COLLÈGE DE FRANCE
1530

Chaire de Physique
de la Matière Condensée
Antoine Georges

Fermions en interaction: Introduction à la théorie de Champ Moyen Dynamique (DMFT)

Cours 1 – Motivations, Concept

Cycle 2018-2019
7 mai 2019

COLLÈGE DE FRANCE
1530

Chaire de Physique
de la Matière Condensée
Antoine Georges

Interacting Fermions: Introduction to Dynamical Mean-Field Theory (DMFT)

Lecture 1 –Motivations, Concept

Slides will be in English

Please don't hesitate to ask questions in French or English

2018-2019 Lectures
May 7, 2019

Today's seminar (11:30)

Michel Ferrero

Ecole Polytechnique, CPHT

and Collège de France

Were Fermions Born Under a Bad Sign ?

Mailing List

(Weekly announcement of lecture and seminar, etc.)

Send email to: listes-diffusion.cdf@college-de-france.fr
Subject line: subscribe chaire-pmc.ipcdf
…or: unsubscribe chaire-pmc.ipcdf

Website:

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

Lectures from this year (and 2016-2017) are video recorded
PDF and Audio of lectures available for all years
PDF for (almost) all seminars

7 mai 2019 Séance de cours
Séminaire : “Were fermions born under a bad sign ?”
Michel FERRERO, *CPHT-Ecole Polytechnique et Collège de France*

14 mai 2019 Séance de cours
Séminaire : “Nonequilibrium extensions of dynamical mean field theory”
Philipp WERNER, *université de Fribourg, Suisse*

21 mai 2019 Séance de cours
Séminaire : “Excitonic condensation of strongly correlated electrons”
Jan KUNES, *TU-Wien and Czech Academy of Sciences, Prague*

Mercredi 22 mai (exceptionnel) Séminaire par Andrew J.Millis – 11h00, Salle 5

28 mai 2019 Deux séances de cours

4 juin 2019 Pas de cours (2 conférences à Paris)

11 juin: Cours, Séminaire et Colloque/Workshop

11 juin 2019 Séance de cours

Séminaire : "Unifying spin-fluctuations and DMFT: TRILEX and vertex-based methods"

Olivier PARCOLLET, *Flatiron Institute, New York et IPhT, CEA-Saclay*

Colloque le mardi 11 juin 2019 de 14h à 18h30

5 séminaires - Salle 2

``Dynamical Mean Field Theory and Beyond: Recent Developments''

Orateurs : Manuel ZINGL, Jernej MRAVLJE, Hugo STRAND, Alessandro TOSCHI, Malte RÖSNER

June 11 workshop - program

Dynamical Mean-Field Theory and Beyond:

Recent Developments

(Talks are 30' plus 15' discussion)

14:00-14:45 Manuel Zingl (CCQ, Flatiron Institute). ***Recent insights on Sr_2RuO_4: High-resolution photoemission and Hall effect***

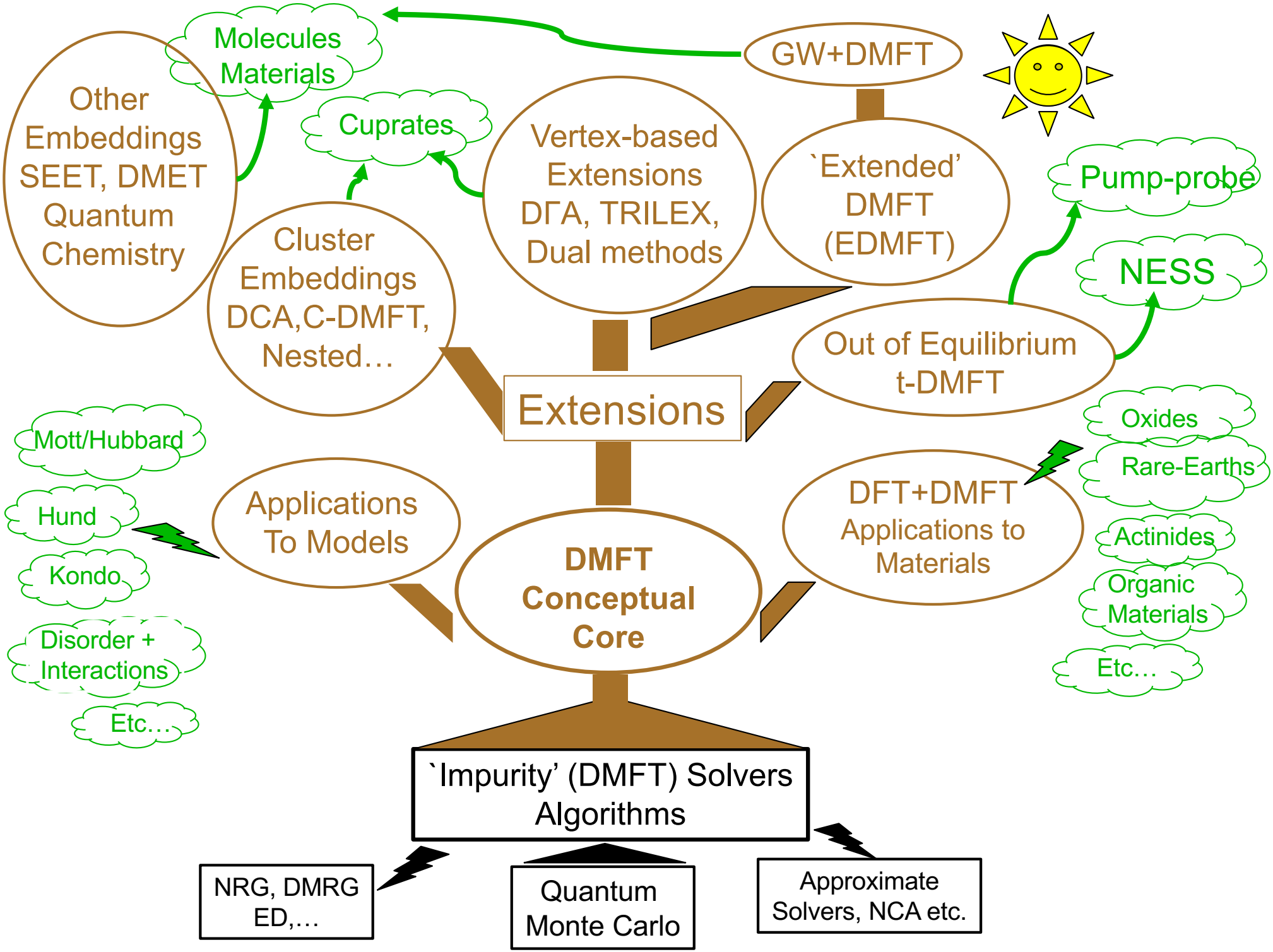
14:45-15:30 Jernej Mravlje (Jožef Stefan Institute, Ljubljana). ***Hund's metals: overview, NRG insights, and the role of spin-orbit coupling***

