COLLÈGE DE FRANCE
1530

Jülich School, Sep 2014
DMFT@25: Infinite Dimensions

Materials from an atomic viewpoint beyond the Landau paradigm - An introduction to Dynamical Mean-Field Theory -

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http://www.cpht.polytechnique.fr/cpht/correl/mainpage.htm

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

European Research Council

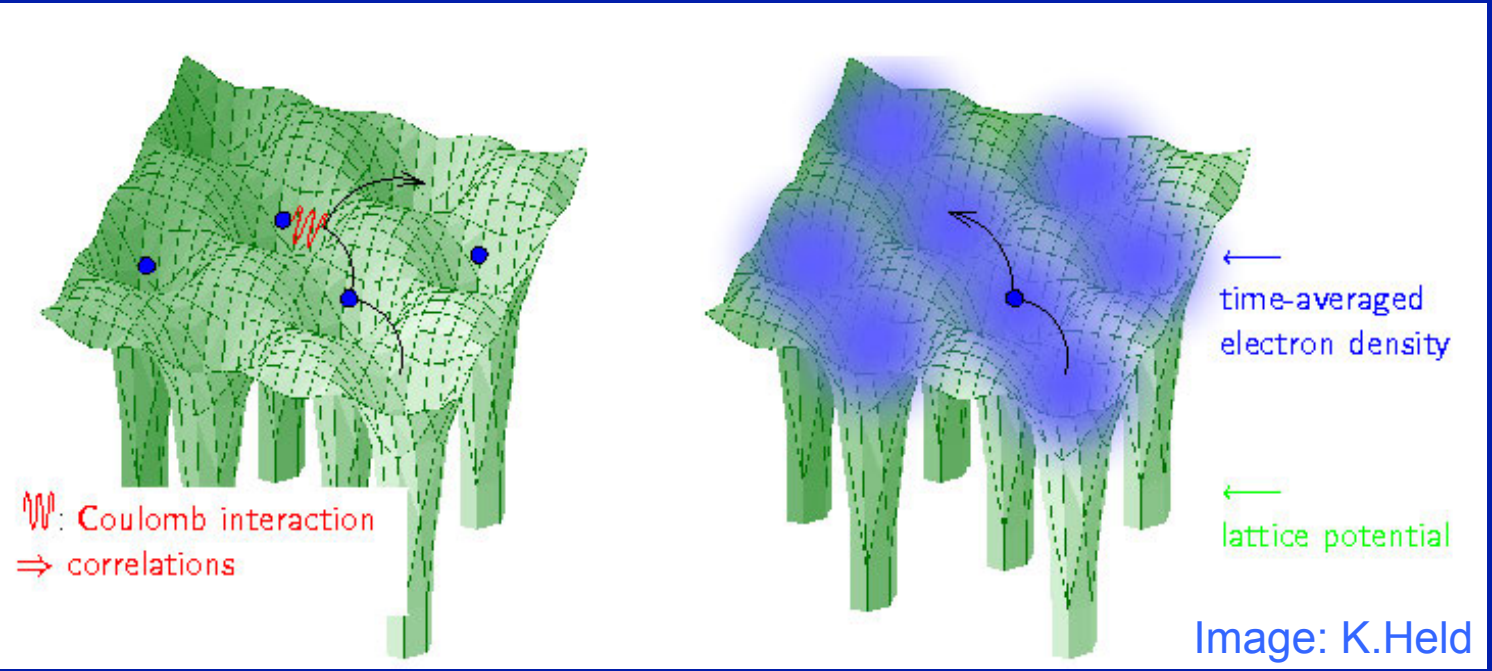
OUTLINE

- Some Physical Motivations
- The DMFT concept: non-technical introduction
- Some success stories for DMFT
- Beyond DMFT

The standard model (most solid-state physics textbooks):

a solid is a kind of electron gas
subject to the periodic potential of ions
→ Bloch wavefunctions, energy bands

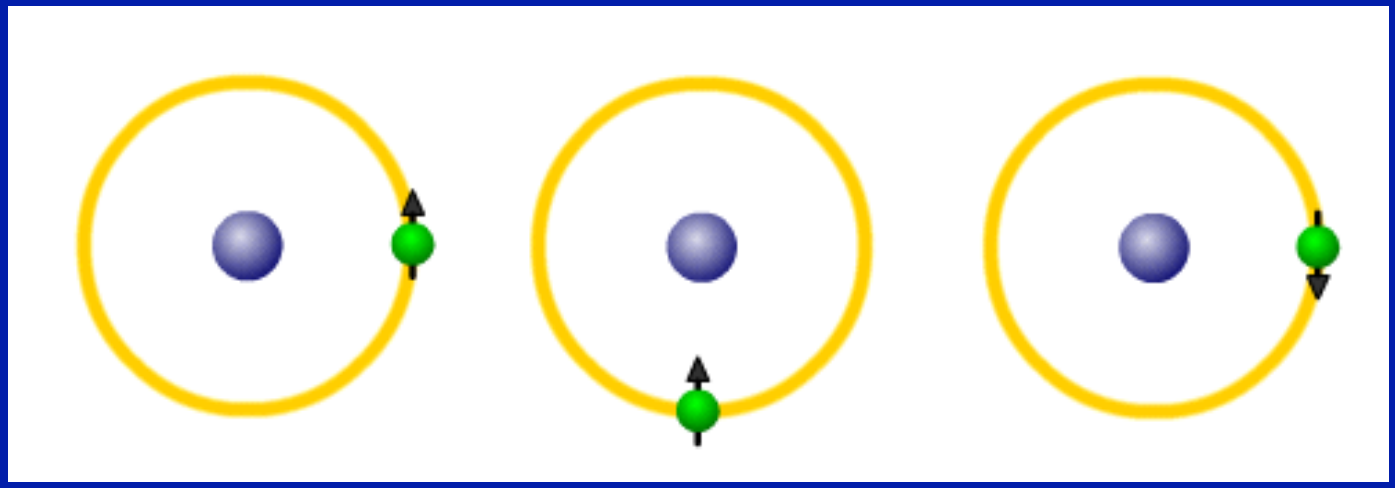
Interactions complicate the matter in a somewhat annoying way



Modern (and most useful) incarnation: DFT-LDA/GGA

In materials with strong correlations
LOCAL ATOMIC PHYSICS
is crucial

Electrons “hesitate”
between being localized
on short-time-scales
and itinerant on long time-scales

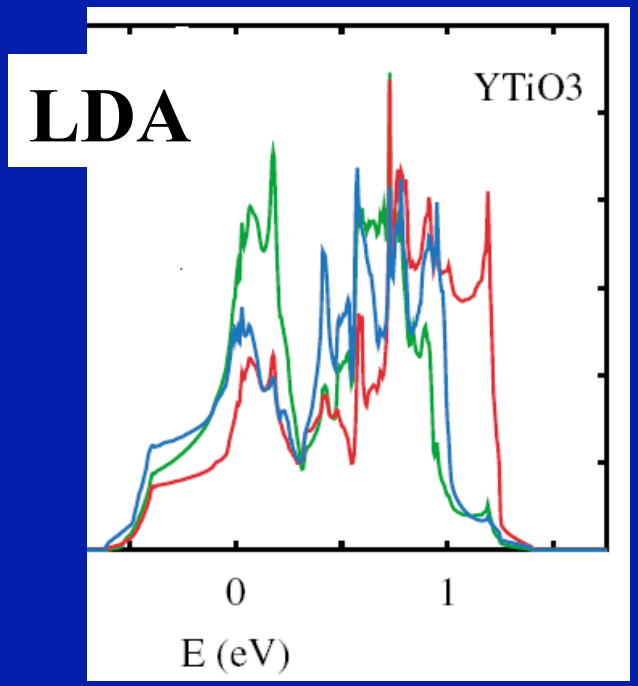


We see this from spectroscopy…

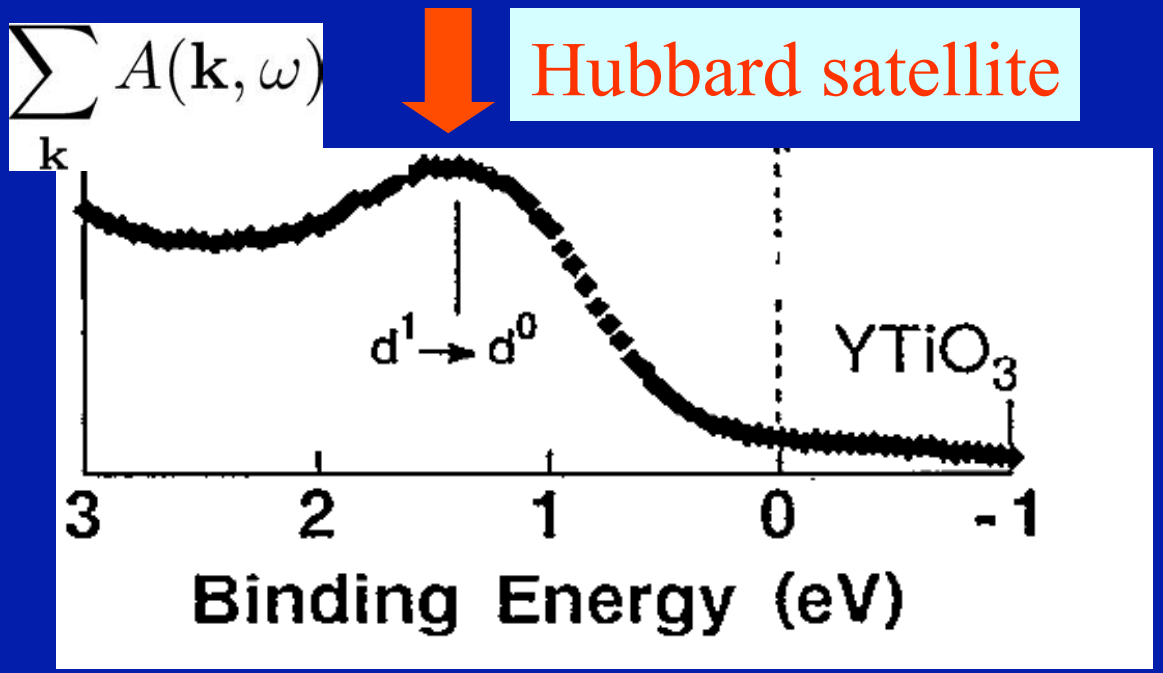
Mott insulators :

Their excitation spectra contain atomic-like excitations

Band structure calculations (interpreting Kohn-Sham spectra as excitations) is in serious trouble for correlated materials !



Metallic LDA (KS) spectrum !

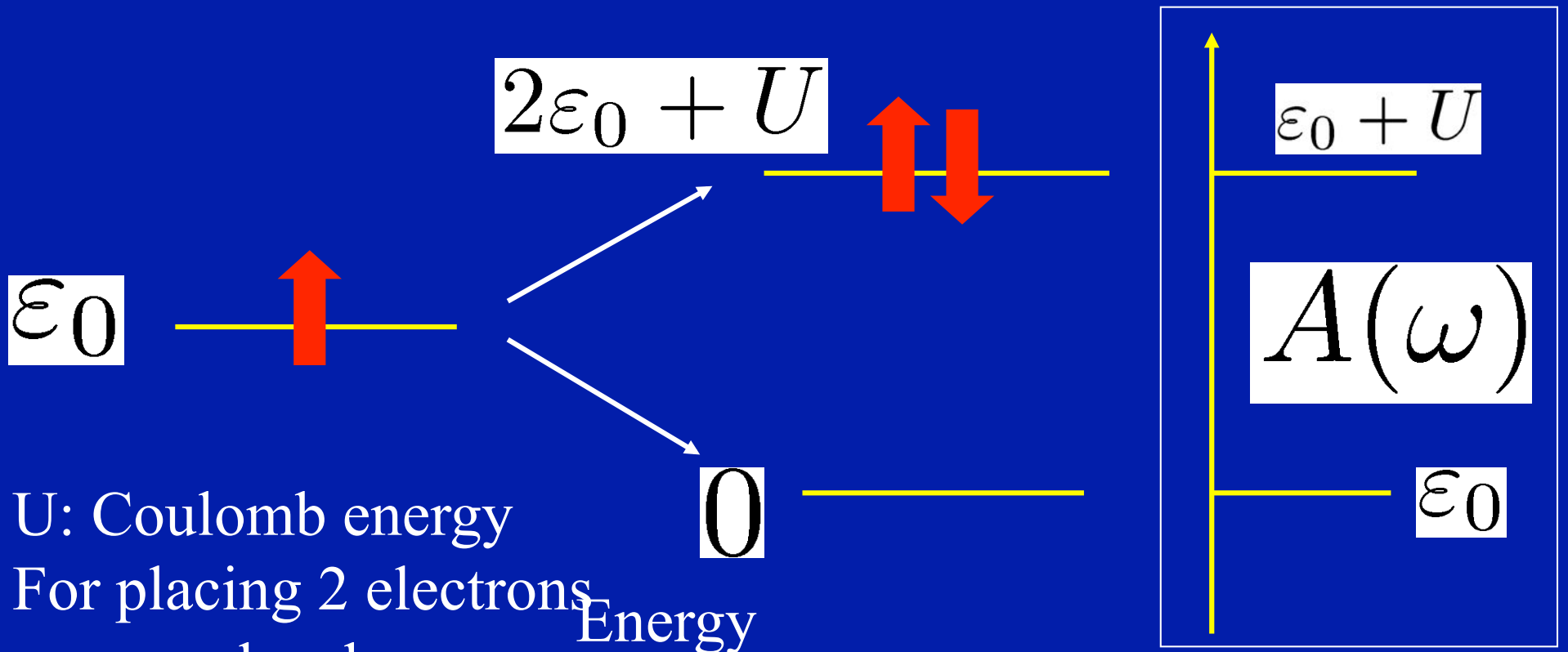


Photoemission: Fujimori et al., PRL 1992

A ``Hubbard satellite'' is nothing but an *atomic transition*

(broadened by the solid-state environment)

Imagine a simplified atom with a single atomic level



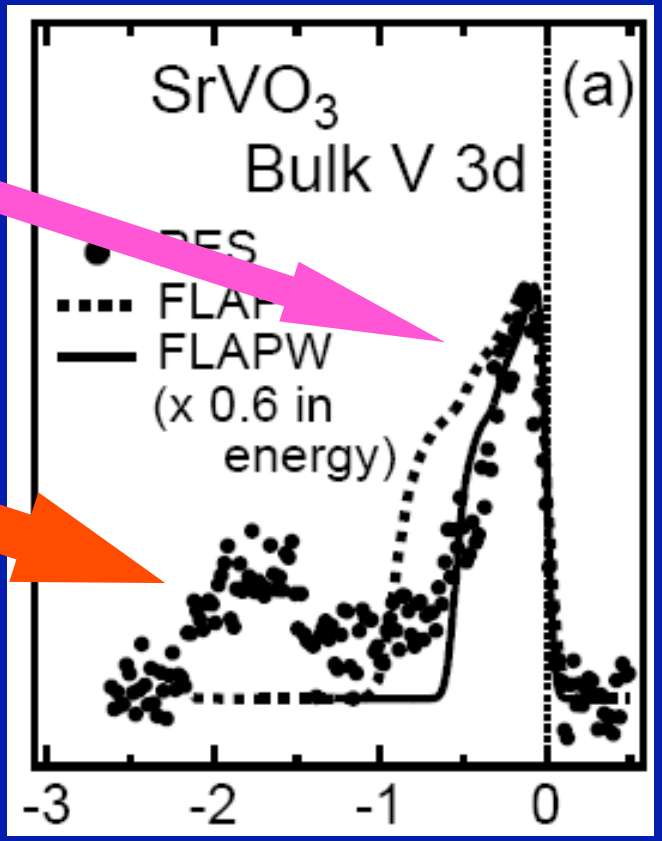
U: Coulomb energy
For placing 2 electrons on same level

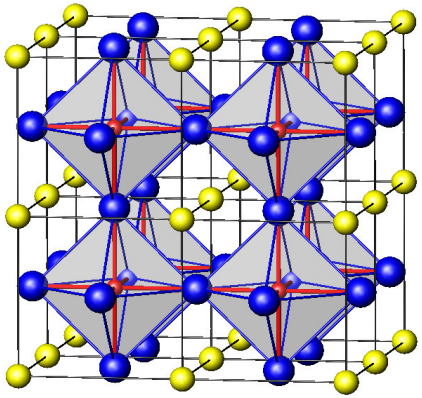
Note: Energetics of the Mott gap requires an accurate description of the many-body eigenstates of single atoms (`multiplets')

→ *cf. `Hund's metals' in the following (see also lecture by G.Kotliar)*

Correlated metals: atomic-like excitations at high energy, quasiparticles at low energy

- **Narrowing of quasiparticle bands** due to correlations (the Brinkman-Rice phenomenon)
- **Hubbard satellites** (i.e extension to the solid of atomic-like transitions)





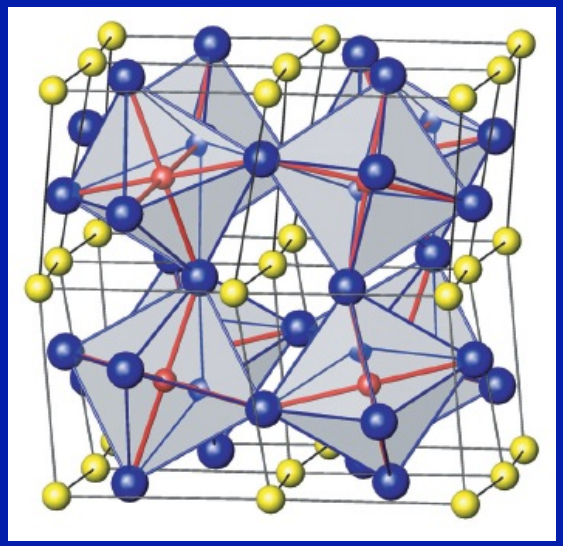
$SrVO_3$

Dashed line:
Spectrum obtained from Conventional band-structure methods (DFT-LDA)

Sekiyama et al., PRL 2004

From weak to strong correlations in d^1 oxides [Fujimori et al. PRL 69, 1796 (1992)]

Puzzle:
Why is $SrVO_3$
a metal
and $LaTiO_3$, $YTiO_3$
Mott insulators ?



