+(U-U'-J_X)T_z^2+(J_X-J)S_z^2+J_P(T_x^2-T_y^2)$$

Hence 2 special cases:

1) $J_P=0$, $J_X=J$, $U'=U-J$

→ Again, Dworin-Narath hamiltonian (see above)

2) $J_P=0$, $J_X=J$, $U'=U$

Hamiltonian introduced by Caroli, Lederer, Saint-James

PRL 23 (1969) 700; see also De Leo and Fabrizio PRB 69 (2004) 245114

$$\frac{U}{2}(\hat{N}-2)^2+J(\vec{T}^2-T_z^2)$$

t_{2g} , spherical symmetry approximation :

U, U', J expressed in terms of Slater (or Racah) parameters:

$$
\begin{aligned}
U &= F^0 + \frac{4}{49}F^2 + \frac{4}{49}F^4 = A + 4B + 3C \\
U' &= F^0 - \frac{2}{49}F^2 - \frac{4}{441}F^4 = A - 2B + C = U - 2J \\
J &= \frac{3}{49}F^2 + \frac{20}{441}F^4 = 3B + C
\end{aligned}
$$

Beware of notations !

Often , for full 3d shell: $U_d=F^0$, $J_H=(F^2+F^4)/14$, $14C_d=9F^2/7-5F^4/7$

Thus, in t_{2g} notations:

$$J = \frac{5}{7} J_H + \frac{1}{9} C_d \simeq 0.77\, J_H$$

Similar expressions for e_g:

$$U = U' + 2J = F^0 + \frac{4}{49}F^2 + \frac{4}{49}F^4 = A + 4B + 3C$$

$$J = \frac{3}{49}F^2 + \frac{5}{147}F^4 = 4B + C$$

RECALL: Lecture 8, 2009-2010 → see slides for more details

Giulio Racah's pioneering work:

Giulio (**Yoel**) **Racah** (Hebrew: גוליו (יואל) רקח, 1909-1965)

Theory of Complex Spectra. I

GIULIO RACAH
The Hebrew University, Jerusalem, Palestine

(Received November 14, 1941)

This paper gives a closed formula which entirely replaces for the two-electron spectra the previous lengthy calculations with the diagonal-sum method. Applications are also made to some configurations with three or more electrons and to the p'' configurations of the nuclei.

Theory of Complex Spectra. IV

GIULIO RACAH
The Hebrew University, Jerusalem, Israel

(Received February 7, 1949)

Isolated atom:

$$V_c(\mathbf{r}-\mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$$

$$\chi_m(\mathbf{r}) = R_{nl}(\mathbf{r})\, Y_{lm}(\theta,\phi)$$

Separate radial and angular variables:

$$V_c(\mathbf{r}-\mathbf{r}') = \sum_{k=0}^{\infty} \frac{4\pi}{2k+1} \frac{r_<^k}{r_>^{k+1}} \sum_{q=-k}^{+k} Y_{kq}(\theta,\phi) Y_{kq}^*(\theta',\phi')$$

$r_>$,$r_<$: largest/smallest of r,r'

This yields:

$$U^{\mathrm{at}}_{m_1 m_2 m_3 m_4} = \sum_k \omega_k(m_1,m_2,m_3,m_4)\, F^k$$

In which:

-The F's are Slater integrals involving radial wave-functions

- The ω's are entirely known numbers (Racah-Wigner)

- The sum involves only F0,F2,F4 for d-shell , F0,F2,F4,F6 for f-shell

$$F^k = e^2 \int_0^\infty r^2 dr \int_0^\infty r'^2 dr' \, \frac{r_<^k}{r_>^{k+1}} \, R_{nl}^2(r) R_{nl}^2(r')$$

$$\omega_k(m_1, m_2, m_3, m_4) = \frac{4\pi}{2k+1} \sum_{q=-k}^{+k} \langle Y_{lm_1} | Y_{kq} | Y_{lm_3} \rangle \langle Y_{lm_2} | Y_{kq}^* | Y_{lm_4} \rangle$$

$$\langle Y_{lm} | Y_{kq} | Y_{lm'} \rangle \equiv \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \, Y_{lm}^*(\theta,\phi) Y_{kq}(\theta,\phi) Y_{lm'}(\theta,\phi)$$

$$= (2l+1)\sqrt{\frac{2k+1}{4\pi}} \begin{pmatrix} l & k & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & k & l \\ -m & q & m' \end{pmatrix}$$

Wigner-
-Racah
3j symbols

If hydrogen atom wave functions are used:

$$F^4/F^2 \simeq 0.625 \;\; (3d - shell)$$

$$F^4/F^2 \simeq 451/675 \simeq\simeq 0.67 \;\; , \;\; F^6/F^2 \simeq 1001/2025 \simeq 0.49$$

(4f-shell)

Orders of magnitude

Determination of screened interaction
→ an active research topic till today, especially from first-principles perspective (cf. S.Biermann's seminar, c-RPA).