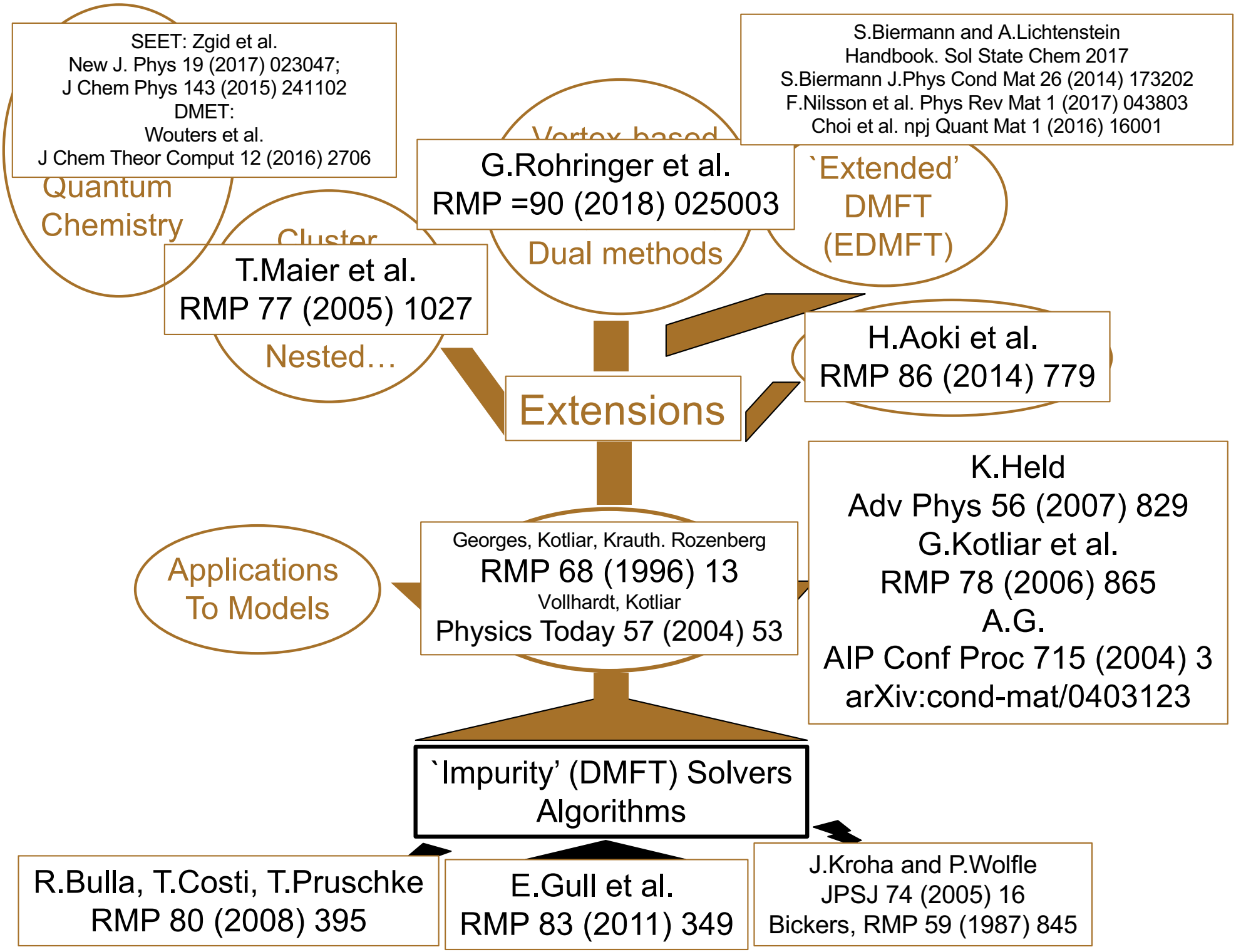
15:30-16:15 Hugo Strand (CCQ, Flatiron Institute). ***Magnetic response of a Hund's metal within DMFT: Sr_2RuO_4***

16:15-17:00 Break

17:00-17:45 Alessandro Toschi (IFP – TU Wien). ***Fluctuation diagnostics of many-electron systems: How to read between the lines of single-particle spectra***

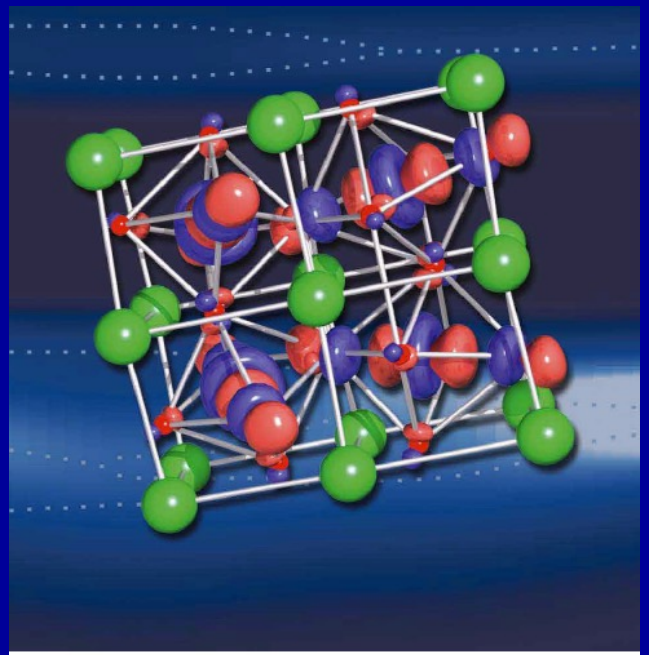
17:45-18:30 TBA


Molecules
Materials
GW+DMFT
Other
Embeddings
SEET, DMET
Quantum
Chemistry
Cuprates
Vertex-based
Extensions
DΓA, TRILEX,
Dual methods
`Extended'
DMFT
(EDMFT)
Pump-probe
NESS
Cluster
Embeddings
DCA,C-DMFT,
Nested…
Out of Equilibrium
t-DMFT
Extensions
Mott/Hubbard
Hund
Kondo
Disorder +
Interactions
Etc…
Applications
To Models
DMFT
Conceptual
Core
DFT+DMFT
Applications to
Materials
Oxides
Rare-Earths
Actinides
Organic
Materials
Etc…
`Impurity' (DMFT) Solvers
Algorithms
NRG, DMRG
ED,…
Quantum
Monte Carlo
Approximate
Solvers, NCA etc.


SEET: Zgid et al.
New J. Phys 19 (2017) 023047;
J Chem Phys 143 (2015) 241102
DMET:
Wouters et al.
J Chem Theor Comput 12 (2016) 2706
Quantum Chemistry
S.Biermann and A.Lichtenstein
Handbook. Sol State Chem 2017
S.Biermann J.Phys Cond Mat 26 (2014) 173202
F.Nilsson et al. Phys Rev Mat 1 (2017) 043803
Choi et al. npj Quant Mat 1 (2016) 16001
G.Rohringer et al.
RMP =90 (2018) 025003
Dual methods
`Extended' DMFT (EDMFT)
T.Maier et al.
RMP 77 (2005) 1027
Nested…
H.Aoki et al.
RMP 86 (2014) 779
Extensions
K.Held
Adv Phys 56 (2007) 829
G.Kotliar et al.
RMP 78 (2006) 865
A.G.
AIP Conf Proc 715 (2004) 3
arXiv:cond-mat/0403123
Applications To Models
Georges, Kotliar, Krauth. Rozenberg
RMP 68 (1996) 13
Vollhardt, Kotliar
Physics Today 57 (2004) 53
`Impurity' (DMFT) Solvers Algorithms
R.Bulla, T.Costi, T.Pruschke
RMP 80 (2008) 395
E.Gull et al.
RMP 83 (2011) 349
J.Kroha and P.Wolfle
JPSJ 74 (2005) 16
Bickers, RMP 59 (1987) 845

Jülich Autumn School on Correlated Electrons

Book series – available as free eBooks

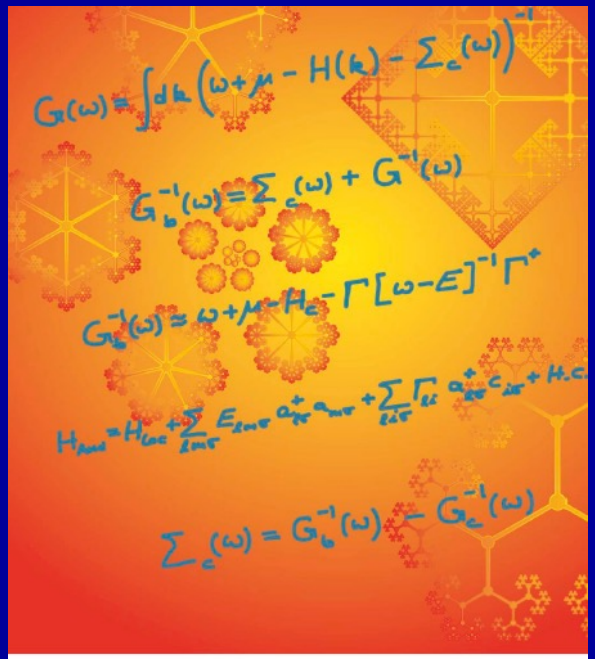


The LDA+DMFT approach to strongly correlated materials

Eva Pavarini, Erik Koch, Dieter Vollhardt, and Alexander Lichtenstein (Eds.)