The Mott phenomenon at strong coupling (U >> t) HAS NOTHING TO DO with magnetism It is due to blocking of density/charge

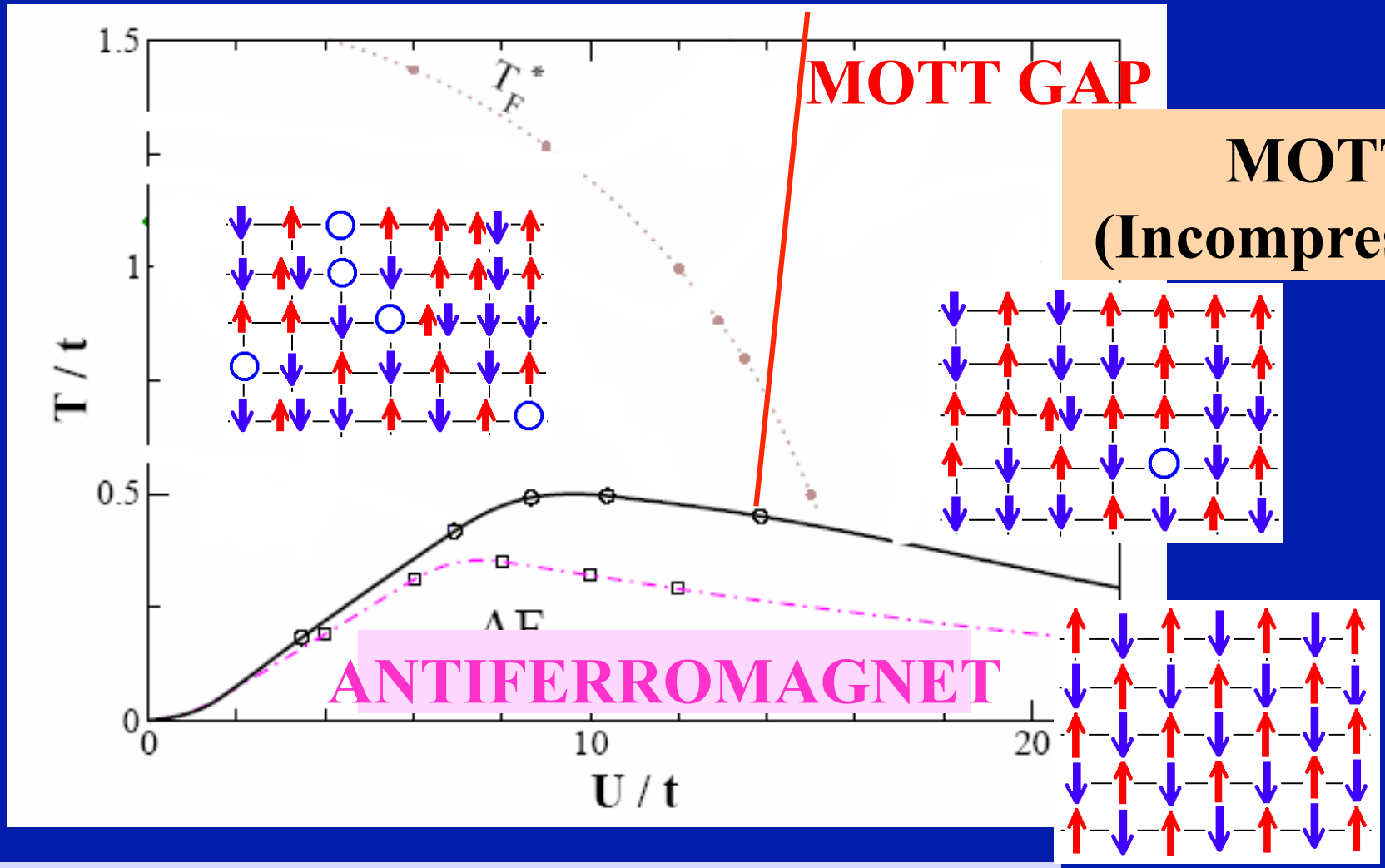
Energy scale for magnetism: superexchange $J \sim t^2/U$

Insulating gap: $\sim U > t >> J$

The system is basically an insulator even well above T_{Neel}

Ex: MANY oxides, e.g. NiO, YTiO3, cuprates etc…

In contrast, LDA+U needs to assume ordering to describe the insulator



Critical boundary calculated for a 3D cubic lattice using:

-Quantum Monte Carlo (Staudt et al. Eur. Phys. J. B17 (2000) 411)

- Dynamical Mean-Field Theory approximation

We need to change our theoretical description
and computational tools
in order to deal with these
« strongly-correlated electron materials »

- Think in terms of atoms, not in terms of an electron gas ! [closer to a chemist point of view]
- Each atom is an interacting (many-body) problem
- Atomic orbitals overlap but motion of electrons is opposed by energy cost for changing the valence of each atom

A theoretical description of the solid-state based on ATOMS rather than on an electron-gas picture: « ***Dynamical Mean-Field Theory*** »

Dynamical Mean-Field Theory:
A.G. & G.Kotliar, PRB 45, 6479 (1992)
Correlated electrons in large dimensions:
W.Metzner & D.Vollhardt, PRL 62, 324 (1989)

Important intermediate steps by: Müller-Hartmann, Schweitzer and Czycholl, Brandt and Mielsch, V.Janis

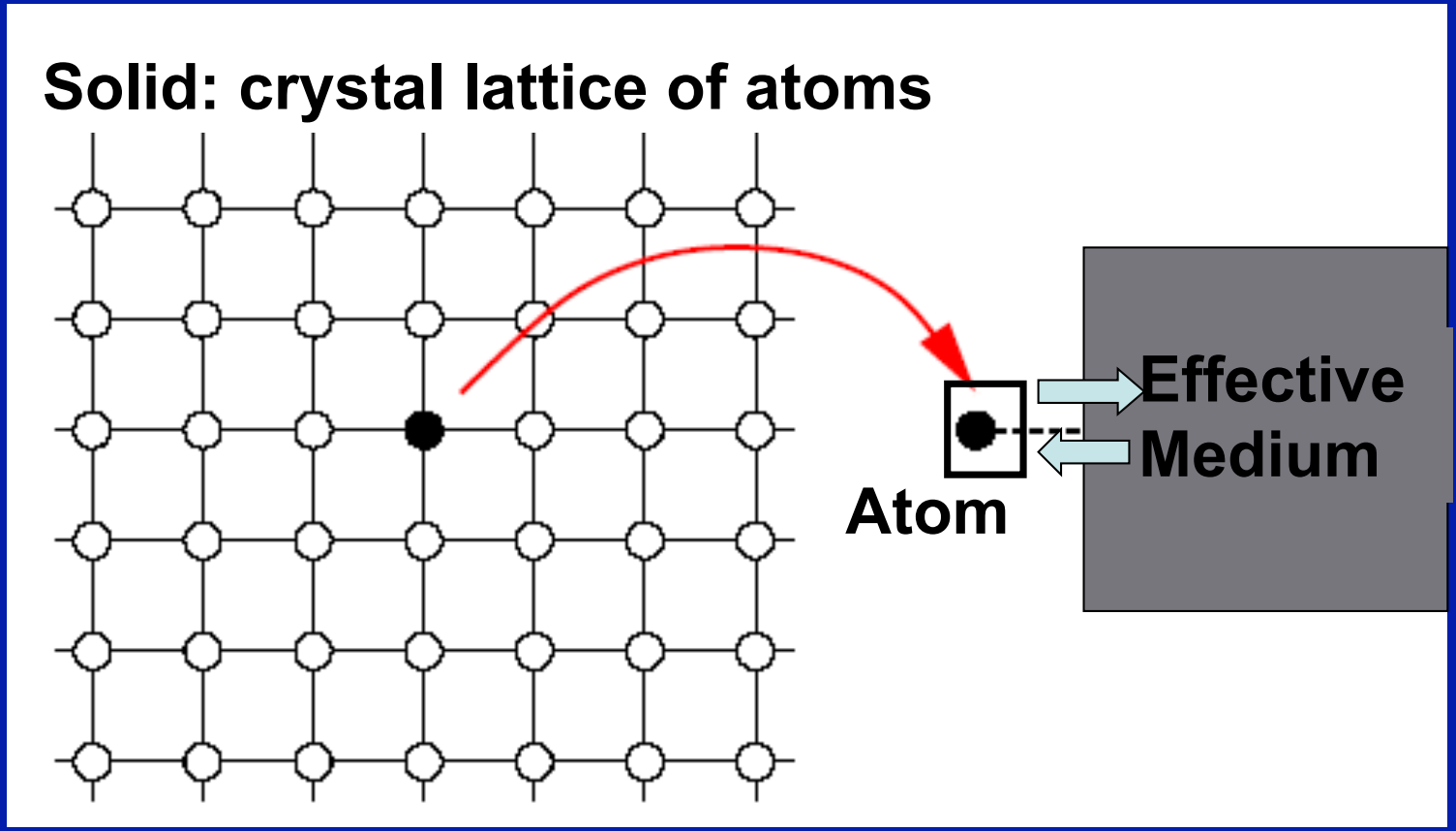
Early review: Georges et al. Rev Mod Phys 68, 13 (1996)

Dresden, 2006 – Europhysics Condensed Matter Prize


Dieter@60 – Augsburg, 2011

Dynamical Mean-Field Theory:

viewing a material as an (ensemble of) atoms coupled to a self-consistent medium



Example: DMFT for the Hubbard model (a model of coupled atoms)

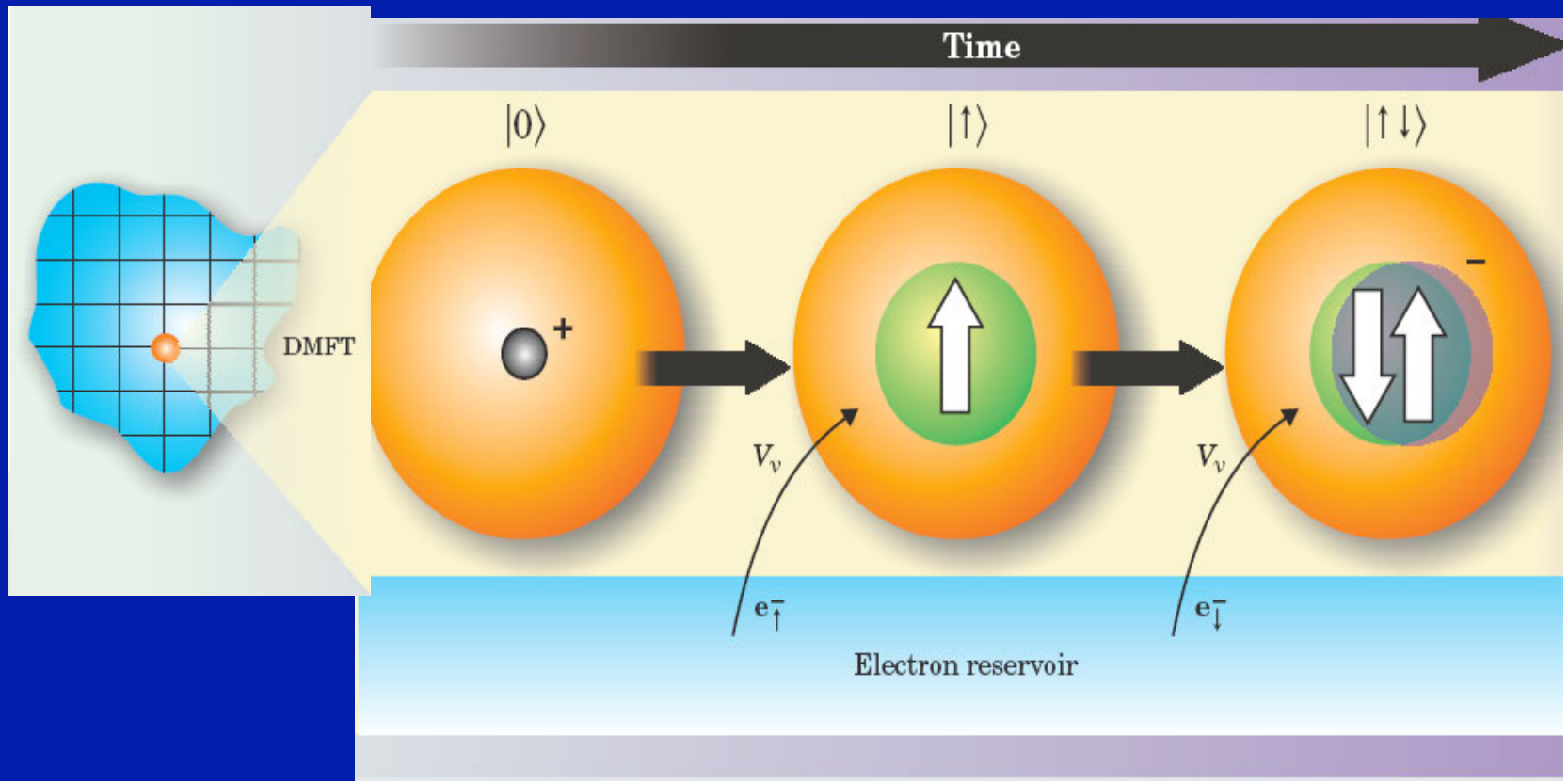
$$H = -\sum_{\mathbf{R}\mathbf{R}'} t_{\mathbf{R}\mathbf{R}'} d^{\dagger}_{\mathbf{R}\sigma} d_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} H^{\mathbf{R}}_{atom}$$

$$H_{atom} = \varepsilon_d \sum_{\sigma} n_{\sigma} + U n_{\uparrow} n_{\downarrow}$$

Focus on a given lattice site:

"Atom" can be in 4 possible configurations: $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$

Describe ``history'' of fluctuations between those configurations



Imaginary-time effective action describing these histories:

$$
\begin{aligned}
S &= S_{\rm at} + S_{\rm hyb} \\
S_{\rm at} &= \int_0^\beta d\tau \sum_\sigma d_\sigma^\dagger(\tau) \left(-\frac{\partial}{\partial \tau} + \varepsilon_d \right) d_\sigma(\tau) + U \int_0^\beta d\tau n_\uparrow n_\downarrow \\
S_{\rm hyb} &= \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d_\sigma^\dagger(\tau') \Delta(\tau - \tau') d_\sigma(\tau)
\end{aligned}
$$

The amplitude Δ(τ) for hopping in and out of the selected site is self-consistently determined: it is the quantum-mechanical Generalization of the Weiss effective field.

$$\mathcal{G}_0^{-1} \equiv \omega + \mu - \Delta(i\omega)$$ Effective `bare propagator'