Pioneering work (experimental/empirical):
D.Van der Marel and G.Sawatzky PRB 37 (1988) 10674 [VdMS]

Because it involves only F^2, F^4 – not F^0 – reduction of J_H
In the solid-state only 20-30%
In contrast: F^0 = 10-25 eV → F^0 = 3-9 eV

VdMS estimate: $J_H = 0.59 + 0.075(Z-21)\,eV$
while Hartree-Fock unscreened: $J_H^{at} = 0.81 + 0.080(Z-21)\,eV$

Hence, J_H ~ 0.6 – 1.2 eV along 3d series ($J(t_{2g})$ ~ 0.77 J_H)

Also, combining these various estimates: J/U ~ 0.11-0.15 for t_{2g}

TABLE IV. Interpolation formulas for F^0, J, and C as a function of atomic number Z.

Row	Parameter	Hartree-Fock	Empirical
$3d$	F^0	$15.31+1.50(Z-21)$	$1.5+0.21(Z-21)$
	J	$0.81+0.080(Z-21)$	$0.59+0.075(Z-21)$
	C	$0.52J$	$0.51J$
$4d$	J	$0.59+0.056(Z-39)$	
	C	$0.50J$	
$5d$	J	$0.60+0.053(Z-71)$	
	C	$0.52J$	
$4f$	F^0	$23.8+0.93(Z-57)$	$6.7+0.033(Z-57)$
	J	$0.90+0.036Z-57)$	$0.69+0.014(Z-57)$
	C	$0.50J$	$0.45J$
$5f$	J	$0.66+0.035(Z-89)$	$0.33+0.070(Z-89)$
	C	$0.41J$	$0.41J$

D.Van der Marel and G.Sawatzky PRB 37 (1988) 10674 [VdMS]

3. Energetic of the Mott gap – a) the atom

cf. VdMS PRB 37 (1998) 10674 ; L. de' Medici PRB 83 (2011) 205112

$$\Delta_g = E_0(N+1) + E_0(N-1) - 2E_0(N)$$

Hund's rule ground-state E_0 not affected by spin-flip and pair-hopping terms.

N<M (N>M) : Max spin state only U'-J = U-3J matters

$$\Delta_g^{at} \equiv U_{eff} = U - 3J$$

→ Atomic gap and U_{eff} REDUCED by J for N<M, N>M

N = M (half-filled shell) :

Excited state with M+1 electrons has higher energy: $|\uparrow\downarrow,\uparrow,\uparrow\rangle$

$$E_0(M+1) = (U'-J)\times M(M-1)/2 + U\times 1 + U'\times(M-1) = (U'-J)M(M+1)/2 + (U-U'+MJ)$$