German Research School for Simulation Sciences

JÜLICH FORSCHUNGSZENTRUM



DMFT at 25: Infinite Dimensions

Eva Pavarini, Erik Koch, Dieter Vollhardt and Alexander Lichtenstein (Eds.)

German Research School for Simulation Sciences

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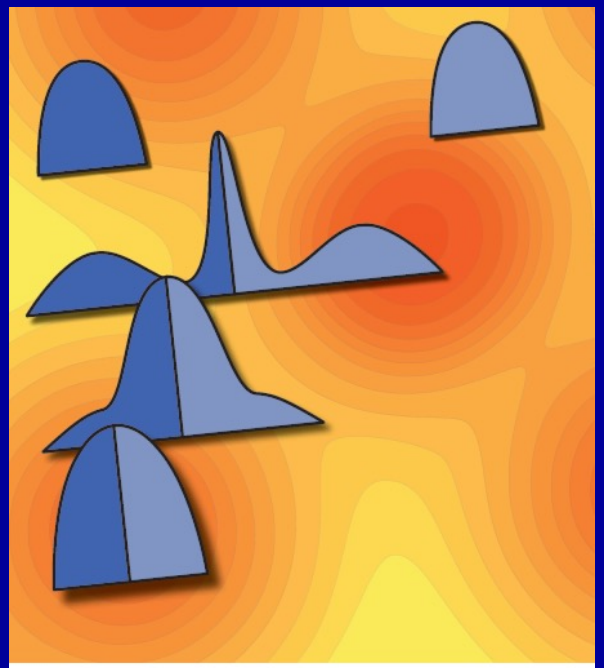
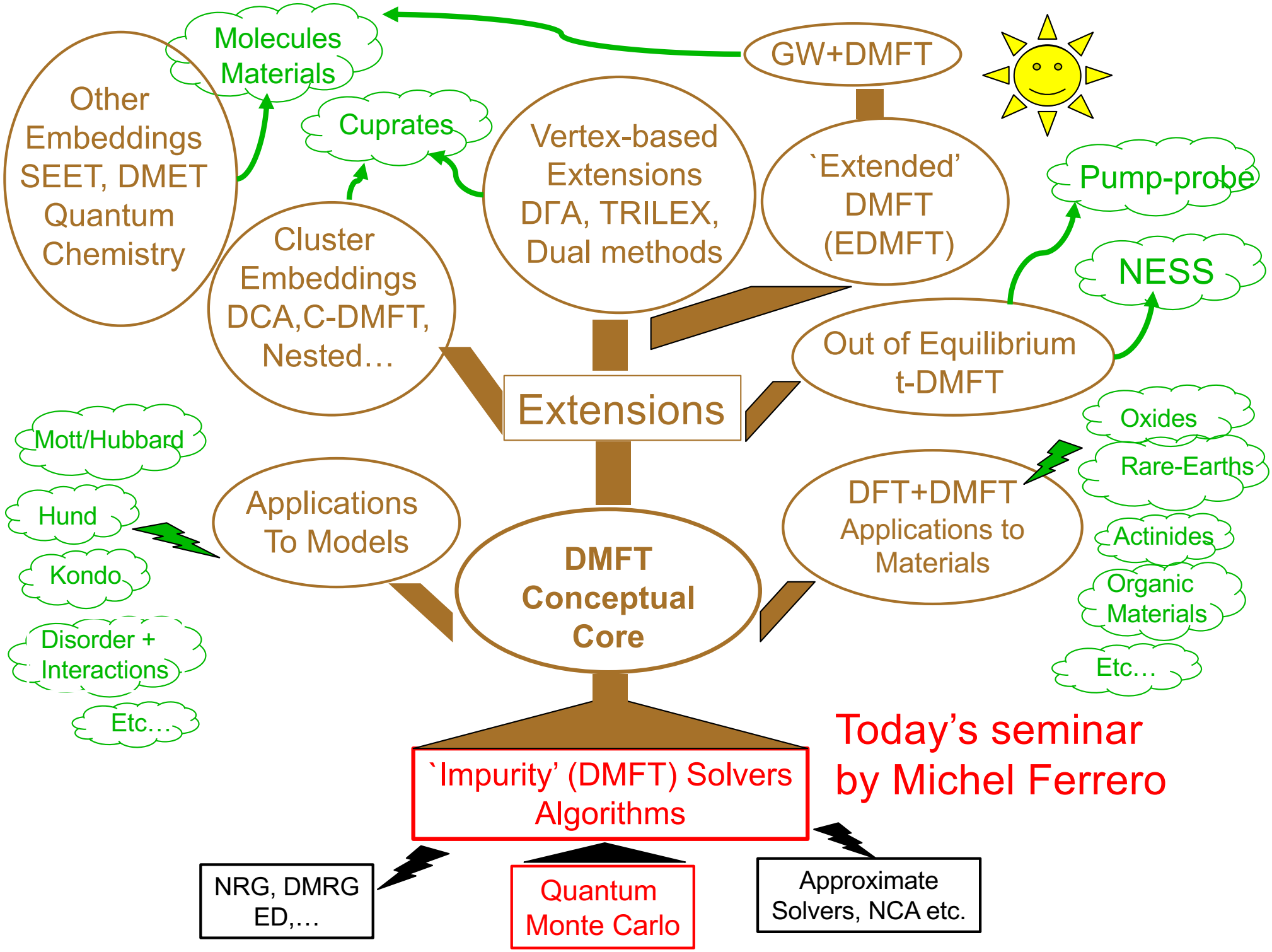


DMFT: From Infinite Dimensions to Real Materials

Eva Pavarini, Erik Koch, Alexander Lichtenstein, and Dieter Vollhardt (Eds.)

JÜLICH Forschungszentrum

https://www.cond-mat.de/events/correl.html


Molecules
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Applications to
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Rare-Earths
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Organic
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Etc…
`Impurity' (DMFT) Solvers
Algorithms
Today's seminar
by Michel Ferrero
NRG, DMRG
ED,…
Quantum
Monte Carlo
Approximate
Solvers, NCA etc.

The `Quantum Many-Body' Research Agenda – Born 1929 !

Quantum Mechanics of Many-Electron Systems.

By P. A. M. Dirac, St. John's College, Cambridge.

(Communicated by R. H. Fowler, F.R.S.—Received March 12, 1929.)

§ 1. *Introduction.*

The general theory of quantum mechanics is now almost complete, the imperfections that still remain being in connection with the exact fitting in of the theory with relativity ideas. These give rise to difficulties only when

P. A. M. Dirac, "Quantum Mechanics of Many-Electron Systems“, Proceedings of the Royal Society of London, Series A, Vol.123, April 1929, pp 714.