Hamiltonian formulation: Anderson impurity model

$$H_c = \sum_{l\sigma} E_l a^+_{l\sigma} a_{l\sigma}$$

$$H = H_{\rm c} + H_{\rm at} + H_{\rm hyb}$$

Conduction electron host (``bath'', environment)

$$H_{\rm at} = \varepsilon_d \sum_{\sigma} d^\dagger_\sigma d_\sigma + U\, n^d_\uparrow n^d_\downarrow$$

Single-level ``atom''

$$H_{hyb} = \sum_{l\sigma} [V_l a^+_{l\sigma} d_\sigma + {\rm h.c.}]$$

Transfers electrons between bath and atom – Hybridization, tunneling

Local effective action:

Focus on dynamics of impurity orbital: integrate out conduction electrons → Effective action for impurity orbital:

$$
\begin{aligned}
S &= S_{\rm at} + S_{\rm hyb} \\
S_{\rm at} &= \int_0^\beta d\tau \sum_\sigma d_\sigma^\dagger(\tau) \left(-\frac{\partial}{\partial \tau} + \varepsilon_d \right) d_\sigma(\tau) + U \int_0^\beta d\tau n_\uparrow n_\downarrow \\
S_{\rm hyb} &= \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d_\sigma^\dagger(\tau') \Delta(\tau - \tau') d_\sigma(\tau)
\end{aligned}
$$

$$
-\frac{1}{\pi} {\rm Im} \Delta(\omega + i0^+) = \sum_l |V_l|^2 \, \delta(\omega - E_l)
$$

$$
\mathcal{G}_0^{-1} \equiv \omega + \mu - \Delta(i\omega)
$$

Effective `bare propagator'

Focus on energy-dependent local observable :

$$G_{RR}(\omega) \equiv G_{\rm loc}$$

On-site Green's function (or spectral function) of the `solid'

Use atom-in-a-bath as a reference system to represent this observable:

→ IMPOSE that ε_d and Δ should be chosen such that:

$$G_{\rm imp}[\omega; \varepsilon_d, \Delta(\omega)] = G_{\rm loc}(\omega)$$

At this point, given G_{loc} of the lattice Hubbard model,
we have just introduced an exact local representation of it

G_{RR} is related to the exact self-energy of the lattice (solid) by:

$$G_{\mathbf{RR}}(\omega) = \sum_{\mathbf{k}} \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega)} = G_{\mathrm{loc}}(\omega)$$

In which ε_k is the tight-binding band (FT of the hopping $t_{RR'}$)

High-frequency → $\varepsilon_d = -\mu + \sum_k \varepsilon_k \, (= -\mu)$

Let us now make the **APPROXIMATION** that the lattice self-energy is **k-independent** and coincides with that of the effective atom (impurity problem):

$$\Sigma(\mathbf{k}, \omega) \simeq \Sigma_{\mathrm{imp}}(\omega)$$

This leads to the following <u>self-consistency condition:</u>

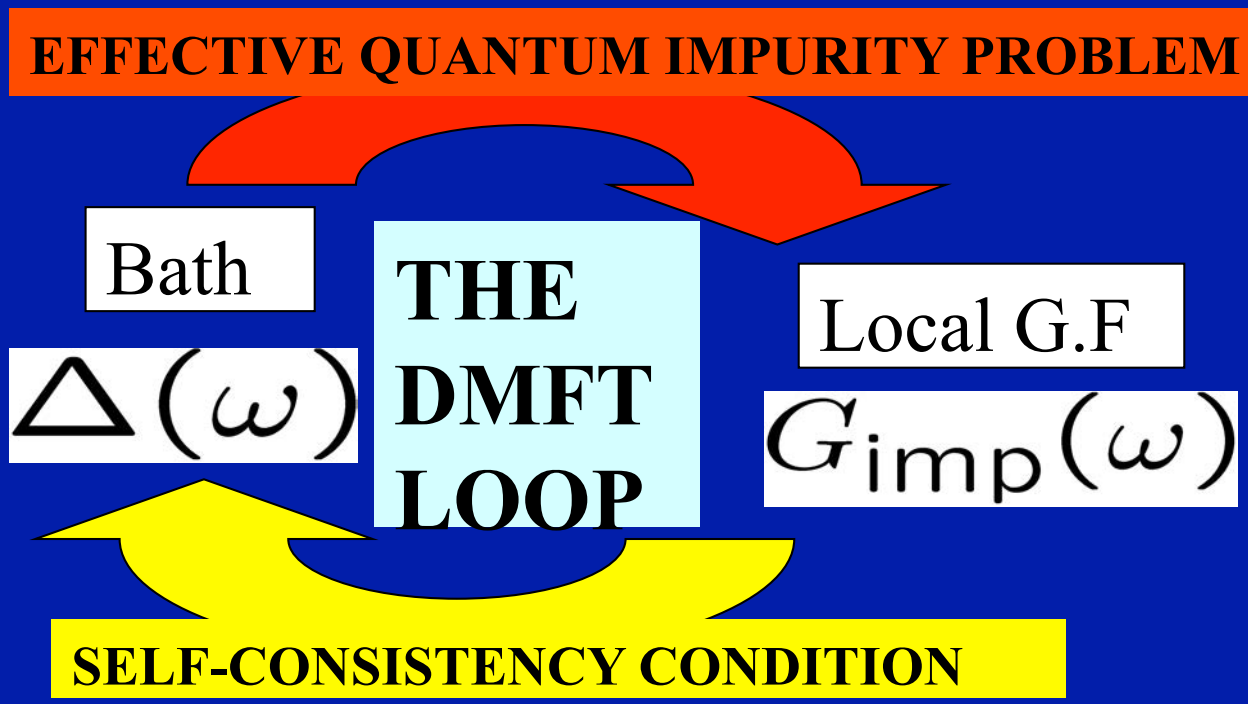
$$G_{\mathrm{imp}}[i\omega; \Delta] = \sum_{\mathbf{k}} \frac{1}{G_{\mathrm{imp}}[i\omega; \Delta]^{-1} + \Delta(i\omega) - \varepsilon_{\mathbf{k}}}$$

The self-consistency equation and the DMFT loop

Approximating the self-energy by that of the local problem : $\Sigma(\mathbf{k},\omega) \simeq \Sigma_{imp}(\omega)$

→ fully determines both the local G and Δ:

$$G_{\mathrm{imp}}[i\omega;\Delta] = \sum_{\mathbf{k}} \frac{1}{G_{\mathrm{imp}}[i\omega;\Delta]^{-1} + \Delta(i\omega) - \varepsilon_{\mathbf{k}}}$$



Δ(ω): generalizing the Weiss field to the quantum world

Pierre Weiss
1865-1940
« Théorie du Champ Moléculaire »
(1907)

Einstein, Paul Ehrenfest, Paul Langevin, Heike Kammerlingh-Onnes, and Pierre Weiss at Ehrenfest's home, Leyden, the Netherlands. From Einstein, His Life and Times, *by Philipp Frank (New York: A.A. Knopf, 1947). Photo courtesy AIP Emilio Segrè Visual Archives.*

Weiss mean-field theory
Density-functional theory
Dynamical mean-field theory

} rely on similar conceptual basis

TABLE 2. Comparison of theories based on functionals of a local observable

Theory	MFT	DFT	DMFT
Quantity	Local magnetization m_i	Local density $n(x)$	Local GF $G_{ii}(\omega)$
Equivalent system	Spin in effective field	Electrons in effective potential	Quantum impurity model
Generalised Weiss field	Effective local field	Kohn-Sham potential	Effective hybridisation

- Exact energy functional of local observable
- Exact representation of local observable:
- Generalized ``Weiss field''
- Self-consistency condition, later approximated

see e.g:
A.G
arXiv cond-mat
0403123

The DMFT construction is EXACT:

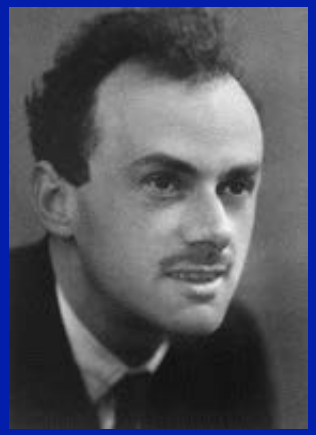
- For the non-interacting system
  (U =0 → Σ = 0 !)
- For the isolated atom
  (strong-coupling limit t=0 → Δ = 0)

→ Hence provides an interpolation from weak to strong coupling

- In the formal limit of infinite dimensionality (infinite lattice coordination) [introduced by Metzner and Vollhardt, 1989]

Proofs: LW functional, Cavity construction (more on board)

In simplest cases (e.g. single-orbital),
the DMFT construction avoids the
fermion minus-sign problem
(absent for simplest quantum impurity problems,
effectively 1+1-dimensional)



`` It therefore becomes desirable
that approximate practical methods
of applying quantum mechanics
should be developed,
which can lead
to an explanation of the main features
of complex atomic systems
without too much computation"

Recent algorithmic breakthroughs

entering a new age for DMFT approaches (and extensions) …

Continuous-time quantum Monte Carlo (CT-QMC)

*Rubtsov 2005 Interaction expansion(CT-INT)

*P. Werner, M.Troyer, A.Millis et al 2006
Hybridization expansion(CT-HYB)

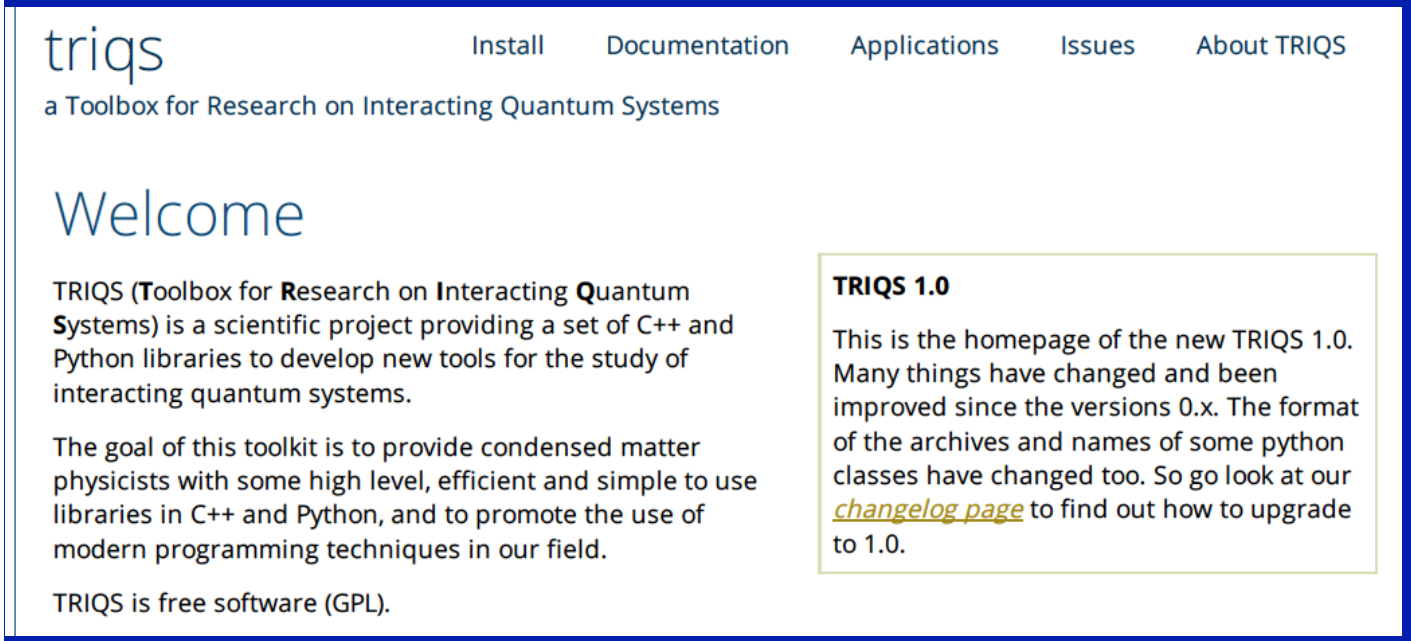
*Gull/Parcollet 2008 Auxiliary field (CT-AUX)

See lecture by F.Assaad

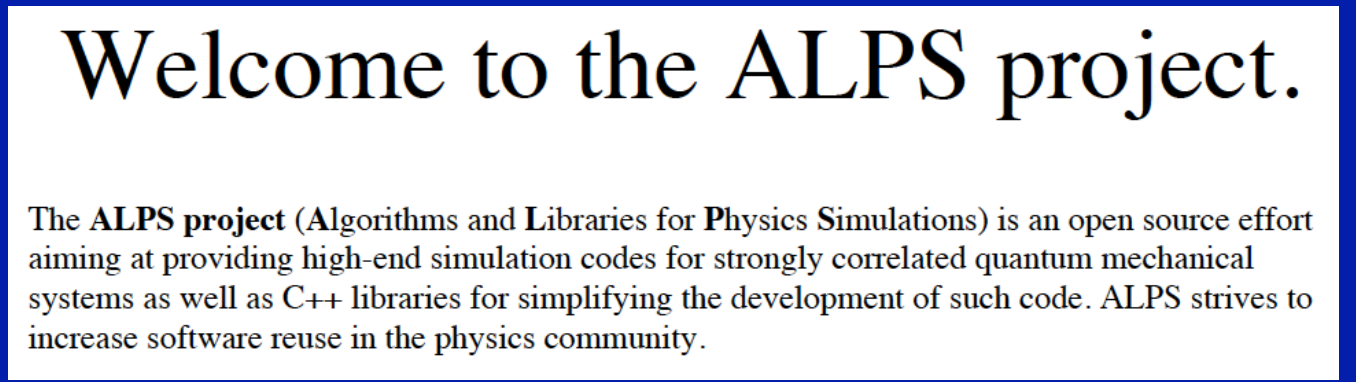
Recent review: Gull et al. Rev Mod Phys 83, 349 (2011)

Need for efficient development and sharing of code libraries

The TRIQS project (O.Parcollet, M.Ferrero et al.)