$$\Delta_g^{at} \equiv U_{eff} = (U'-J) + (U-U'+MJ) = U + (M-1)J$$

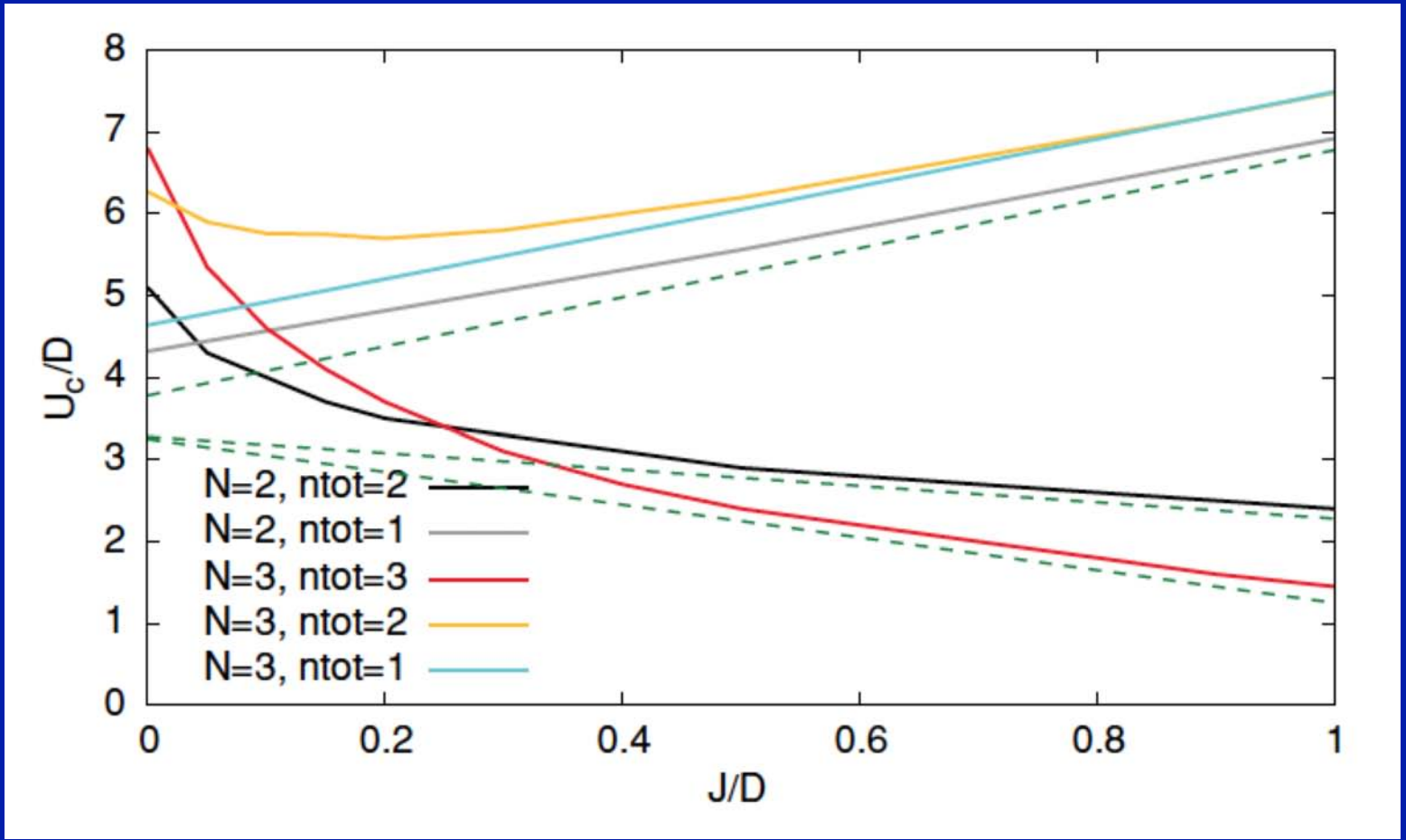
→ Atomic gap gap and U_{eff} INCREASED by J for N<M, N>M

Conclusion remains for d-shell, full hamiltonian:

	Effective Coulomb interaction U_{eff} for Hund's rule ground-state				
	Full Hamiltonian		Simple	Kanamori	Kanamori mean field
d^1	$F^0-\frac{8}{49}F^2-\frac{9}{441}F^4$	$U_0- J_H-C$	$U_0- J_H$	U'- J	U'- J
d^2	$F^0+\frac{1}{49}F^2-\frac{54}{441}F^4$	$U_0- J_H+C$	$U_0- J_H$	U'- J	U'- J
d^3	$F^0+\frac{1}{49}F^2-\frac{54}{441}F^4$	$U_0- J_H+C$	$U_0- J_H$	U'- J	U'- J
d^4	$F^0-\frac{8}{49}F^2-\frac{9}{441}F^4$	$U_0- J_H-C$	$U_0- J_H$	U'- J	U'- J
d^5	$F^0+\frac{14}{49}F^2+\frac{126}{441}F^4$	U_0+4J_H	U_0+4J_H	U+4J	U+4J
d^6	$F^0-\frac{8}{49}F^2-\frac{9}{441}F^4$	$U_0- J_H-C$	$U_0- J_H$	U'- J	U'- J
d^7	$F^0+\frac{1}{49}F^2-\frac{54}{441}F^4$	$U_0- J_H+C$	$U_0- J_H$	U'- J	U'- J
d^8	$F^0+\frac{1}{49}F^2-\frac{54}{441}F^4$	$U_0- J_H+C$	$U_0- J_H$	U'- J	U'- J
d^9	$F^0-\frac{8}{49}F^2-\frac{9}{441}F^4$	$U_0- J_H-C$	$U_0- J_H$	U'- J	U'- J

VdMS (1988) ; M.Haverkort PhD (2005)

Consequences for Mott gap in the solid:



L. de' Medici, PRB 83, 205112 (2011)
[values above from `slave-spin' method]

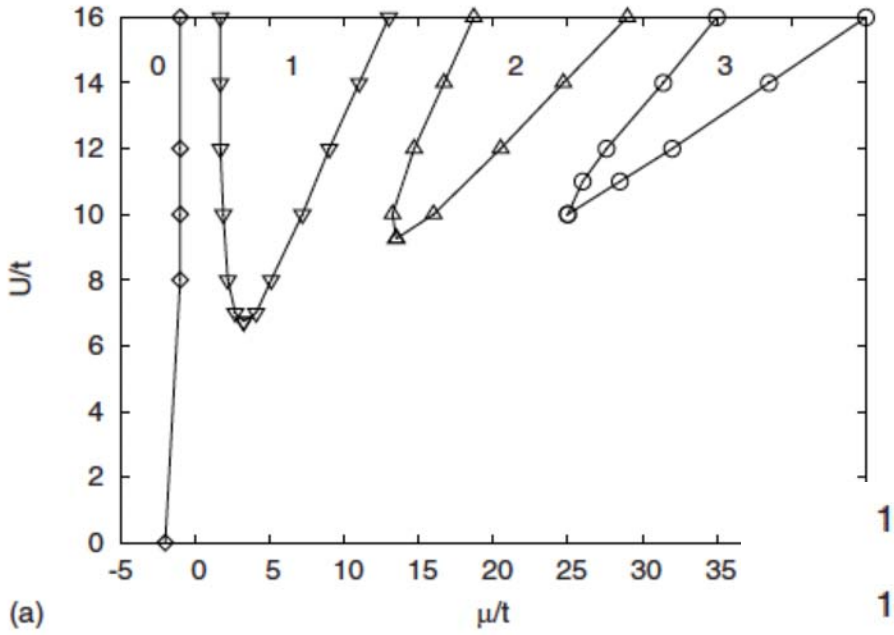
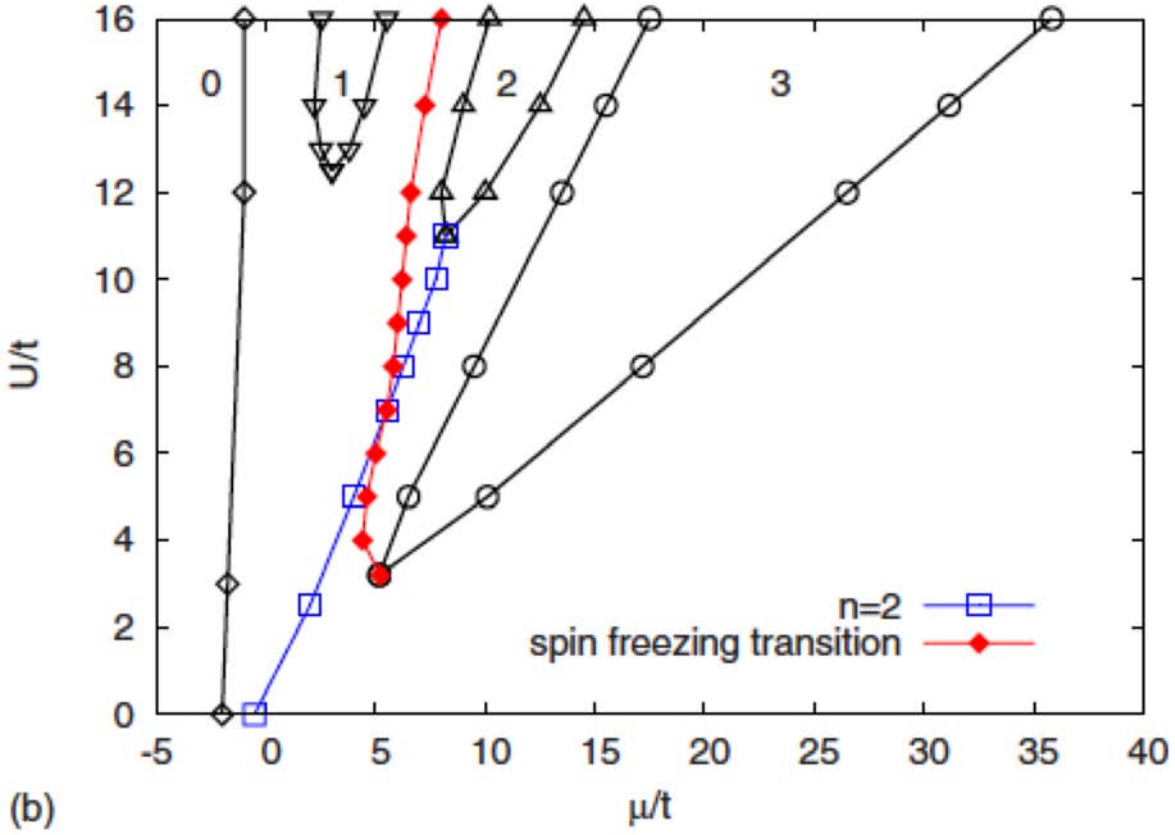