Paul Dirac, 1929
``Quantum Mechanics of Many-Electron Systems''

``The general theory of quantum mechanics is now almost complete (...). The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

P. A. M. Dirac, "Quantum Mechanics of Many-Electron Systems“, Proceedings of the Royal Society of London, Series A, Vol.123, April 1929, pp 714.

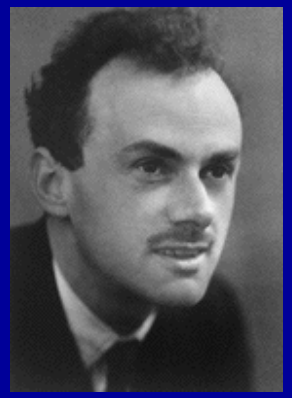
Quantum Mechanics of 10^{21} interacting particles !

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_i v_{ion}(\vec{r}_i) + \frac{1}{2}\sum_{i,j}\frac{e^2}{4\pi\varepsilon_0|r_i - r_j|}$$

$$H\Psi(r_1, \cdots, r_N) = E\Psi(r_1, \cdots, r_N)$$

Eigenstates (wave-functions)
and Eigenvalues (Energy spectrum)

`Dirac's program' (same 1929 article):



`` 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."

Dirac's program is not yet fully implemented but key progress has been made.
Note that ``*without too much computation*" has an entirely different meaning now than in the 1930's ☺

Why are interacting fermion systems hard problems ?

- Exponential size of the Hilbert space ~ $\exp(10^{23})$

→ Exact diagonalisation only handles (very) small systems

- Alternating sign of fermionic quantum-mechanical amplitudes

→(Direct) Quantum Monte-Carlo is in trouble

→See seminar by Michel Ferrero

Continuous progress in algorithms and computational methods: a crucial line of research !

Why is diagonalizing the Hamiltonian (very) hard ?

Consider a `simple' model: a chain of N electrons, which are localized so the only remaining degree of freedom is their spin – can take two values on each site

Basis of configuration space:

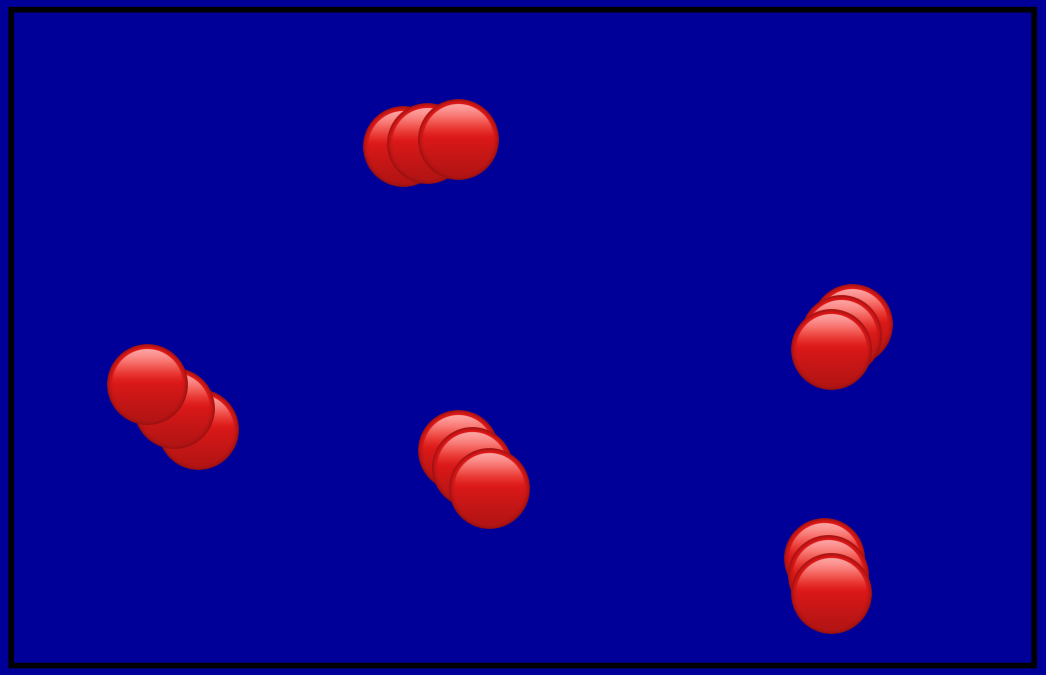
$$|\sigma_1, \cdots, \sigma_N\rangle \quad , \quad \sigma_i = \pm 1$$

2^N states ! Grows exponentially in N...Try thinking of Exp[10^{21}] …

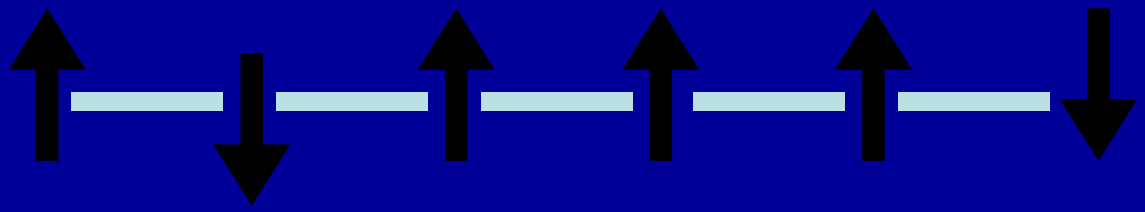
State vector (wave-function):

$$|\Psi\rangle = \sum_{\sigma_1 \cdots \sigma_N} c_{\sigma_1 \cdots \sigma_N} |\sigma_1, \cdots, \sigma_N\rangle$$

Storing it is already very hard, let alone computing it…



From particles… to spins in a line



In Quantum Mechanics, the Hamiltonian is an operator acting on these state vectors

Heisenberg Model:

$$\hat{H} = J \sum_i S_i^z S_{i+1}^z + J_\perp \sum_i \left[S_i^+ S_{i+1}^- + S_{i+1}^+ S_i^- \right]$$

$$S^z|\sigma\rangle = \sigma|\sigma\rangle \ , \ S^+|-\rangle = |+\rangle \ , \ S^-|+\rangle = |-\rangle$$

With only J-term: energy spectrum easy to evaluate classical Ising)