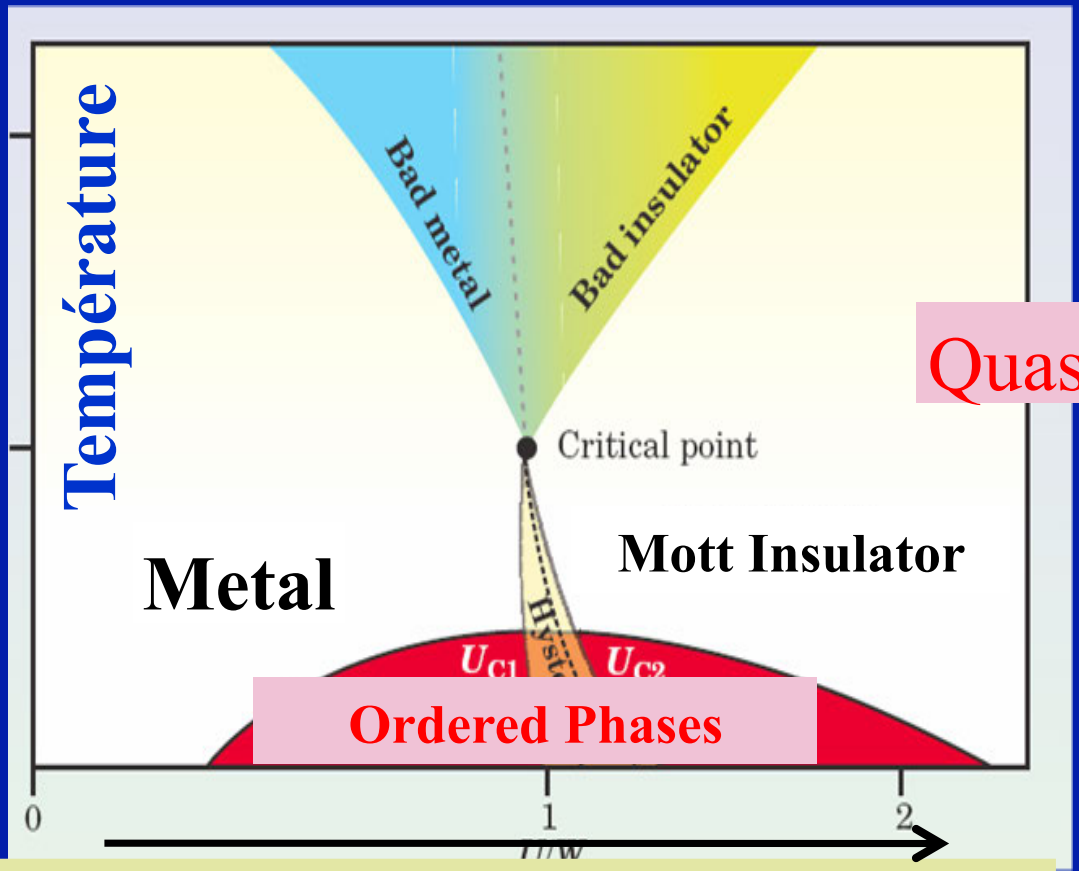


ipht.cea.fr/triqs



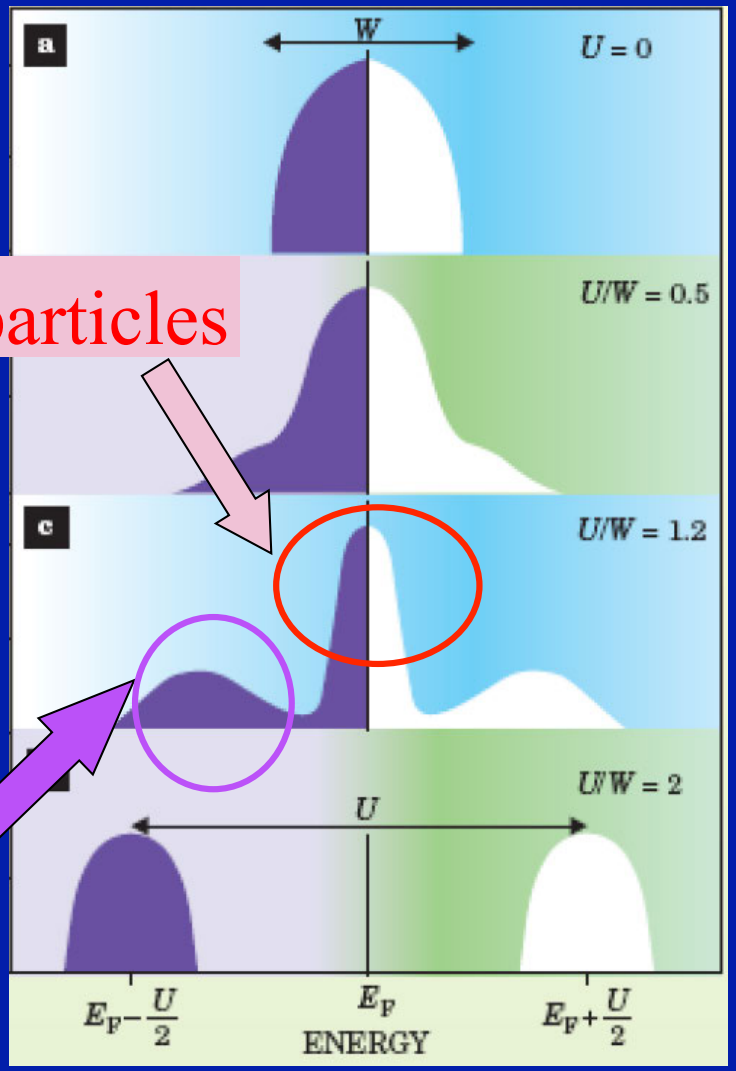
alps.comp-phys.org

An early success of DMFT (1992-1999)
Complete theory of the Mott transition



Interaction strength/kinetic energy

Quasiparticles

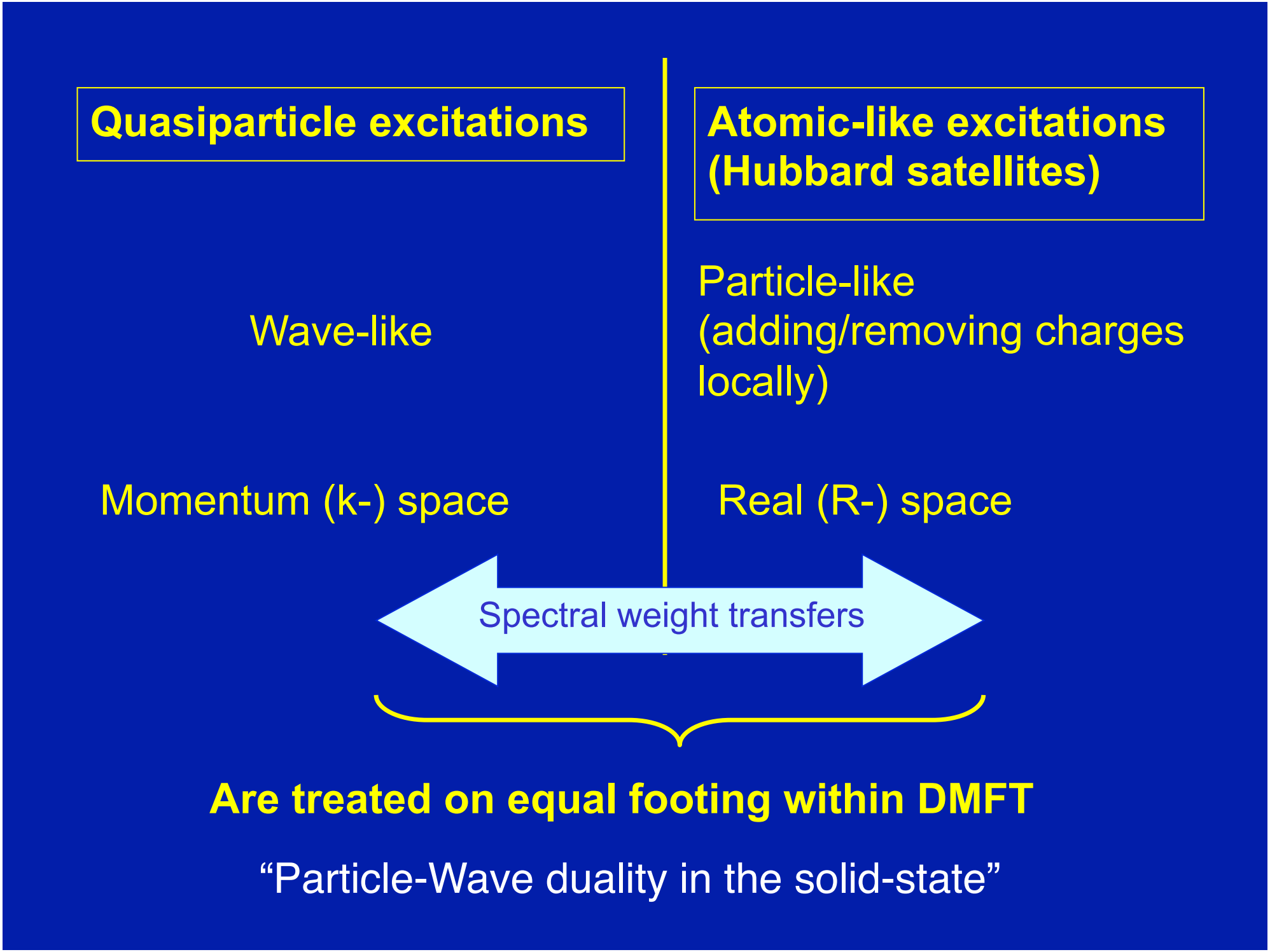


Quasi atomic excitations

Low-frequency behavior of $\Delta(\omega)$ determines nature of the phase

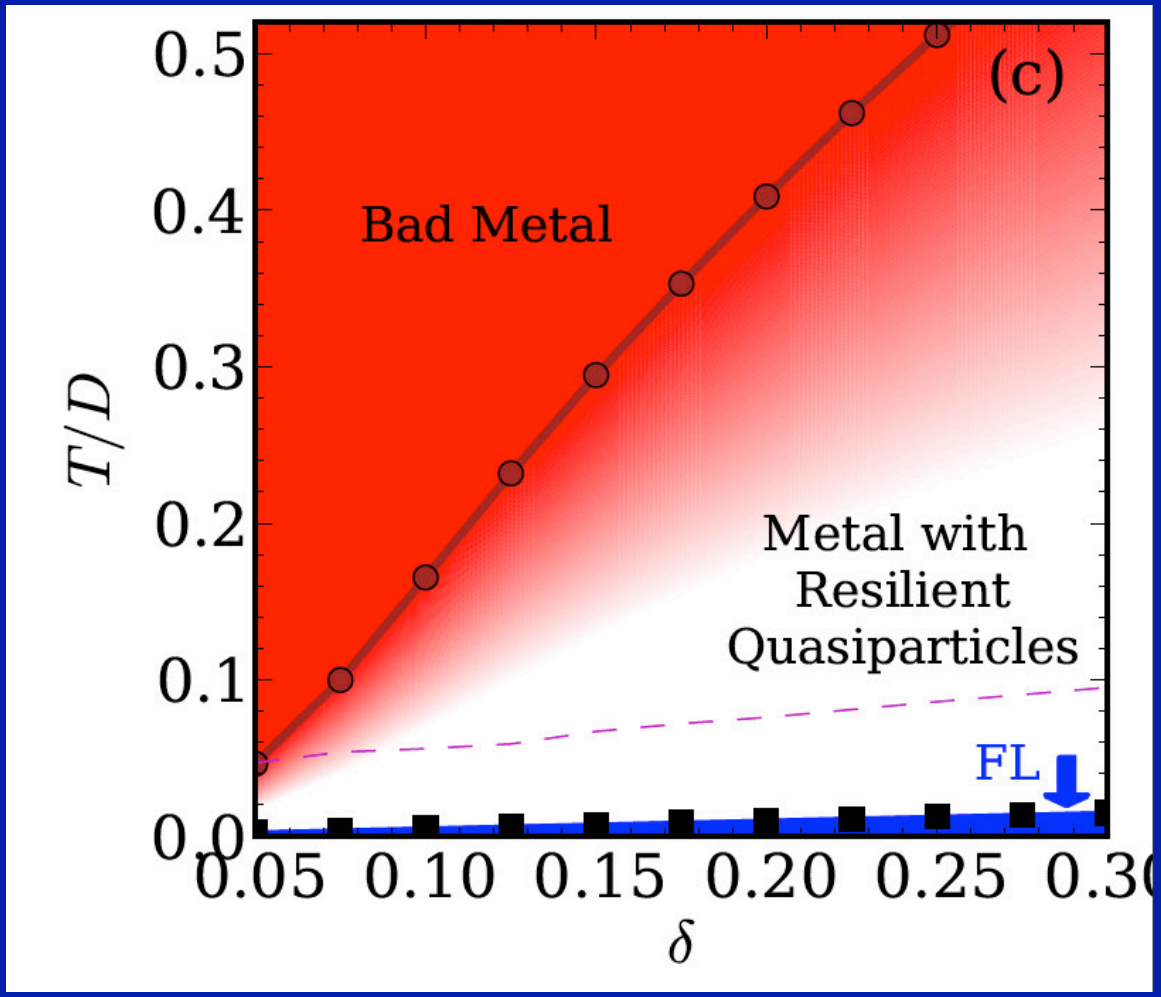
- $\Delta(\omega \to 0)$ finite → local moment is screened. `Self-consistent' Kondo effect. Gapless metallic state.

- $\Delta(\omega)$ gapped → no Kondo effect, degenerate ground-state, insulator with local moments

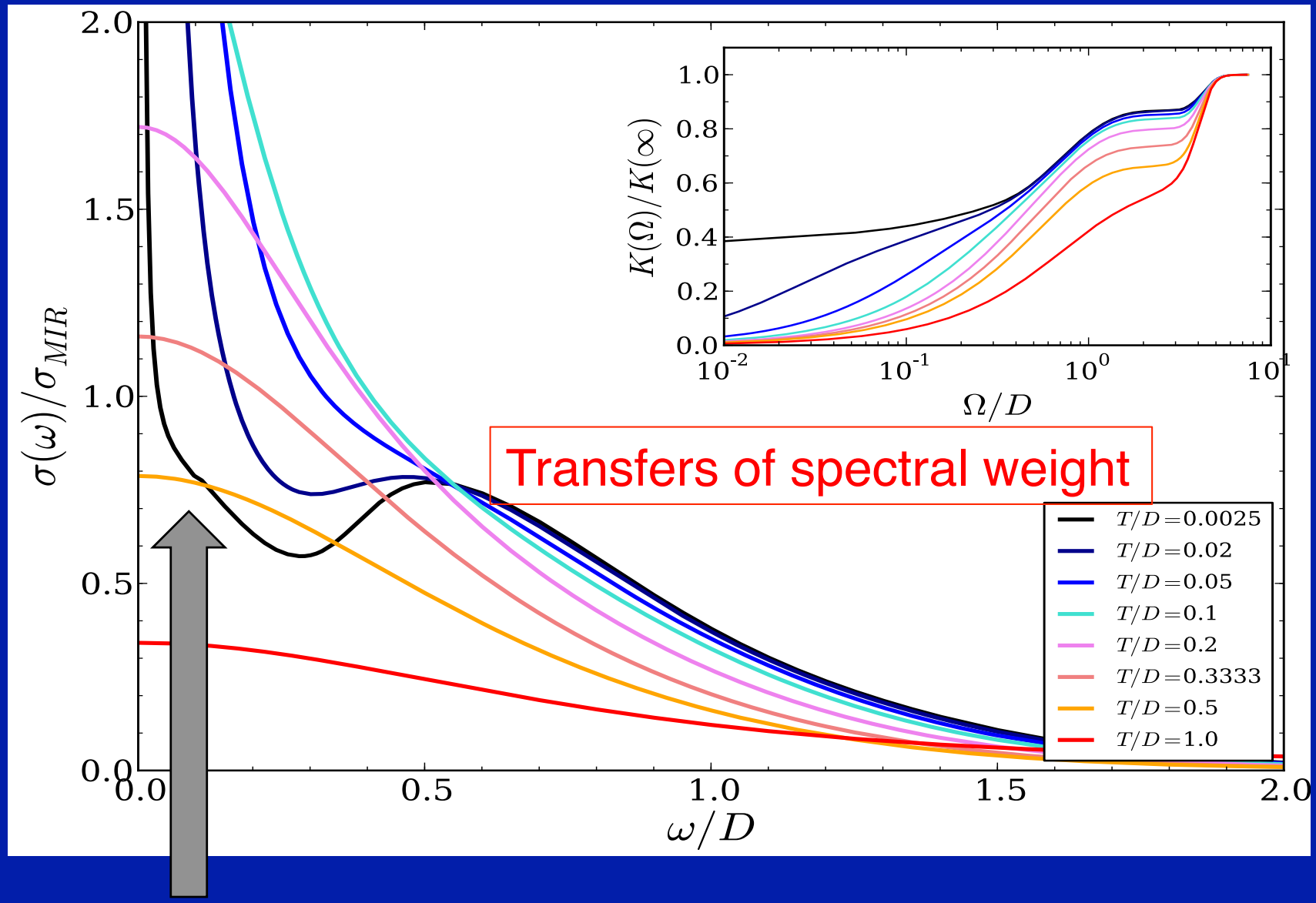

Quasiparticle excitations
Atomic-like excitations (Hubbard satellites)
Wave-like
Particle-like (adding/removing charges locally)
Momentum (k-) space
Real (R-) space
Spectral weight transfers
Are treated on equal footing within DMFT
"Particle-Wave duality in the solid-state"

Recent insights into an old problem: "How bad metals become good"

`Resilient' *quasiparticles* *beyond Landau Theory*



Deng et al.
PRL 110 (2013)
086401



This non-Drude ``foot'' is actually the signature of Landau's Fermi liquid in the optical spectrum !