FIG. 2. (Color online) Metal-insulator phase diagram presented in the space of chemical potential μ and interaction strength U (measured in units of the quarter bandwidth t) for $\Delta_a=0$ and $\beta t=50$ at Hund coupling $J=0$ (upper panel) and $J=U/6$ (lower panel). Orbital and spin symmetries were enforced in the calculation. Error bars are on the order of the symbol size. The numerals in the lobes indicate the electron concentration per site in the insulating phases. In the lower panel the solid diamonds indicate the boundary of a spin freezing transition discussed in Ref. 28, while the line with squares plots the locus of μ and U corresponding to the density $n=2$.

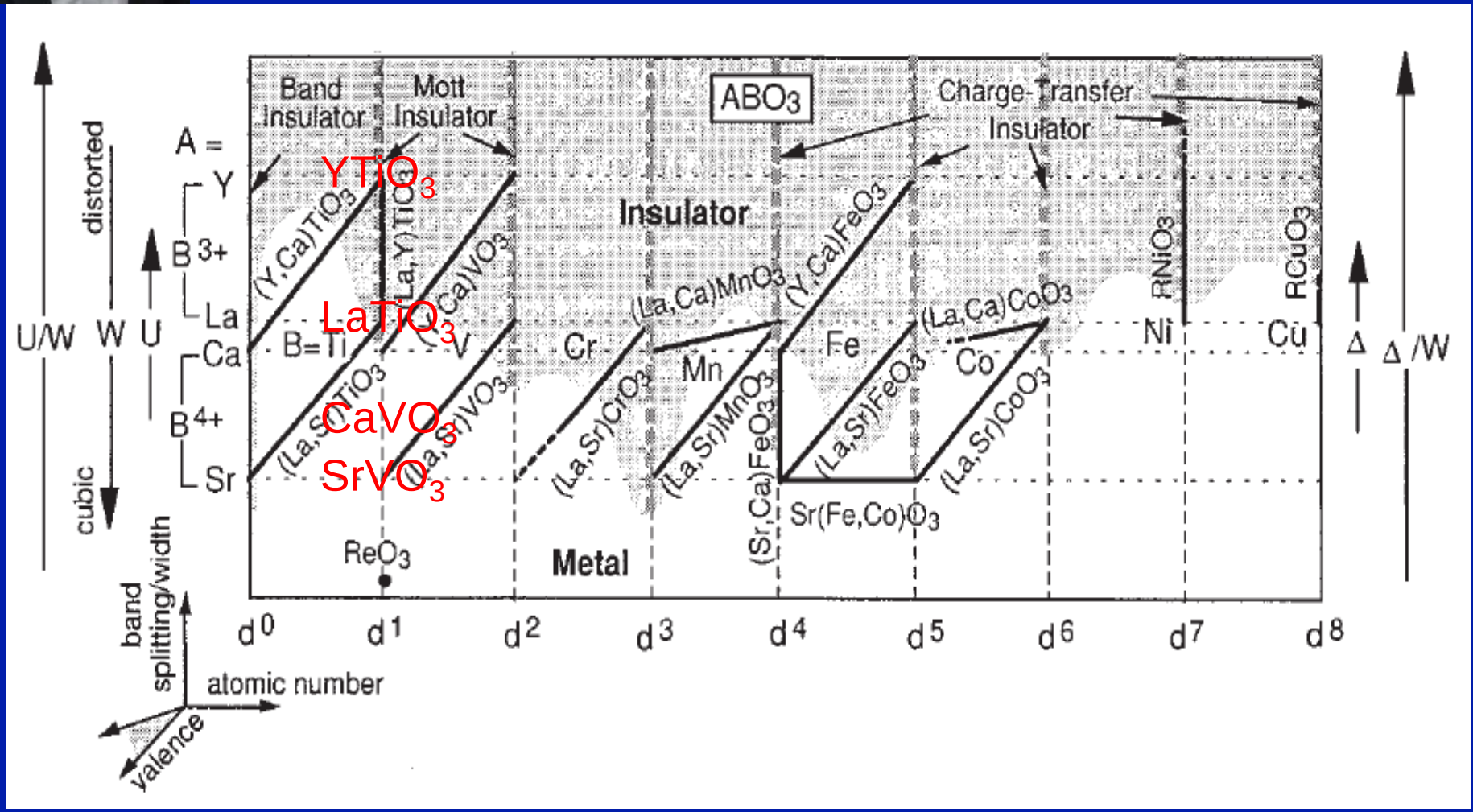
Contrast J=0 to finite J

Werner, Gull & Millis
PRB 79 (2009) 115119

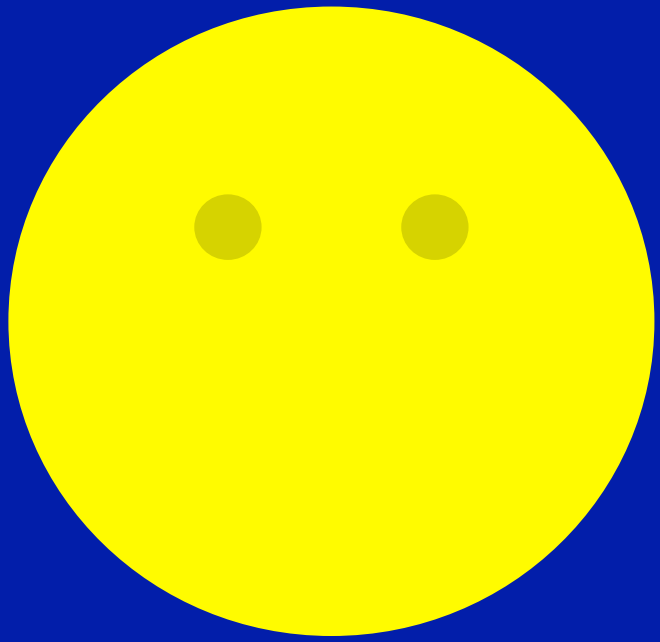


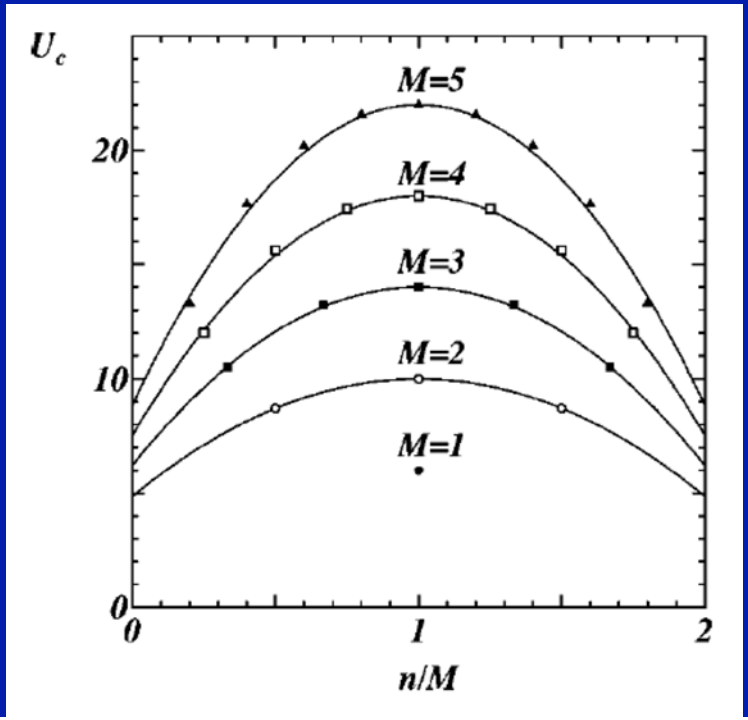
Cf. ``Atsushi Fujimori's map of RMO_3 perovskites''