With second term: diagonalization of a $2^N * 2^N$ (sparse) matrix

Model is directly relevant to (quantum) Magnets

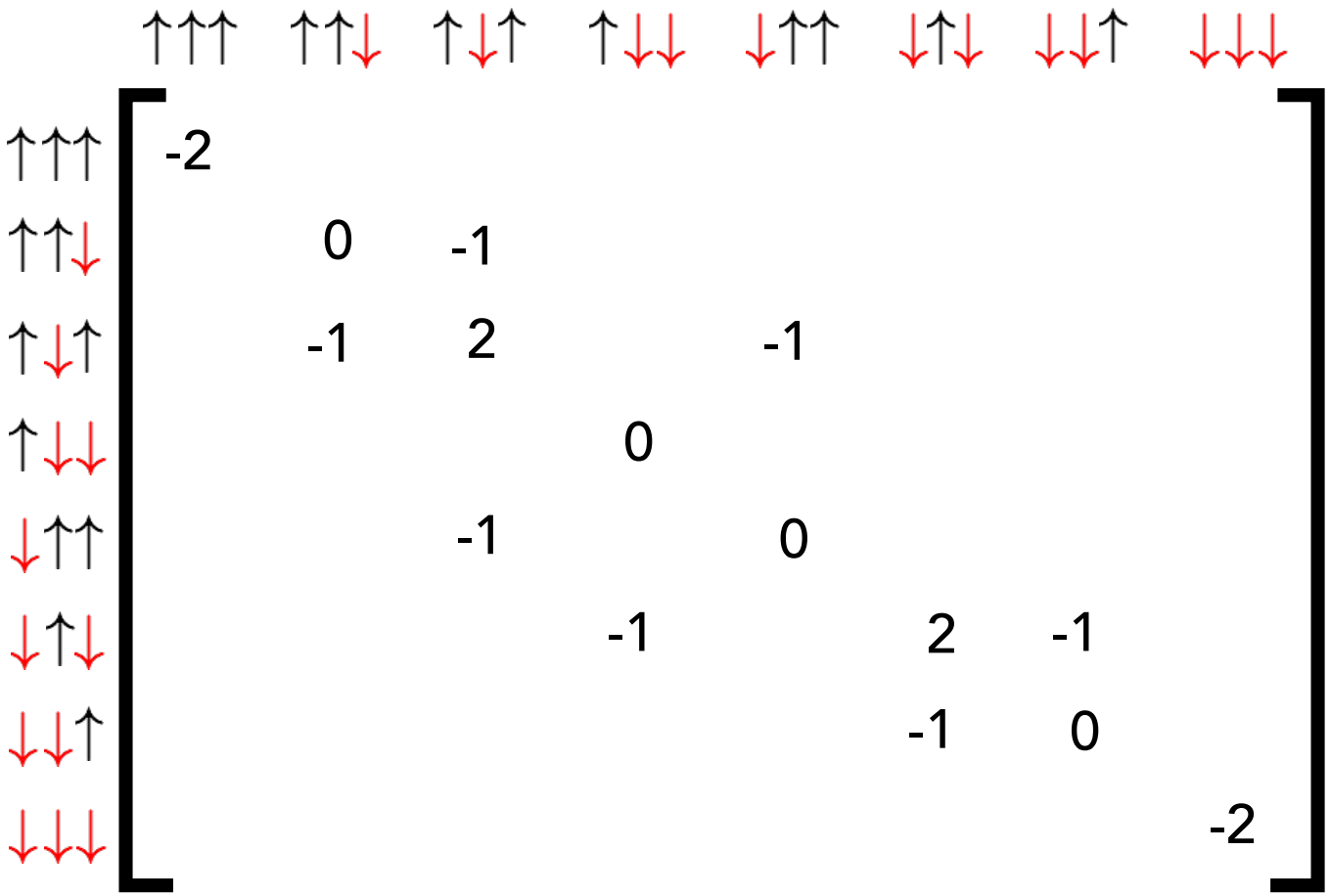
Energy matrix (Hamiltonian $\hat{H}$) acts on space of all configurations

$N = 2$ example

$$\hat{H} = \begin{array}{c} \\ \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{array} \begin{array}{c} \begin{array}{cccc} \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow \end{array} \\ \begin{bmatrix} -1 & & & \\ & 1 & -1 & \\ & -1 & 1 & \\ & & & -1 \end{bmatrix} \end{array}$$

Energy matrix (Hamiltonian $\hat{H}$) acts on space of all configurations

$N = 3$ example



N=4 case can hardly fit on slide…

Efficient algorithms for evaluating eigenvectors of sparse matrices e.g. Lanczos

Current record, using symmetries and many tricks

50 spins !

… not quite 10^{21}

PHYSICAL REVIEW E **98**, 033309 (2018)

Sublattice coding algorithm and distributed memory parallelization for large-scale exact diagonalizations of quantum many-body systems

Alexander Wietek* and Andreas M. Läuchli
Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria

(Received 18 April 2018; published 26 September 2018)

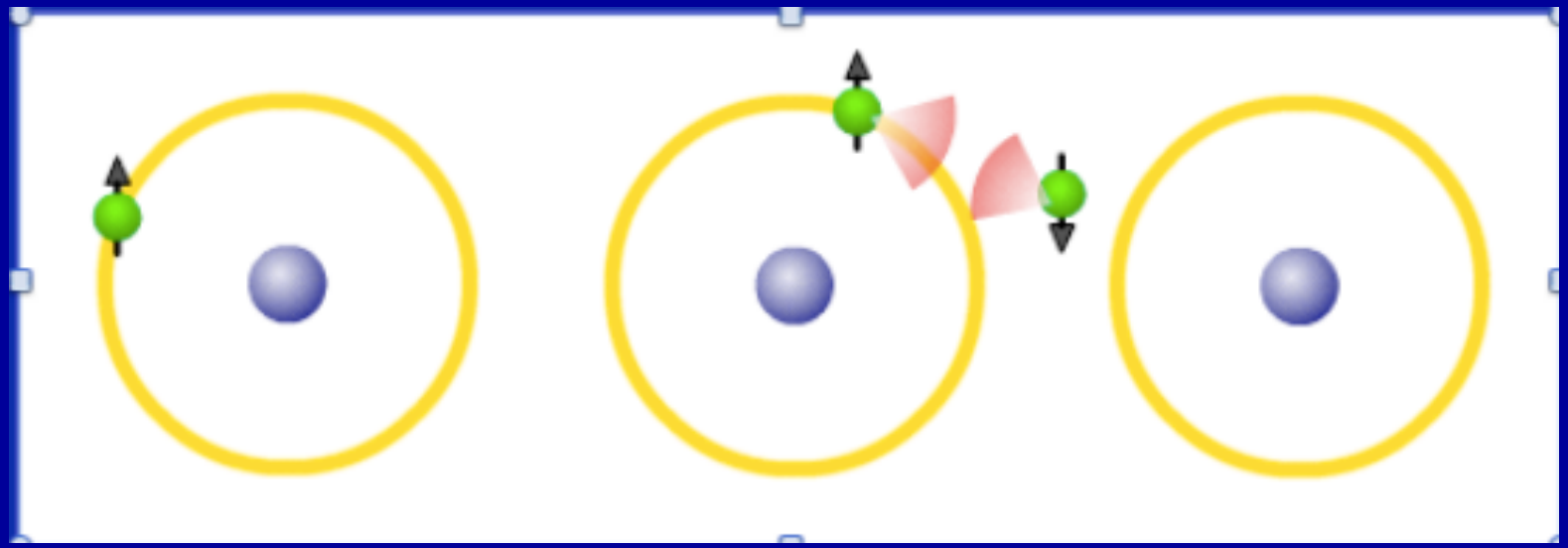
We present algorithmic improvements for fast and memory-efficient use of discrete spatial symmetries in exact diagonalization computations of quantum many-body systems. These techniques allow us to work flexibly in the reduced basis of symmetry-adapted wave functions. Moreover, a parallelization scheme for the Hamiltonian-vector multiplication in the Lanczos procedure for distributed memory machines avoiding load-balancing problems is proposed. We demonstrate that using these methods low-energy properties of systems of up to 50 spin-1/2 particles can be successfully determined.