Recent interest in signatures of Fermi Liquid Theory in optical spectroscopy:

- A.Chubukov and D.Maslov, PRB 86 (2012) 155136 & 155137
- U.Nagel et al. (T. Timusk's group) PNAS 109, 19161 (2012)
- M.Dressel and M.Scheffler Ann. Phys. 15, 535 (2006)
- M.Schneider et al. arXiv:1312.3809 [PRL 2014] [$CaRuO_3$]

PHYSICAL REVIEW B **87**, 115109 (2013)

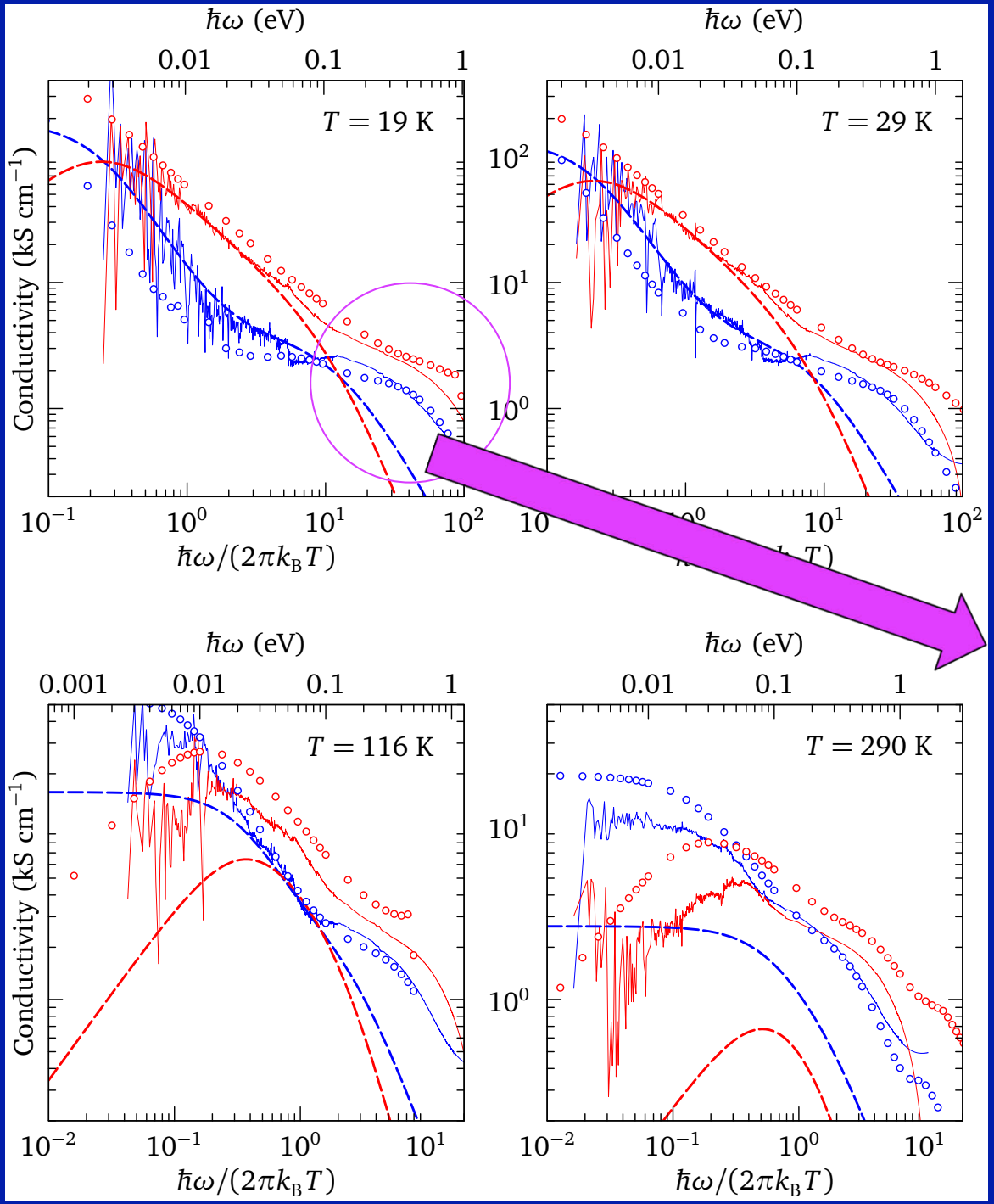
Non-Drude universal scaling laws for the optical response of local Fermi liquids

Christophe Berthod,[1] Jernej Mravlje,[2,3,4] Xiaoyu Deng,[5] Rok Žitko,[4] Dirk van der Marel,[1] and Antoine Georges[1,2,3]

PRL **113,** 087404 (2014) PHYSICAL REVIEW LETTERS week ending 22 AUGUST 2014

Optical Response of Sr_2RuO_4 Reveals Universal Fermi-Liquid Scaling and Quasiparticles Beyond Landau Theory

D. Stricker,[1] J. Mravlje,[2] C. Berthod,[1] R. Fittipaldi,[3] A. Vecchione,[3] A. Georges,[4,5,1] and D. van der Marel[1]



Optical spectra of Sr_2RuO_4 D.Stricker et al.

arXiv:1403.5445

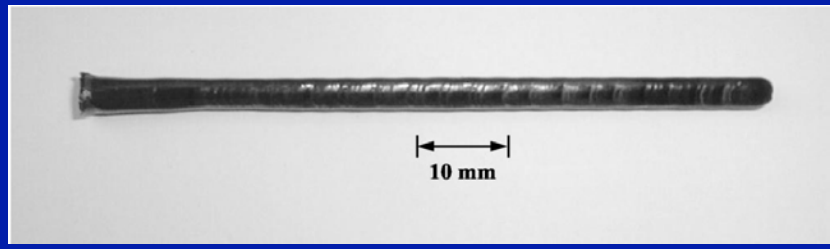
Dashed lines :
universal FL form
→ Beautiful agreement
→ At low T, low ω

Clear deviations from FL for ω above ~ 0.1 eV
Very well described by DMFT !

Dots:
LDA+DMFT calculation for this material

Sr_2RuO_4: the `Helium 3' of transition-metal oxides !

cf. Andy McKenzie's talk yesterday

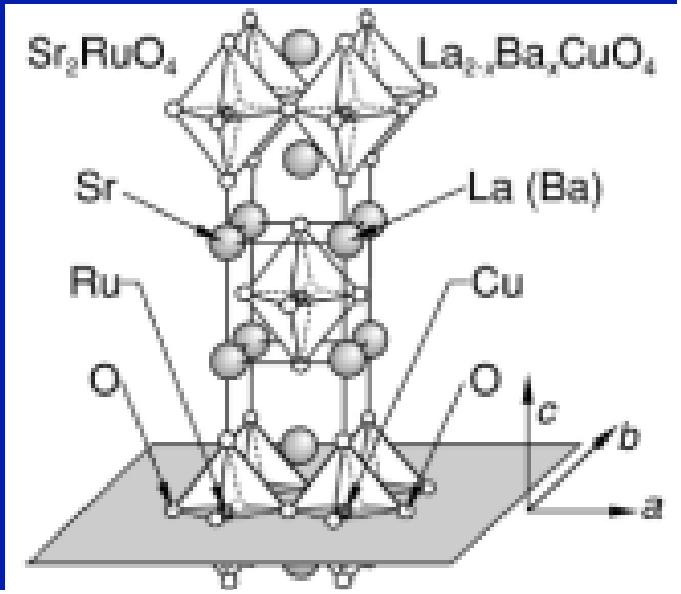


- Huge high-quality crystals !
- Has been investigated with basically all techniques in the experimentalist's toolbox
- 4d-row structural analogue of La_2CuO_4
- Beautiful review articles:

- A.Mackenzie and Y.Maeno

  RMP 75, 657 (2003)
- Bergemann, Adv. Phys. 52, 639 (2003)

  [Focus on dHvA quantum oscillations]

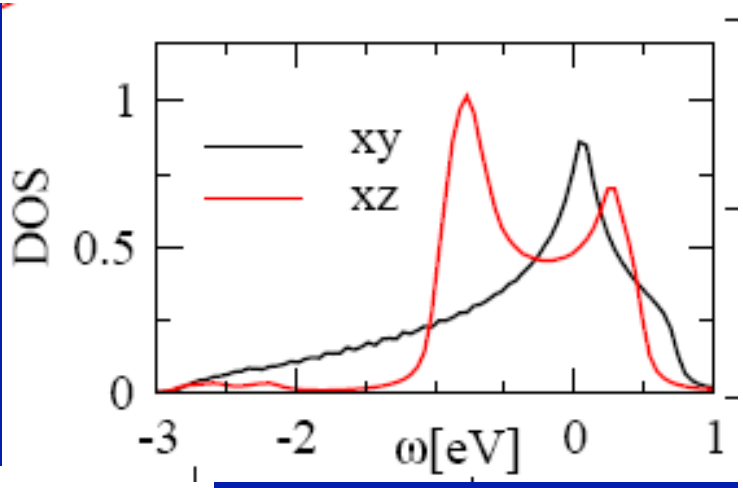


Puzzle:

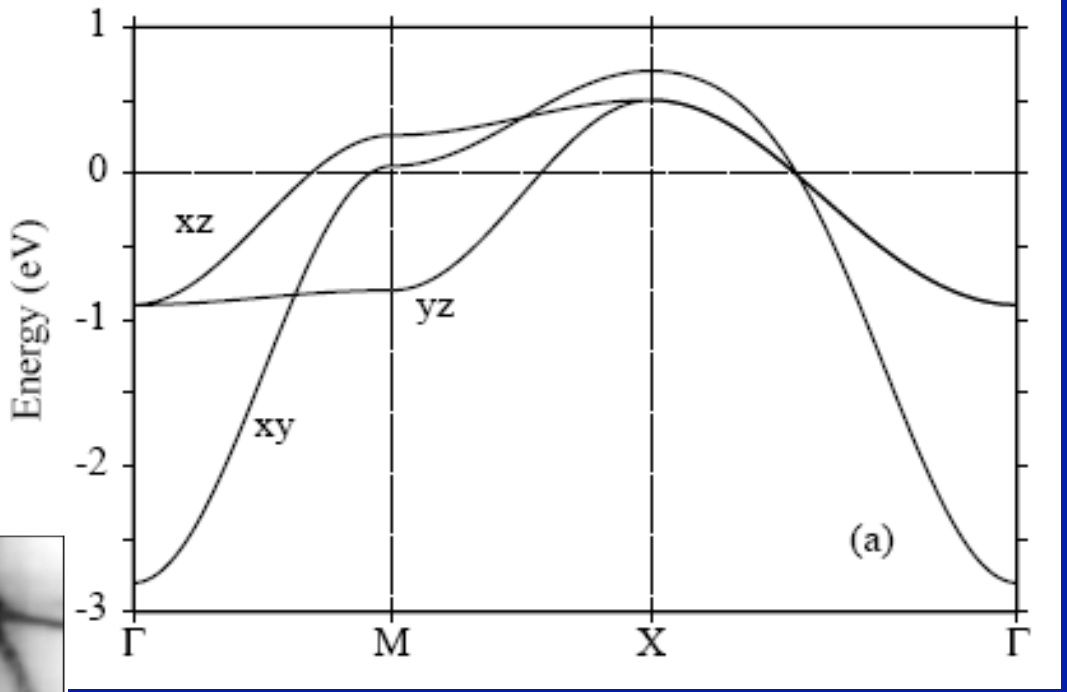
Why are transition-metal oxides of the 4d series (such as ruthenates) strongly correlated metals, while not being close to a Mott insulating state ?

Example: Sr_2RuO_4 has t_{2g} bandwidth ~ 4eV,
And estimated U for t_{2g} shell about 2.5 eV at most.
Nevertheless effective mass enhancement (over LDA)
of xy-band is ~ 5 !!

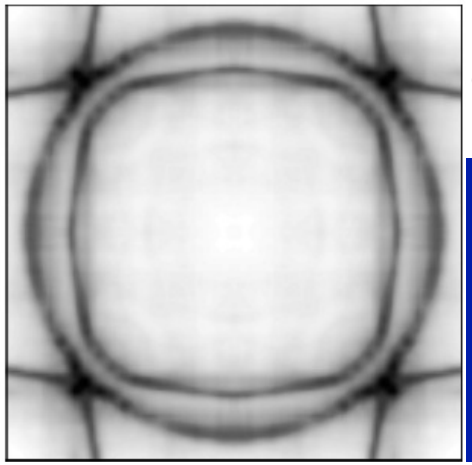
Bands (LDA)



~ 1.5 eV
(xz,yz)



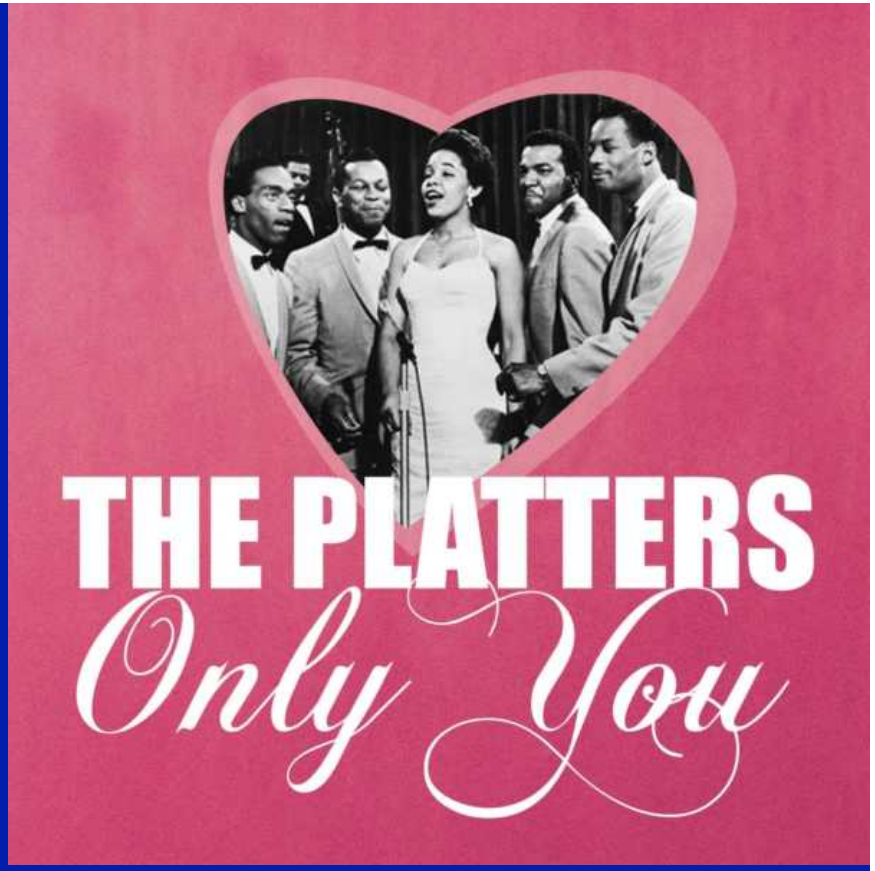
~ 3.6 eV
(xy band)

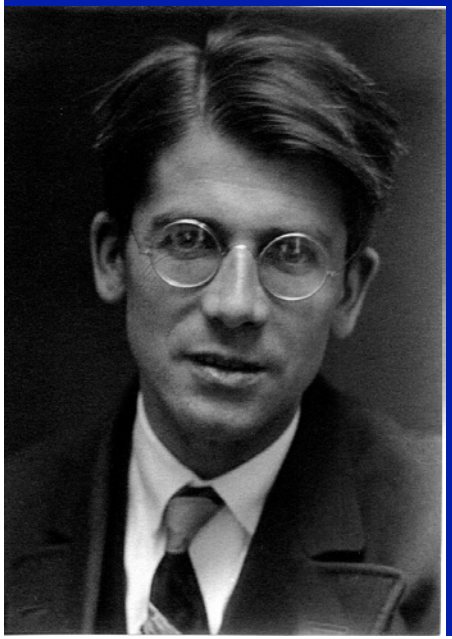


But kinetic energies of all bands comparable

The Platters said:

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





… Take-home message here:

« Not only U, also J_H matters » !