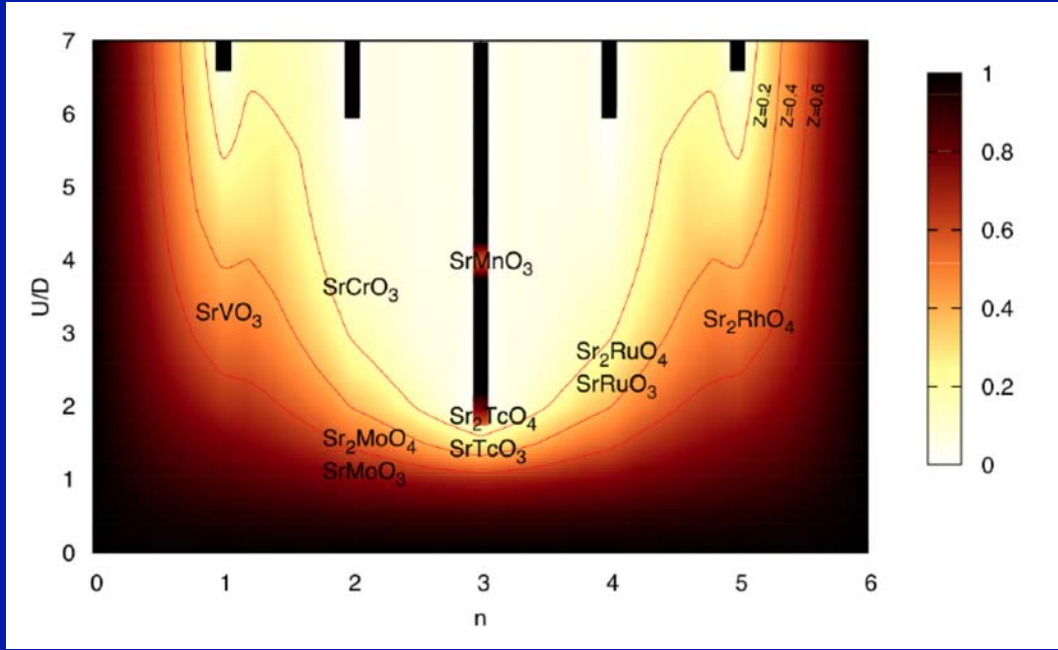
J.Phys Chem Sol. 53 (1992) 1595

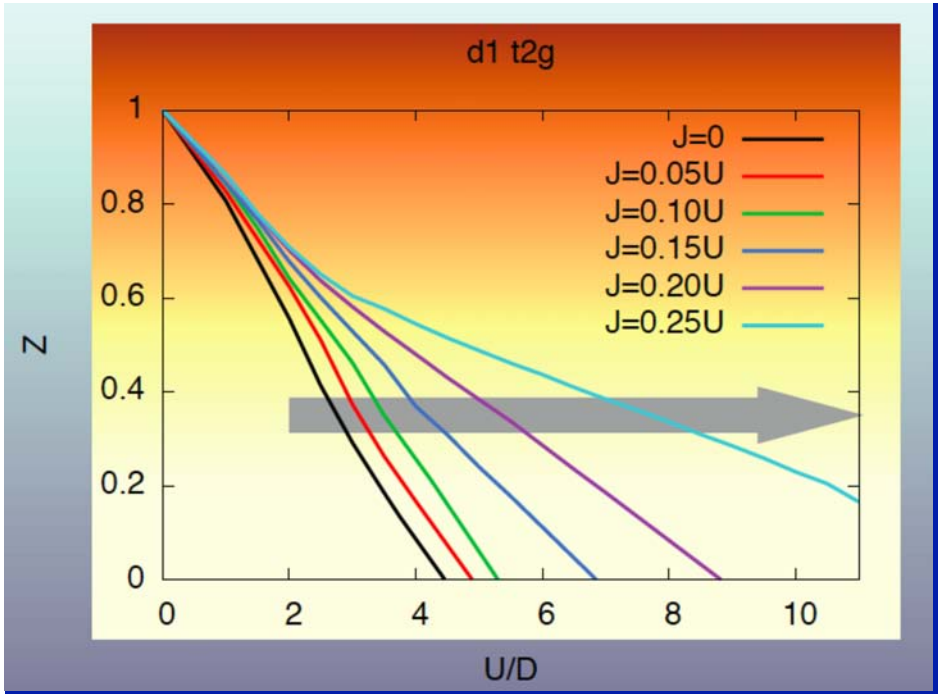


Finte J is crucial to make contact with real-life !