DOI: 10.1103/PhysRevE.98.033309

Simplest « toy model » with mobile electrons: The Hubbard model (Hilbert space: 4^N)

$$-t \sum_{\langle ij \rangle} \sum_{\sigma=\uparrow,\downarrow} (c^+_{i\sigma} c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

4 states per site: $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$



t: Tunnel amplitude (electron hopping between sites)

U: On-site matrix element of screened Coulomb interaction

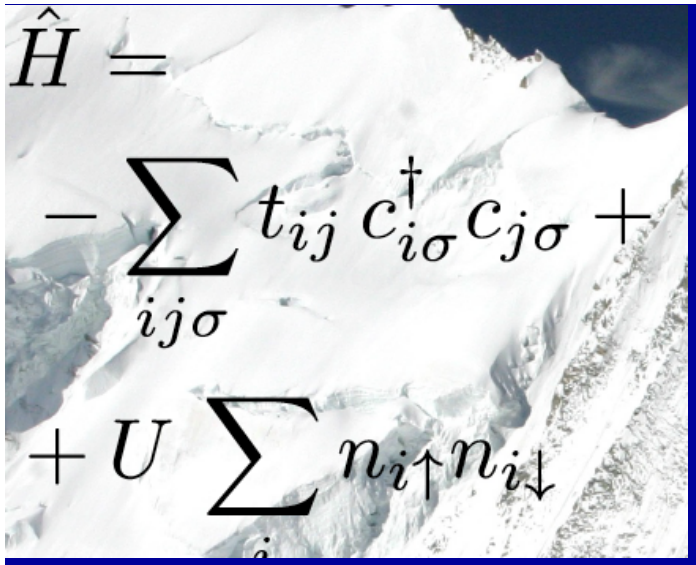
Despite its simple formulation
the Hubbard model
is far from being `solved'
and even qualitatively understood

Except in some cases such as:

- ONE spatial dimension
- INFINITE spatial dimensions

Especially relevant: d=2

The Hubbard model plays a somewhat similar role
for many-body quantum physics
to that of the Ising model in classical statistical mechanics
And we are living in pre-Onsager days (< 1942)…

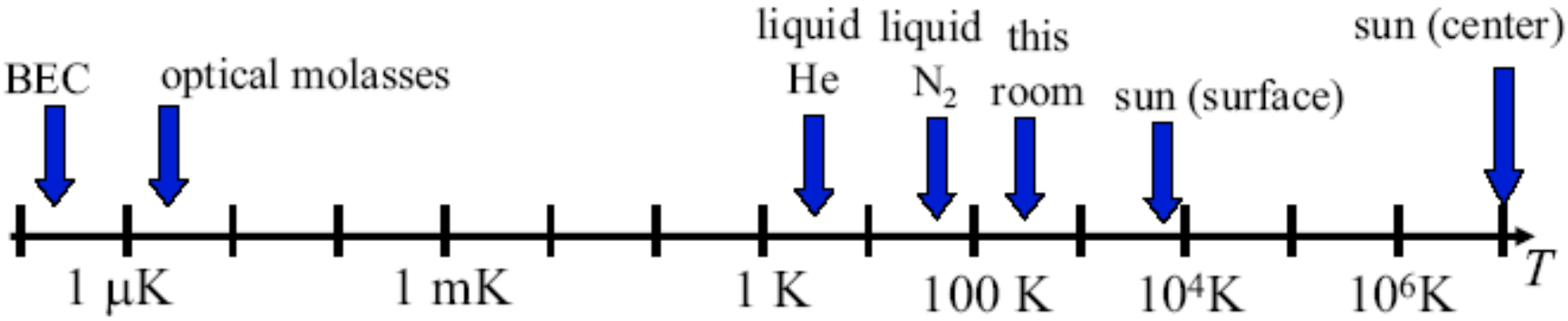


The Hubbard model is no longer only a Toy Model !

A new frontier at the interface of Condensed Matter Physics and Quantum Optics:

Ultra-Cold Atomic Gases in Optical Lattices

Ultra-Cold Atomic Gases



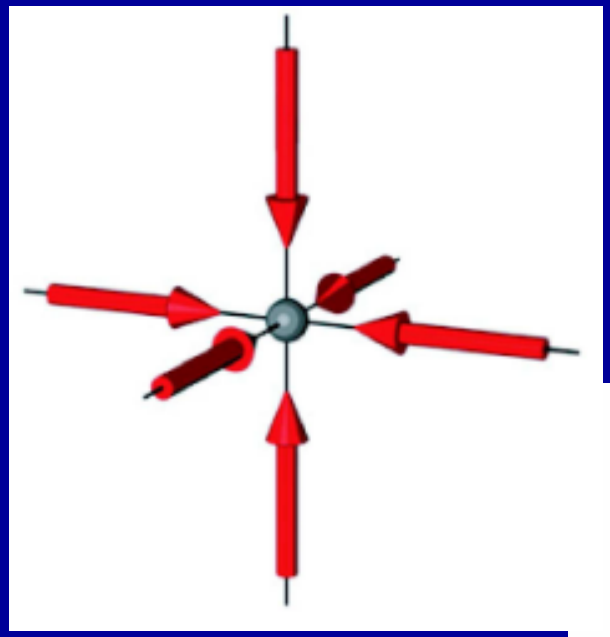
BEC

Nobel 2001
E. Cornell , W. Ketterle , C. Wieman

COOLING

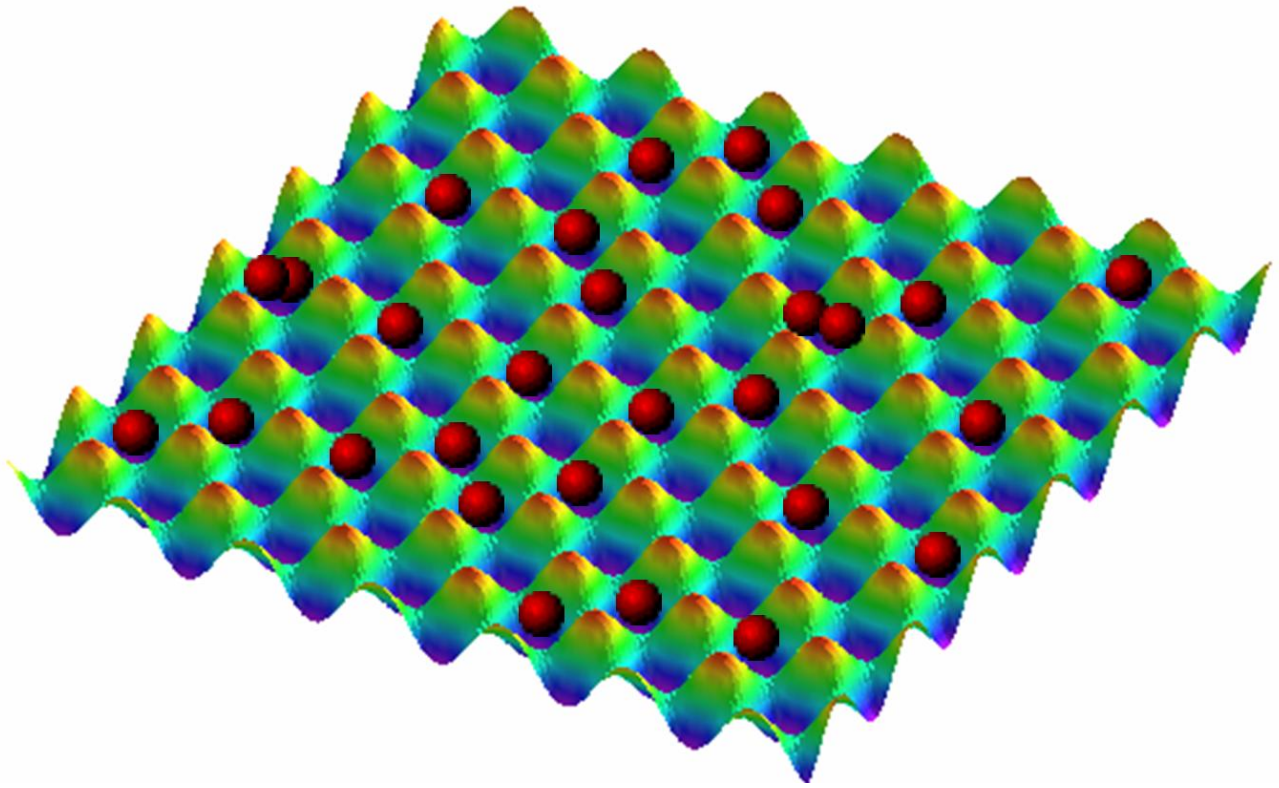
Nobel 1997
S. Chu, C. Cohen-Tannoudji, W. Phillips

The Hubbard model can now be realized using quantum optics techniques !