Friedrich Hund
1896-1997

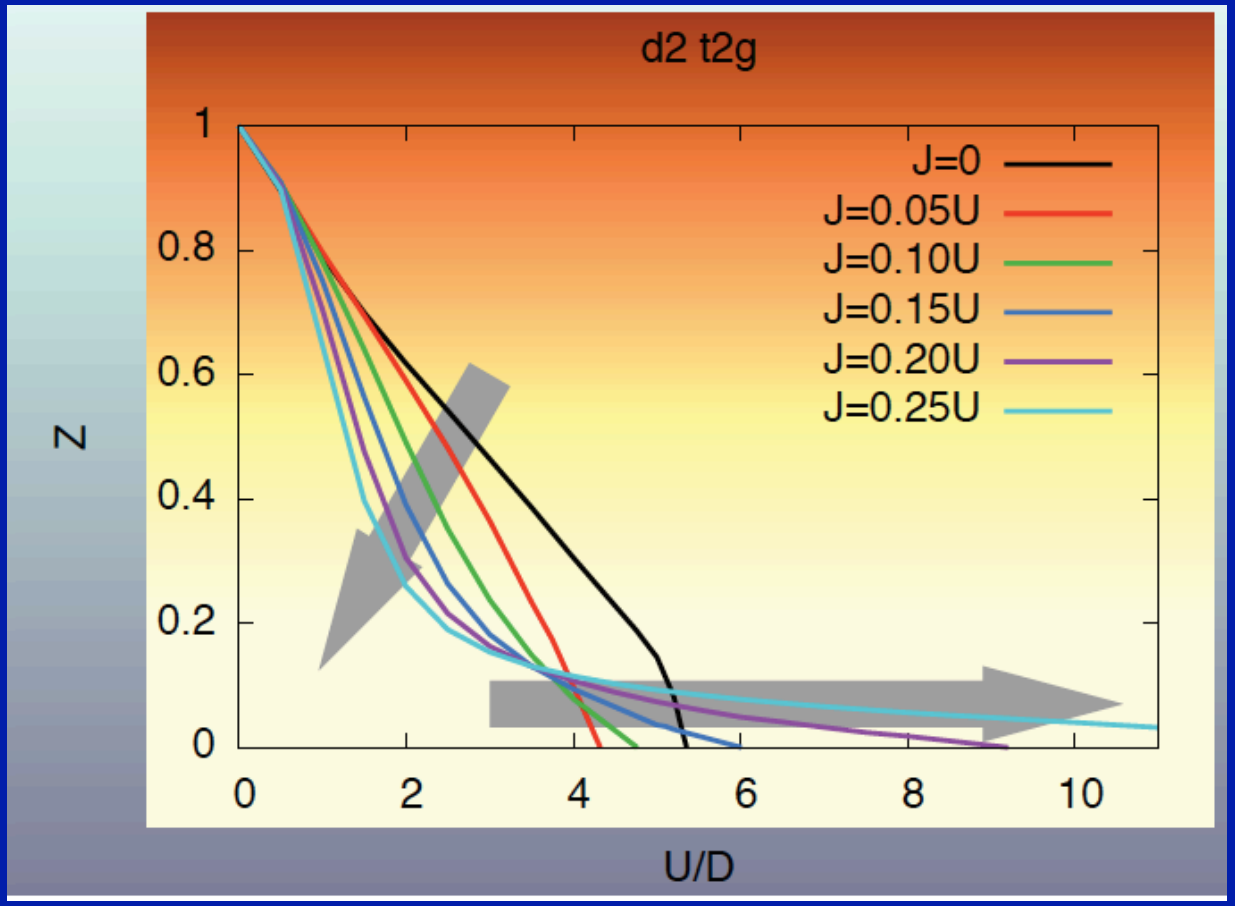
Some articles of the `Hund's metals' saga…

- Haule and Kotliar New J. Phys. 11, 025021 (2009)
- Werner, Gull Troyer and Millis, PRL 101, 166405 (2008)
- Mravlje et al.PRL 106, 096401 (2011)
- de'Medici et al. PRL 107, 256401 (2011)

Recent review article:
AG, de'Medici and Mravlje
Annual Reviews Cond. Mat. Phys Vol 4 (2013)
arXiv:1207.3033

For all filling except ½-filling and a single electron and hole:

1. Hund's coupling suppresses coherence scale → reduces quasiparticle coherence scale, smaller Z



2. But also increases U_c → Enhances range of metallic state !

J is « Janus-faced » : it has two ANTAGONISTIC effects

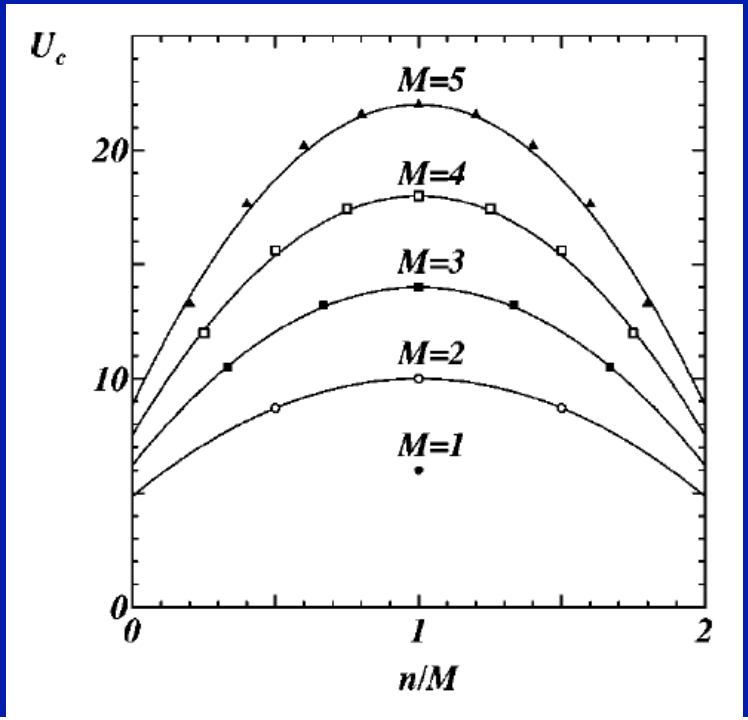
Janus is the latin god of beginnings/ transitions and is often associated with doors and entrances and has two faces.
He was first promoted to being a physicist by Pierre-Gilles de Gennes (“Janus grains”)

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

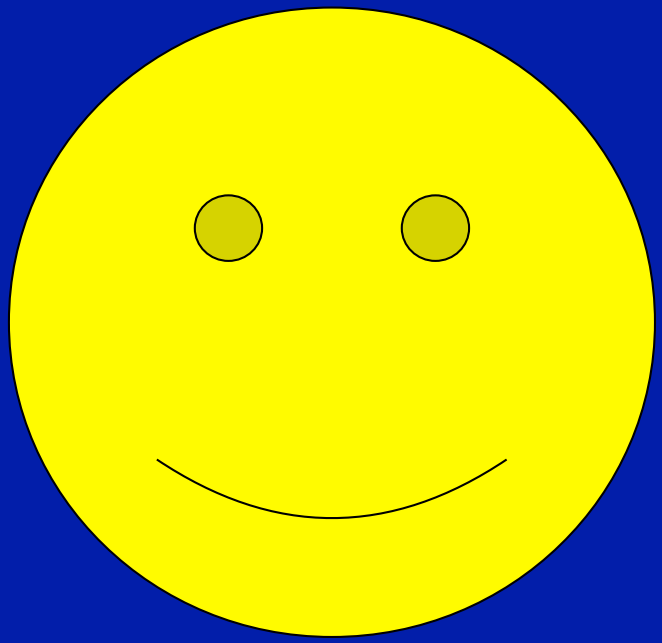
Janus-Faced Influence of Hund’s Rule Coupling in Strongly Correlated Materials

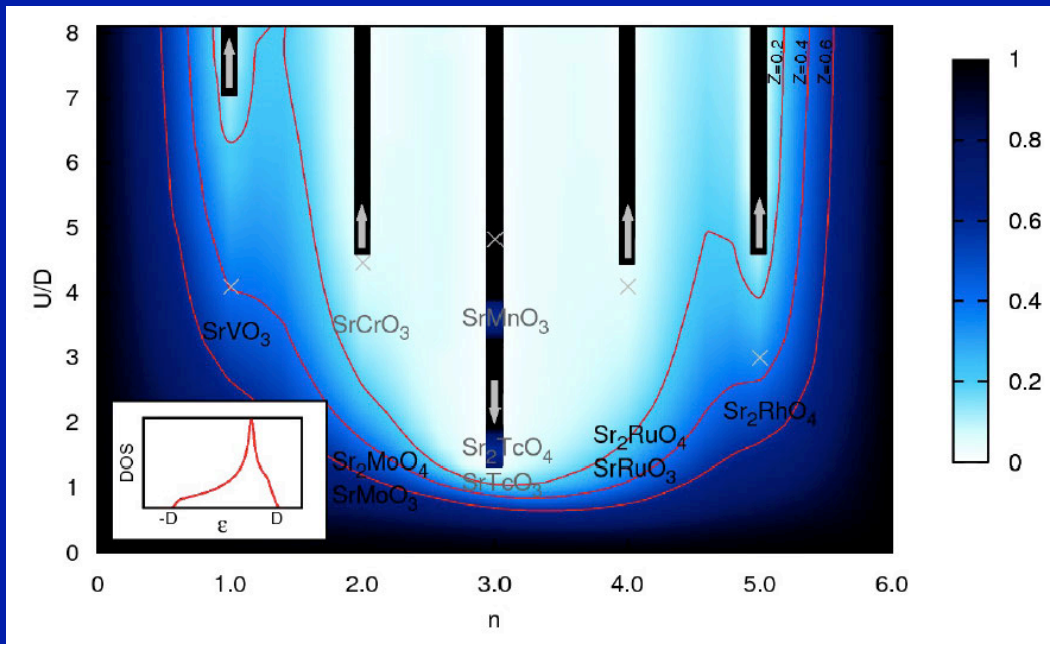
Luca de’ Medici,[1] Jernej Mravlje,[2,3,4] and Antoine Georges[2,4,5,6]

J=0


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

J≠0

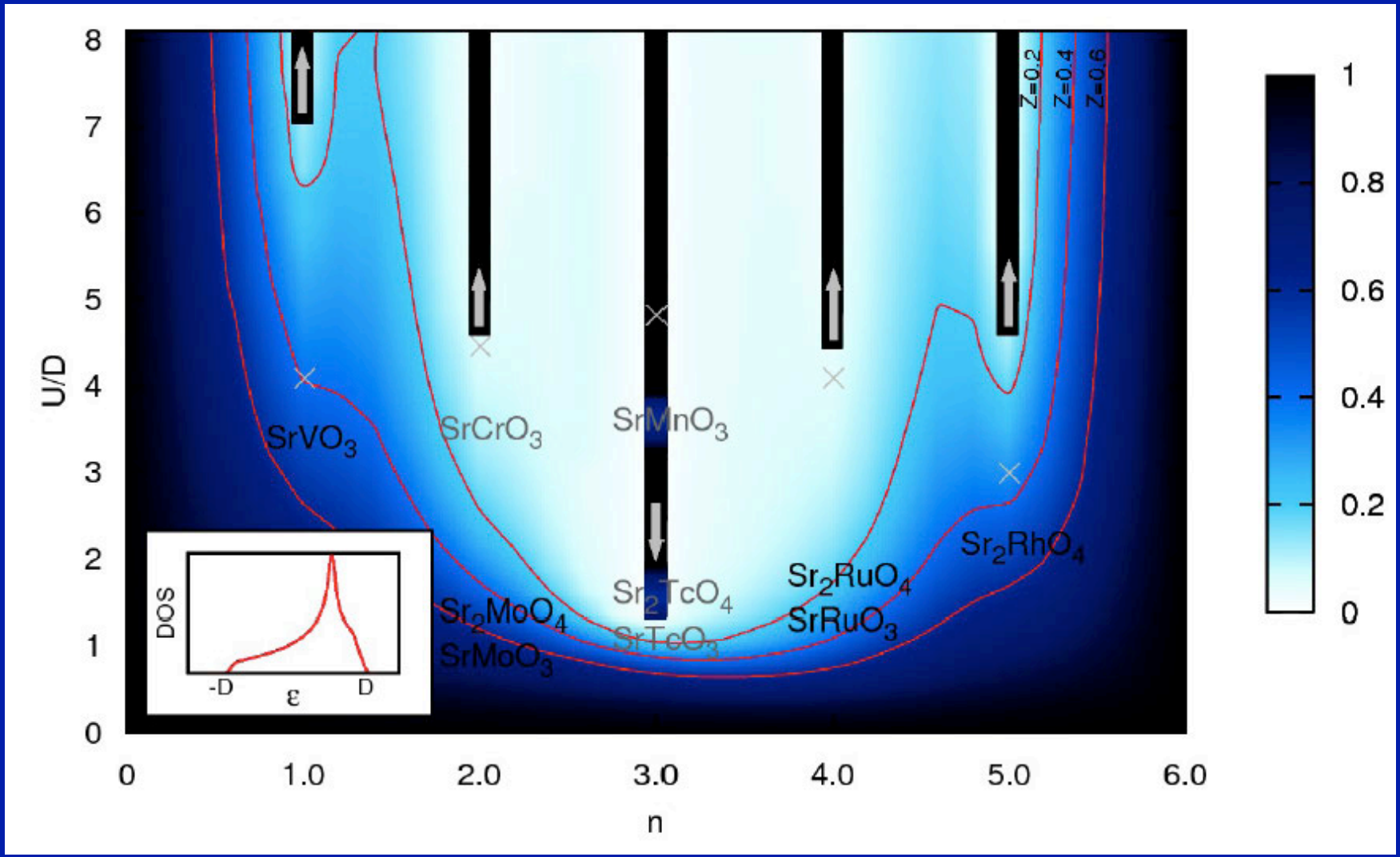



U/D
n
SrVO3
SrCrO3
SrMnO3
Sr2TcO4
SrTcO3
Sr2MoO4
SrMoO3
Sr2RuO4
SrRuO3
Sr2RhO4
Z=0.2
Z=0.4
Z=0.6
DOS
-D
ε
D

→ *Drawing a map of early transition-metal oxides (both 3d and 4d) with Hund's rule coupling as guidance*

and based on dynamical mean-field theory electronic-structure calculations

Color-intensity map of quasiparticle weight Z (~ m/m*)



3d oxides: U/D ~ 4 ; 4d oxides: U/D ~ 2

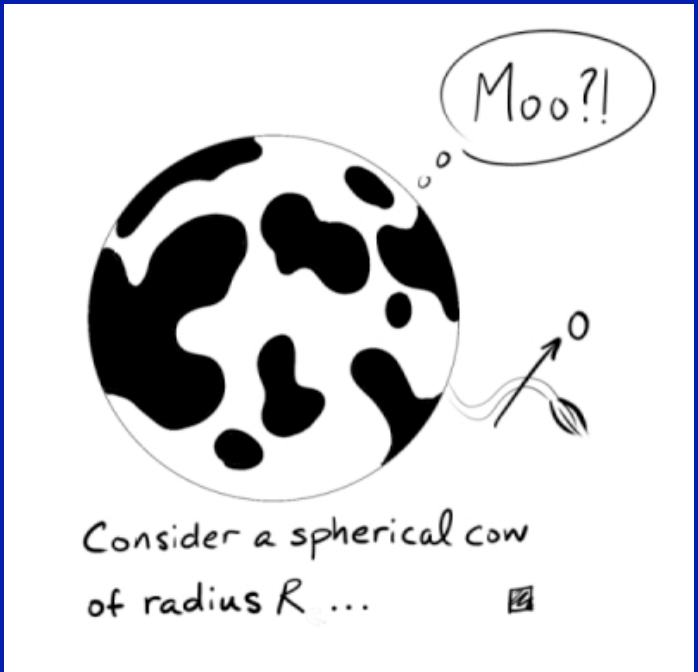
The happy marriage of DMFT with electronic structure (DFT)

An interdisciplinary effort
started in 1996 and still continuing today

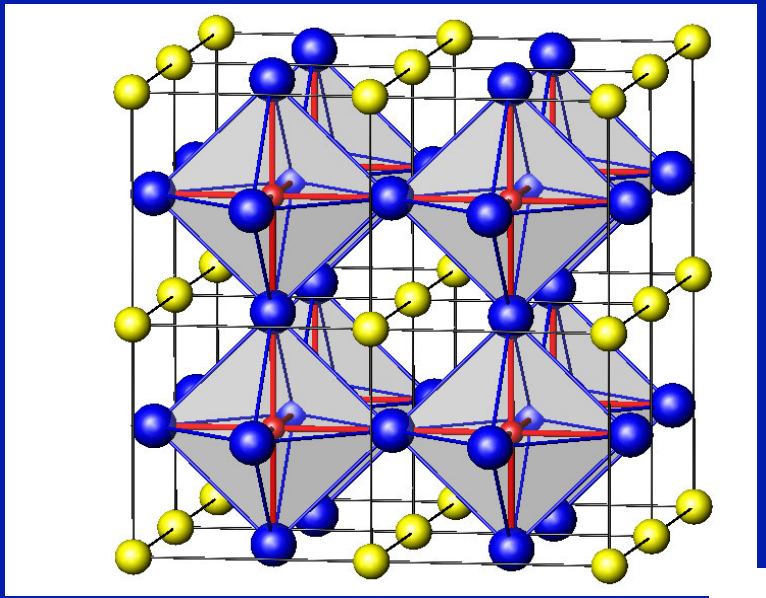
Anisimov, Kotliar et al. J.Phys Cond Mat 9, 7359 (1997)
Lichtenstein and Katsnelson Phys Rev B 57, 6884 (1998)

cf. lectures by A.Lichtenstein and by G.Kotliar

From spherical cow models…



… to real materials



$SrVO_3$

→ Rich interplay between: structural aspects, orbital degrees of freedom, various intra- and inter-orbital interactions, spin degrees of freedom, etc…

Real materials raise many fascinating puzzles…

Puzzle :
Why are 113 Vanadates Metallic while 113 Titanates are insulating ?