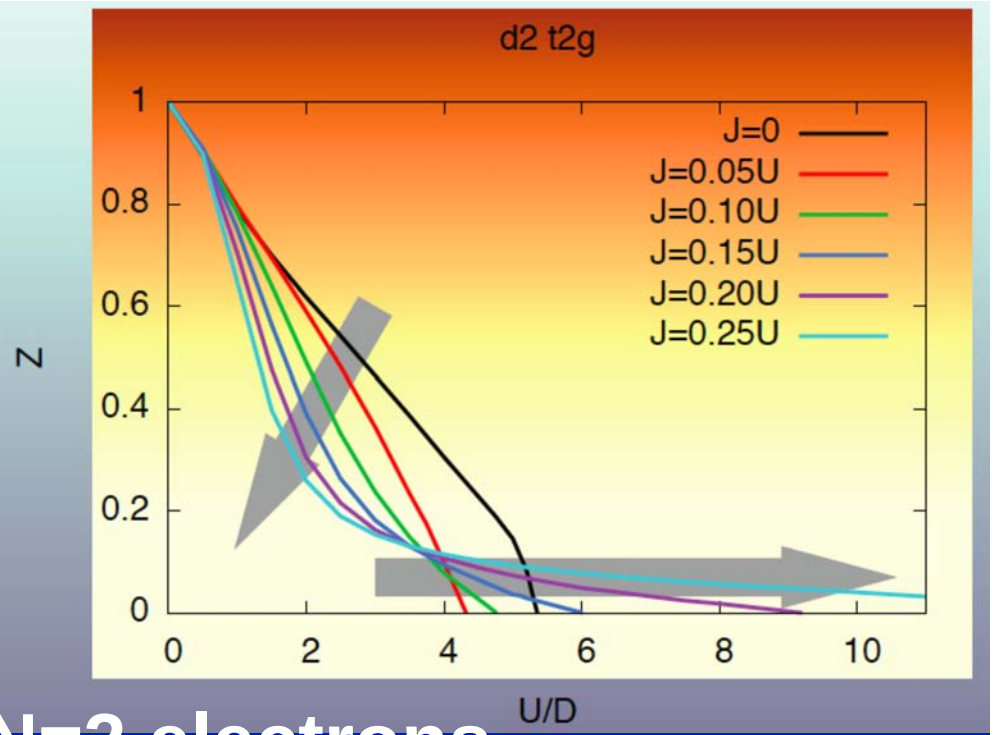



U_c
M=5
M=4
M=3
M=2
M=1
20
10
0
0
1
2
n/M


U/D
n
SrVO3
SrCrO3
SrMnO3
Sr2MoO4
SrMoO3
Sr2TcO4
SrTcO3
Sr2RuO4
SrRuO3
Sr2RhO4
Z=0.2
Z=0.4
Z=0.6
1
0.8
0.6
0.4
0.2
0

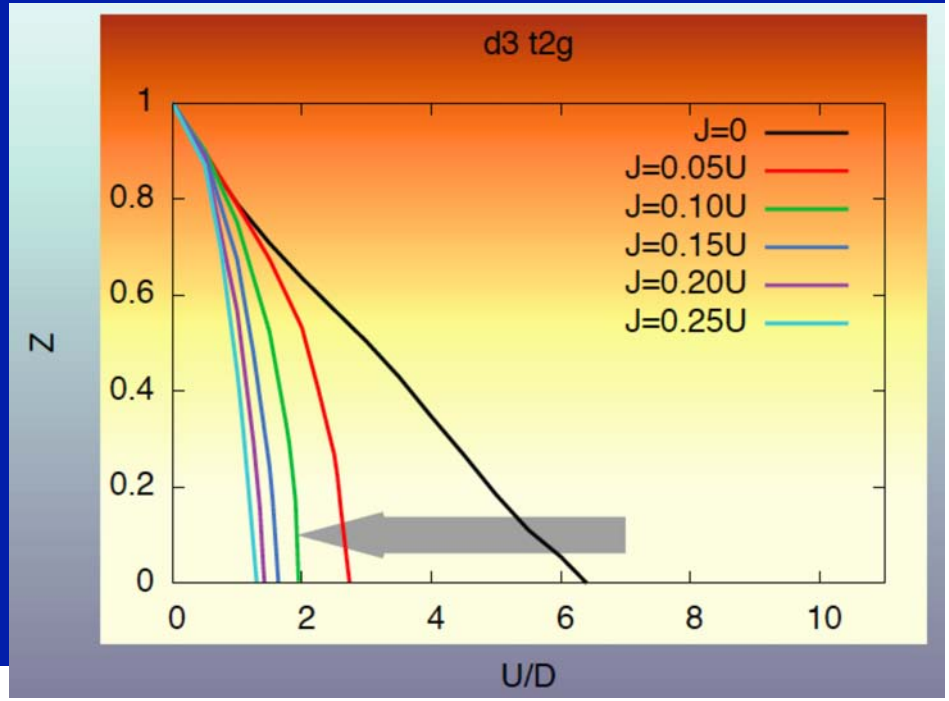


N=1 electron



N=2 electrons

Quasiparticle weight Z vs. U/D



N=3 electrons

Rationalizing the behaviour of U_c

→ On blackboard, cf. lecture notes/review