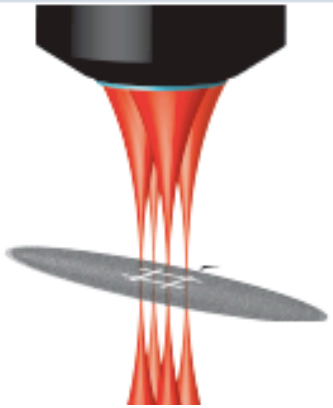
A new frontier: cold atoms in optical lattices: «artificial crystals of atoms and light »

D.Jaksch et al.
PRL, 1998



Cold Atoms and Condensed Matter Physics: very different characteristic scales

	Cold Fermionic atoms	Electrons in a solid
Density	10^{12} cm^{-3}	10^{22} cm^{-3} (Metals)
Mass	6 (Li), 40 (K)	$5.4\ 10^{-4}$
Fermi Temperature	μK	10^{4} K
Temperature	100 nK	10 mK
Charge	0	-1
Interactions	Contact, *tunable*	Coulomb, material dep.
Potential shaping	Laser light	growing, lithography



Slide: courtesy
J-P Brantut

Highly controllable systems:

- Interaction strength (U) can be tuned (e.g. through Feshbach resonances)

- Hopping (t) can be tuned by changing lattice depth (laser intensity)

-Geometry of lattice can be changed

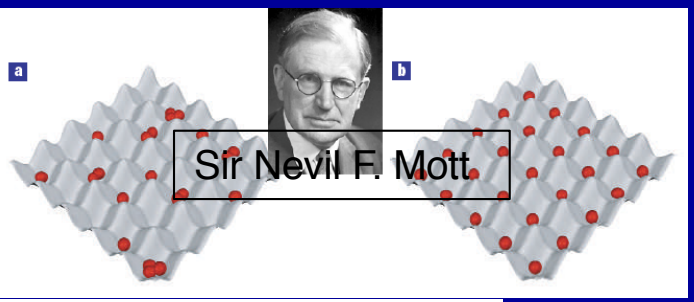
- Controlled time-dependent perturbations

- BUT… still quite `hot': T ~ t / 5 ~ a few nK (aka room temperature in the solid-state!)

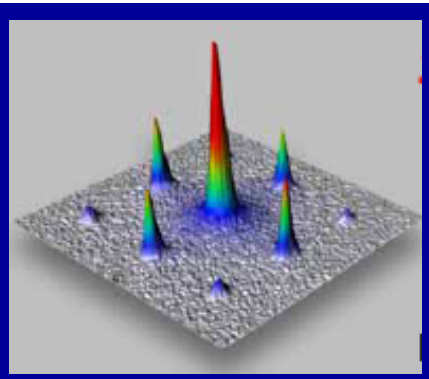
Experimental observation of the Superfluid to Mott insulator transition for cold bosonic atoms

Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms

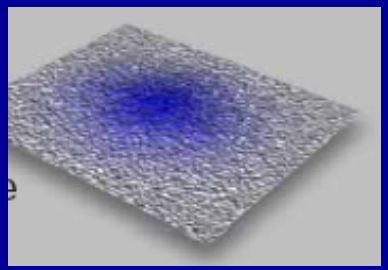
Markus Greiner*, Olaf Mandel*, Tilman Esslinger†, Theodor W. Hänsch* & Immanuel Bloch*