Interplay:
Structural distortion
→ Energetics of orbitals
→ Mott transition

Pavarini et al. PRL 92, 176403 (2004); NJP 7, 188 (2005)
See also recent work by Dang et al. arXiv:1309. 2995

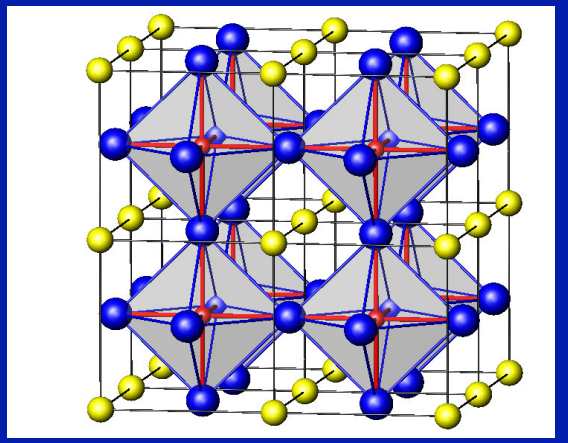
Vanadates and Titanates commonalities:

- 1 electron in the 3d shell
- Very similar values of the Hubbard U
- Similar electronic structure …

- $SrVO_3$ [V^{4+}, d^1]: A metal with signatures of sizeable but moderate e-e correlations ($m^*/m \sim 2.5$)
- $CaVO_3$ [V^{4+}, d^1]: A metal with stronger electronic correlations ($m^*/m \sim 3.5$)
- $LaTiO_3$ [Ti^{3+}, d^1]: A small-gap insulator (~0.2 eV)
- $YTiO_3$ [Ti^{3+}, d^1]: A larger gap insulator (~ 1eV)

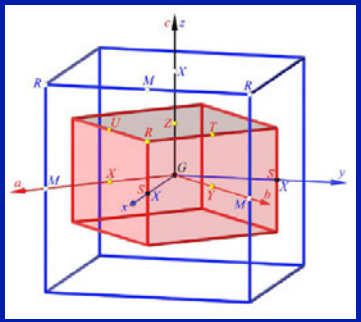
WHY ?

From a band-structure (DFT-LDA) point of view, they are all metals with a single electrons in t_{2g}-like bands…



$SrVO_3$

Pavarini et al.
PRL 92 (2004) 176403
New J.Phys 7 (2005) 188
Amadon et al.
PRB 77 (2008) 205112



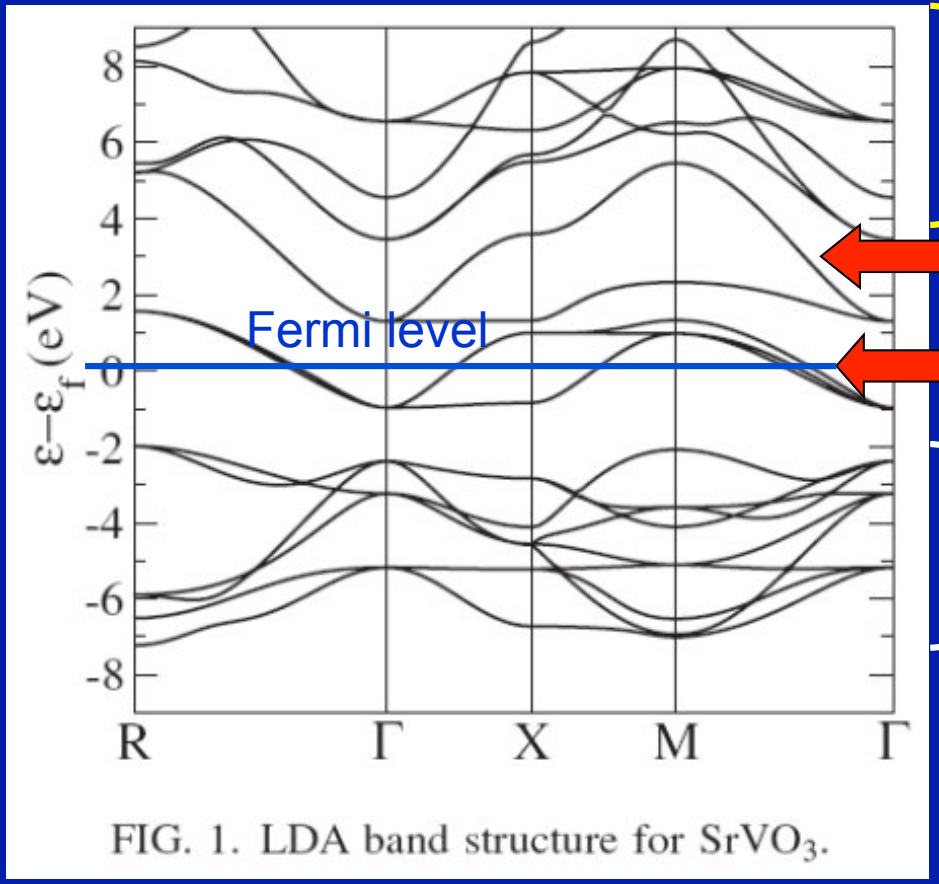


FIG. 1. LDA band structure for $SrVO_3$.

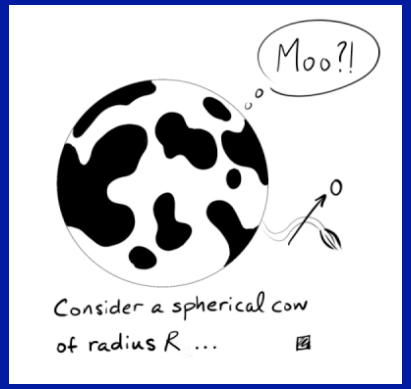
Sr 5s and 4d

2 V-eg bands

3 V-t2g bands

9=3*3 Oxygen bands

The answer…



``It's the bandwidth reduction, stupid…"

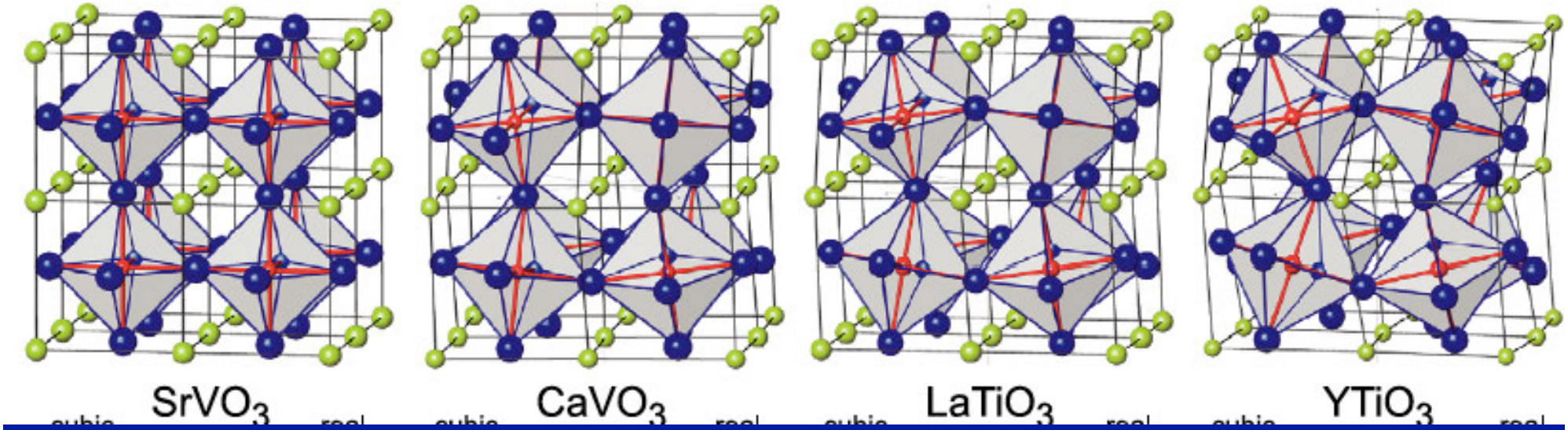


Table 8. t_{2g} edge-to-edge ($W_{t_{2g}}$) and rms (W) bandwidths in eV.

	$SrVO_3$ [42]	$CaVO_3$ [43]	$LaTiO_3$ [44]	$LaTiO_3$ [12]	$YTiO_3$ [20]
$W_{t_{2g}}$	2.85	2.45	2.09	1.92	2.05
W	2.85	2.39	2.18	2.08	1.87

Important effect but insufficient to explain MIT (U ~ 3-4 eV)

Key to solving the puzzle:
lifting of t_{2g} degeneracy
due to structural distortion
→ lowers considerably critical U

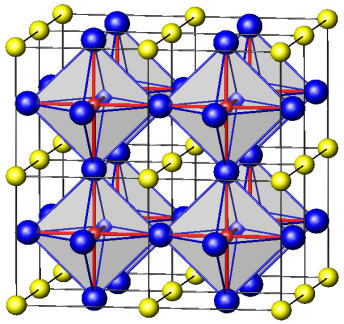
Splitting: up to 200 meV for LaTiO3, up to 330 meV for YTiO3

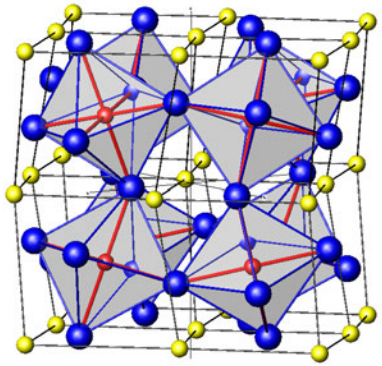
1 electron in:
3 degenerate orbitals, J/U=0.15 → $U_c/W \sim 3.5$
1 single orbital → $U_c/W \sim 1.5$

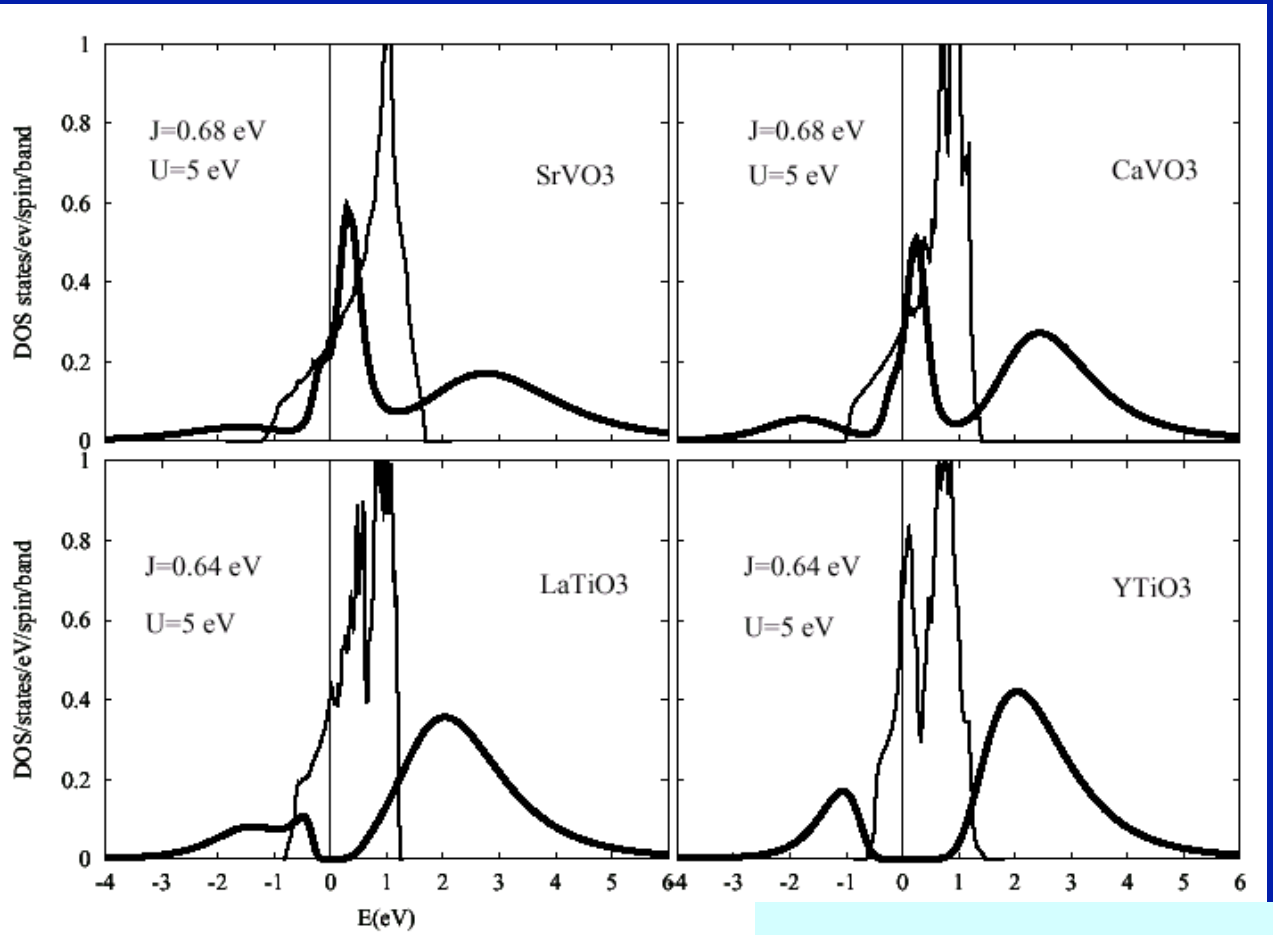
Pavarini et al. PRL 92, 176403 (2004); NJP 7, 188 (2005)

Maybe Andy will comment and elaborate on related aspects
In his talk on transition-metal oxides ?

Electronic structure + Many-Body (DMFT) calculations: accouting for metallic/insulating nature of vanadates/titanates







E.Pavarini et al., PRL 2004

cf. also Sekiyama et al. (Ca/SrVO3) PRL 2004

- **Narrowing of quasiparticle bands** due to correlations (the Brinkman-Rice phenomenon)
- **Hubbard satellites** (i.e extension to the solid of atomic-like transitions)

Quantitative comparison with experiments

quasiparticles + lower Hubbard band clearly resolved
in bulk-sensitive photoemission experiments

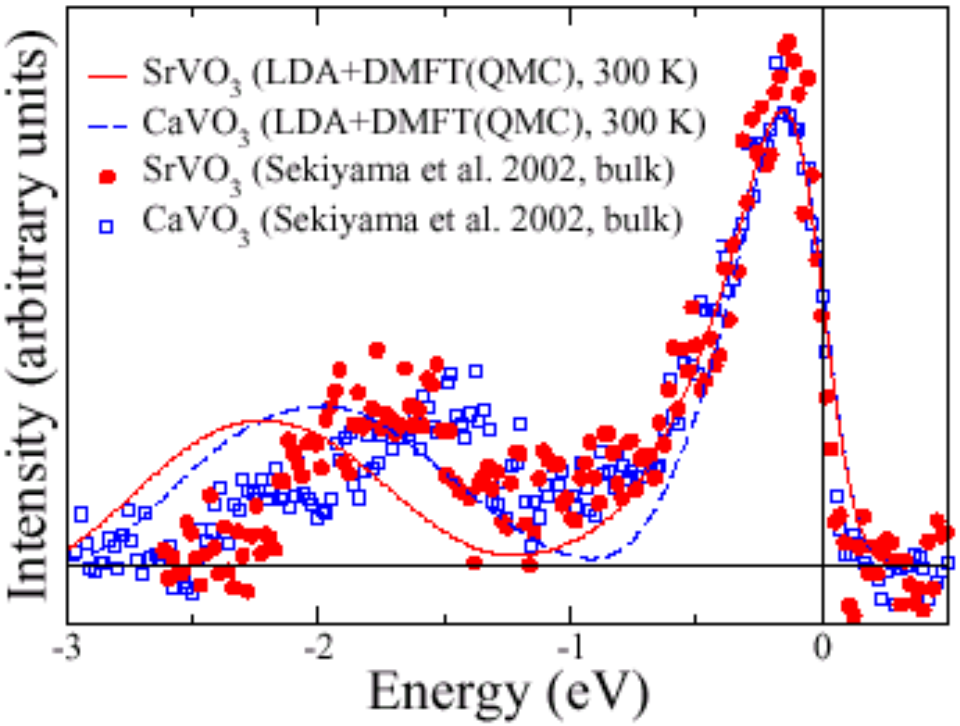


FIG. 4: Comparison of the calculated, parameter-free LDA+DMFT(QMC) spectra of $SrVO_3$ (solid line) and $CaVO_3$ (dashed line) with bulk-sensitive high-resolution PES ($SrVO_3$: circles; $CaVO_3$: rectangles) [4]. Horizontal line: experimental subtraction of the background intensity.

Sekiyama et al,
Ca/SrVO3

Beyond single-site DMFT:
- Momentum-dependence
- How magnetic correlations affect quasiparticles

From a single-site embedding to a cluster: "Molecular" DMFTs

cf. lectures by E.Koch, M.Potthoff

Accounting for short-range correlations and momentum dependence: Cluster extensions of DMF T.

For reviews see:

→ Talk by Andre-Marie Tremblay

[27] T. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, Rev. Mod. Phys. **77**, 1027 (2005).

[28] G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianett, Rev. Mod. Phys. **78**, 865 (2006).

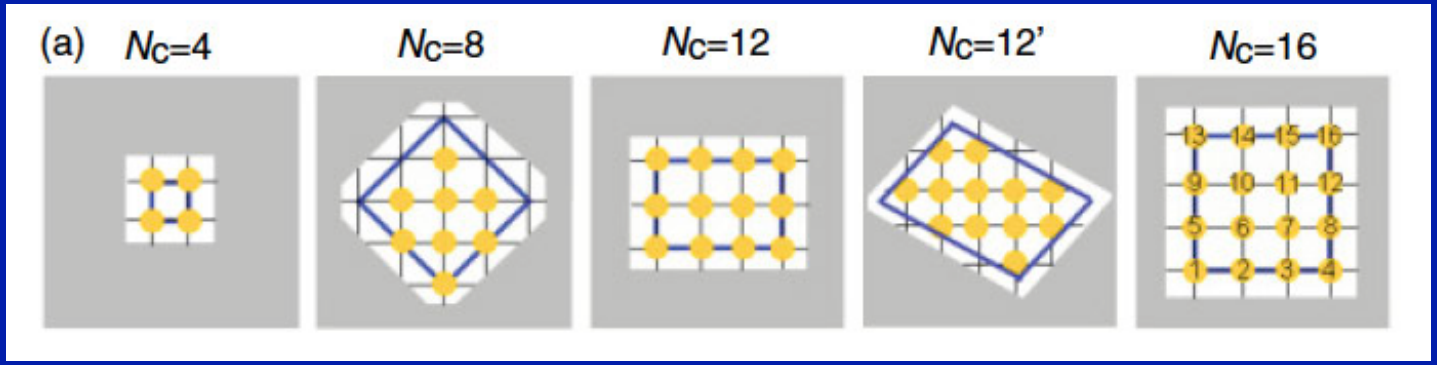
[29] A. M. S. Tremblay, B. Kyung, and D. Senechal, Low Temp. Phys. **32**, 424 (2006).

Numerous works by several groups in the last ~ 12 years:
Cincinatti/Baton Rouge (Jarrell et al.), Rutgers (Kotliar, Haule et al.), Sherbrooke (Tremblay, Senechal et al., Kyung, Sordi), Columbia (Millis et al., Gull)., Oak Ridge (Maier et al.), Tokyo (Imada, Sakai et al.) Hamburg(Lichtenstein et al.), Rome (Capone et al.) Paris/Saclay/Orsay (Parcollet, Ferrero, AG, Civelli et al.), etc…

Single-site mean-field → `Molecular' mean-field (cf. Bethe-Peierls, Kikuchi)

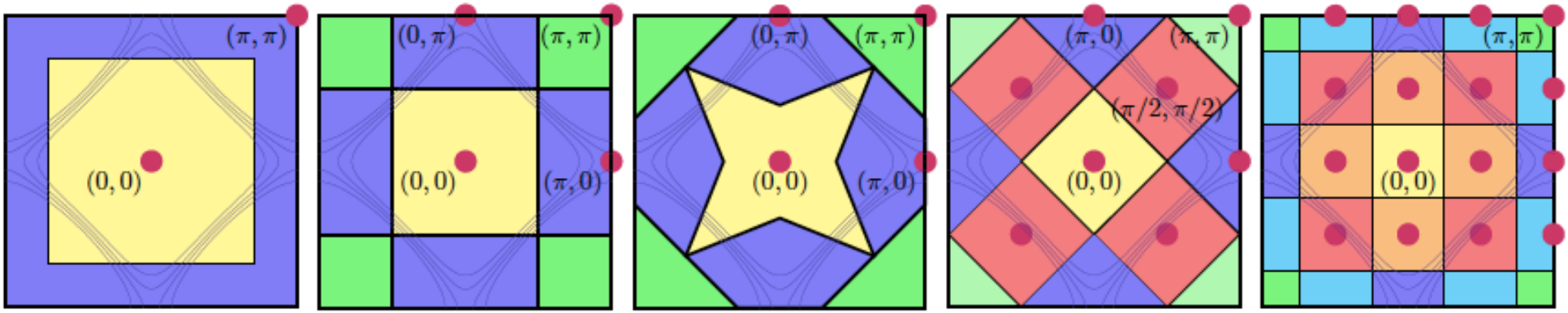
A cluster of sites coupled to an environment

C-DMFT: real-space cluster (cf. "cavity construction").



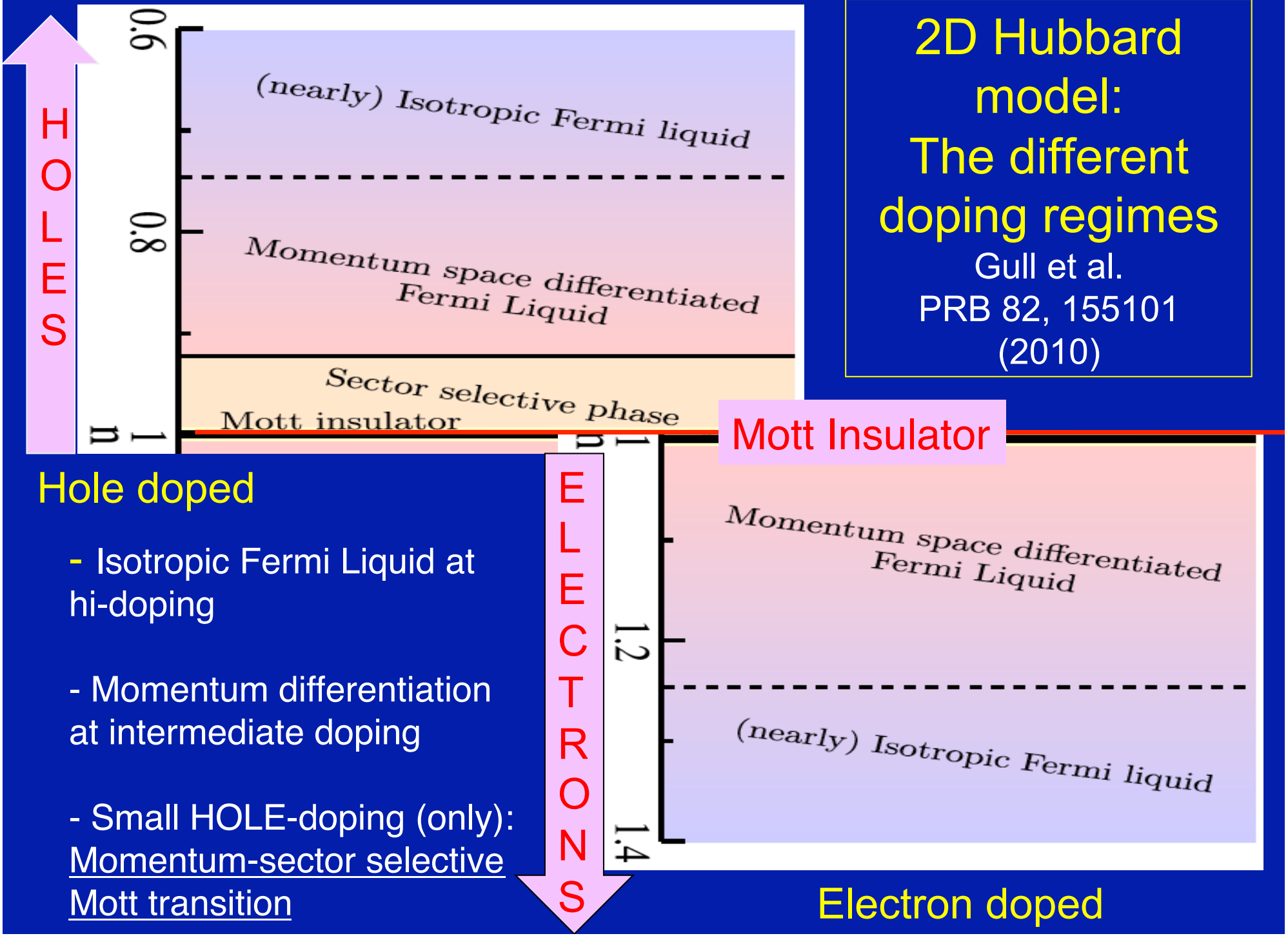
DCA: Patching momentum-space, cluster used to calculate self-energy at cluster momenta. PBC by construction.

Note: patches can be adapted to best capture the physics.



2D Hubbard model: The different doping regimes

Gull et al.
PRB 82, 155101 (2010)



Hole doped

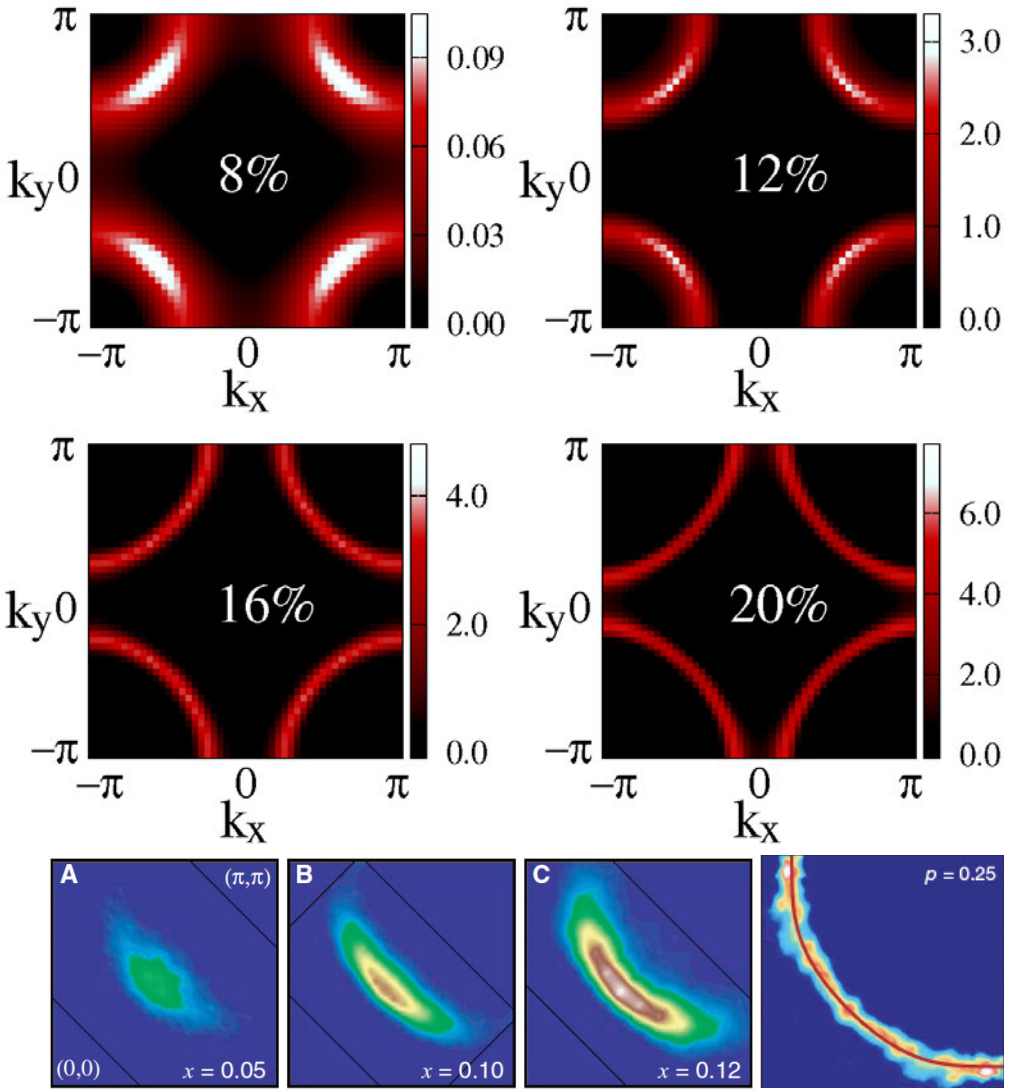
- Isotropic Fermi Liquid at hi-doping

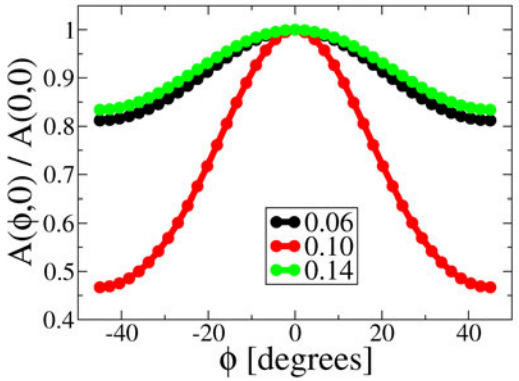
- Momentum differentiation at intermediate doping

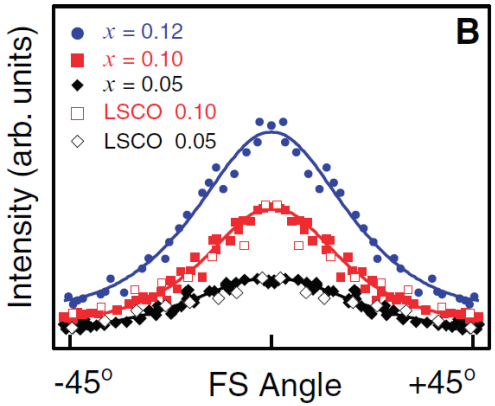
- Small HOLE-doping (only): Momentum-sector selective Mott transition

Electron doped

Calculated ARPES intensity maps [many cluster studies, e.g. early work by Rutgers group (Civelli, Parcollet et al) and Sherbrooke group]







Shen et al., Science (2005)

Shrinking of Fermi arcs as doping is reduced:
a very different route to the Mott insulator than Brinkman-Rice

As we flow down from high energy to lower energy, range of spatial correlations will grow and 1-site DMFT may become increasingly inaccurate

Starting from:
- High-temperature /
- High-energy /
- High-doping level /
- Large frustration t’ /t, etc.

All these can be viewed as control parameters
~ range of spatial correlations

cf. A.G Ann. Phys. 523, 672 (2011)
arXiv:1112.5212
cf. W.Metzner’s lecture

DMFT is a compass to orient oursleves when flowing down in energy

…or perhaps a booster rocket (W.Metzner’s lecture)

What’s next ?

(Much) advance needed on momentum-dependence (i.e. including spatial correlations)

- Cluster extensions of DMFT are now reaching their limits (in my opinion)
- Possibly promising route: using DMFT in the context of lattice diagrammatic Monte-Carlo, i.e. resum all local diagrams using DMFT
- Other routes: dual fermions, dynamical vertex approximation, etc.

Electronic Structure; Materials; New Directions

- Get rid of DFT-LDA ! (and associated double-counting issues)
- Fully diagrammatic / Green's function based approaches e.g. GW+DMFT

→ Lectures by A.Lichtenstein, G.Kotliar

- Non-equlibrium → Lecture by M.Kollar
- Applications to other fields e.g. molecular (bio-)chemistry e.g. transition metal ions in enzymes

Take-home message

- Quantitative theory has come a long way in 2 decades…
- Tremendous progress on materials and on experimental/instrumental techniques
- Theory is coming of age: semi-quantitative calculations become possible, with material-specific realism, with predictive capabilities
- Creative techniques and ideas around for control and materials design

We now have a theoretical and practical framework, which :

- Takes a radically different point of view on the electronic structure of solids than the “standard model” of solid-state physics
- Is not faced with the limitations of the `standard model’ when dealing with strongly correlated systems/localized orbitals
- Uses a language much closer to that of the chemist: ATOMS - atomic orbitals, bonding and hybridization (rather than Bloch bands)
- → Hence making realistic understanding, perhaps even design of correlated materials possible

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