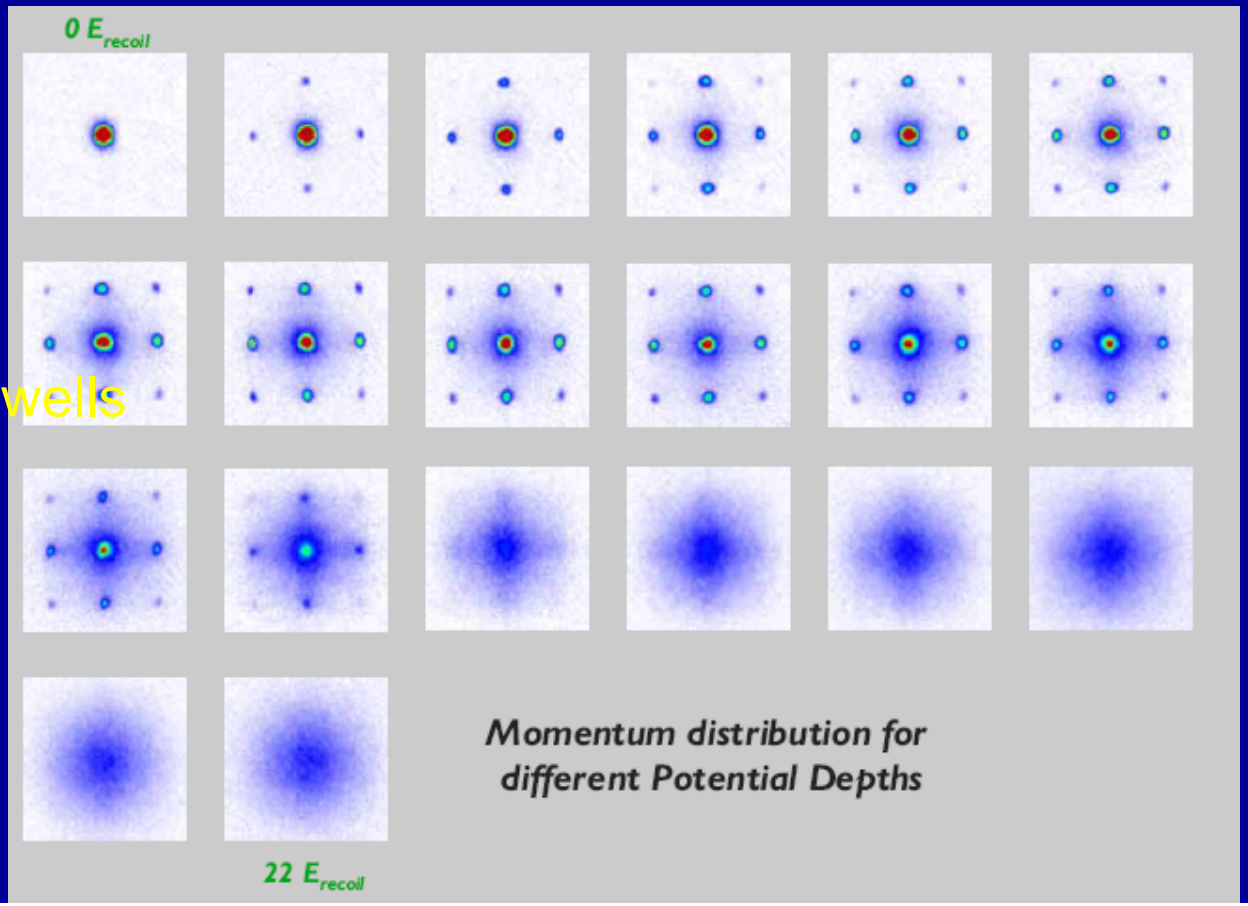


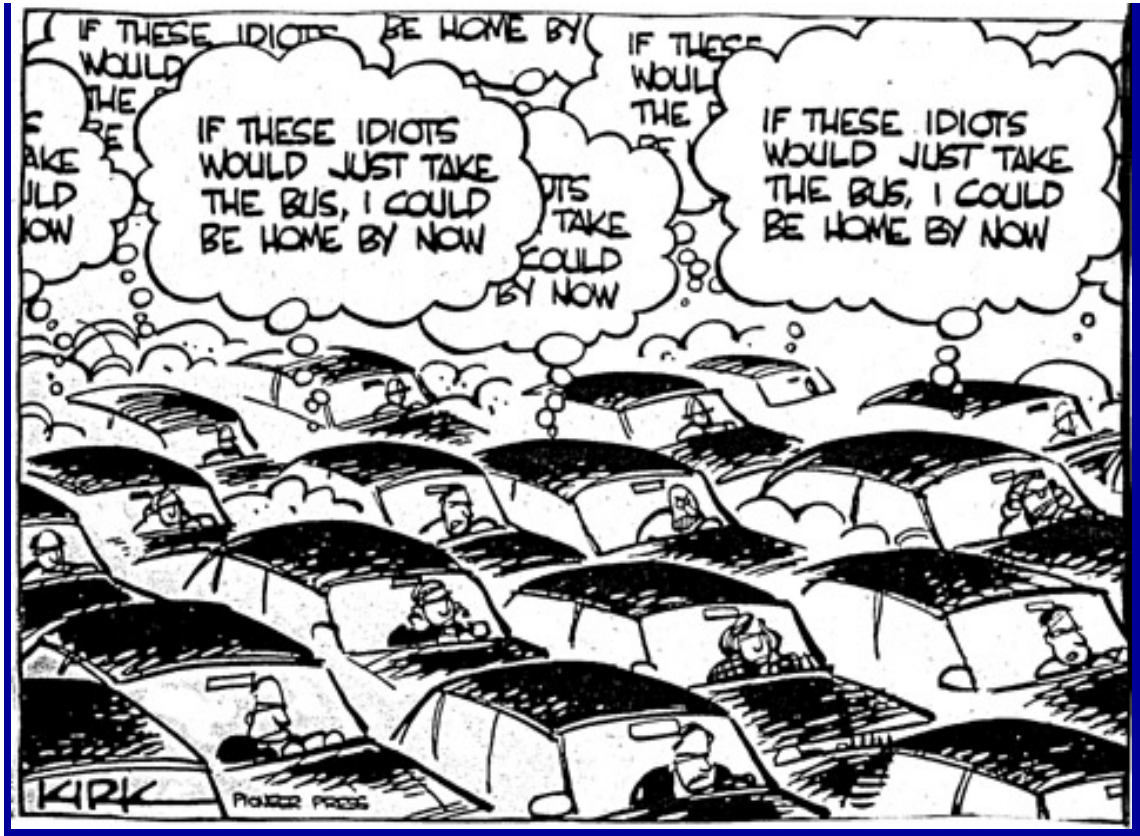
NATURE | VOL 415 | 3 JANUARY 2002



Phase coherence between wells in superfluid phase >interference pattern







A Mott insulator is an incompressible state of matter

LA's highways

The RER-subway in Paris at rush hours

How to make progress ?

- 1. Approximations – In best cases: sequence of approximations that will converge (at lest in principle) to the exact answer

  → *`Dynamical Mean-Field Theory' and `Embedding Methods'*
- 2. Find clever ways of doing Quantum Monte Carlo → *`Diagrammatic QMC'*
- 3. Data compression methods for the full wave-function → *`Tensor Networks'*

Computational Quantum Physics and Chemistry

- Computational methods for many-body quantum systems have seen considerable progress in the last ~ 30 years
- Moore's law increase in computing power is not the main reason for these advances
- RATHER:
- New algorithms
- New Concepts and Approximations

More Physics Motivations

Materials with Strong Electronic Correlations

INTERACTIONS lead to COLLECTIVE EFFECTS

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_i v_{ion}(\vec{r}_i) + \frac{1}{2}\sum_{i,j}\frac{e^2}{4\pi\varepsilon_0|r_i - r_j|}$$

Wave-function NOT well approximated
by a single Slater determinant (~product): ENTANGLEMENT
→ CORRELATIONS between particles

$$H\Psi(r_1, \cdots, r_N) = E\Psi(r_1, \cdots, r_N)$$

Approximation of (quasi) independent electrons

$$\Psi(r_1, \cdots, r_N) \simeq \mathrm{Det}\left[\phi_{\nu_i}(r_j)\right]$$
$$(i, j = 1, \cdots, N)$$

The many-body wave-function is approximated as a product of single-particle Bloch waves (antisymmetrized → Slater determinant)

Works OK for many materials, but here we shall focus on those for which this approximation FAILS !

Materials with Strong Electron Correlations do "BIG THINGS"

- Because of the strong interdependence of electrons, collective phenomena take place
- Such as: *metal-insulator transitions, magnetism, superconductivity, etc.*
- → Interesting functionalities
- → Fundamental questions in physics and chemistry

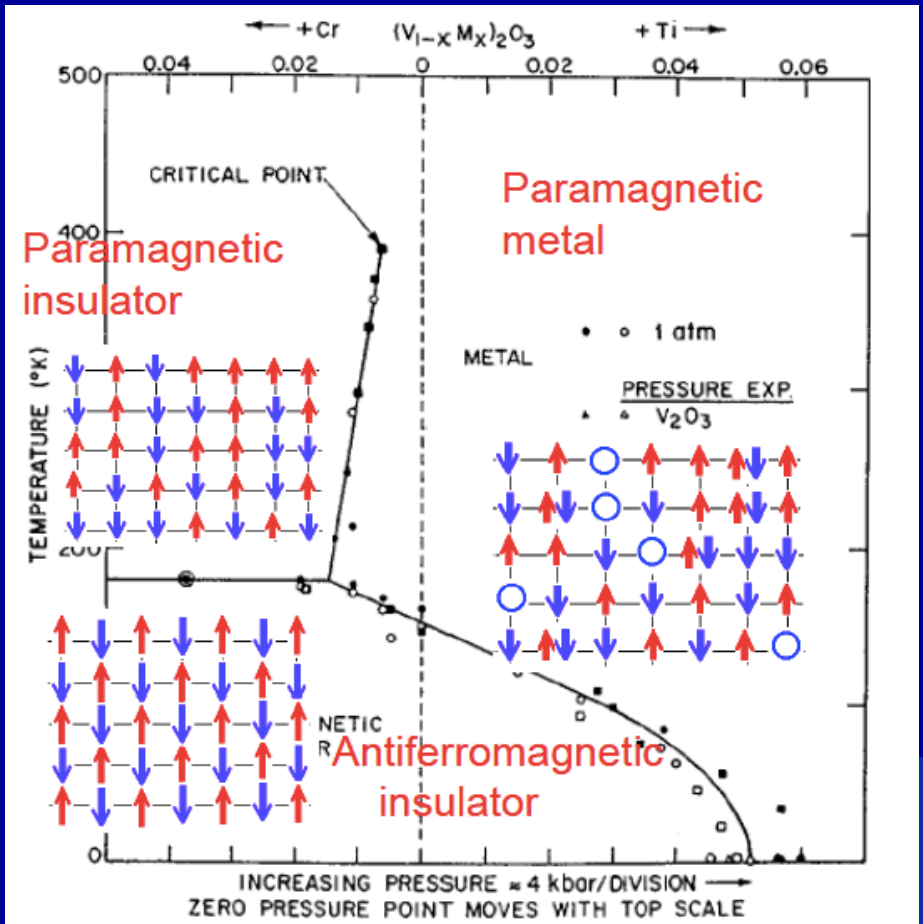
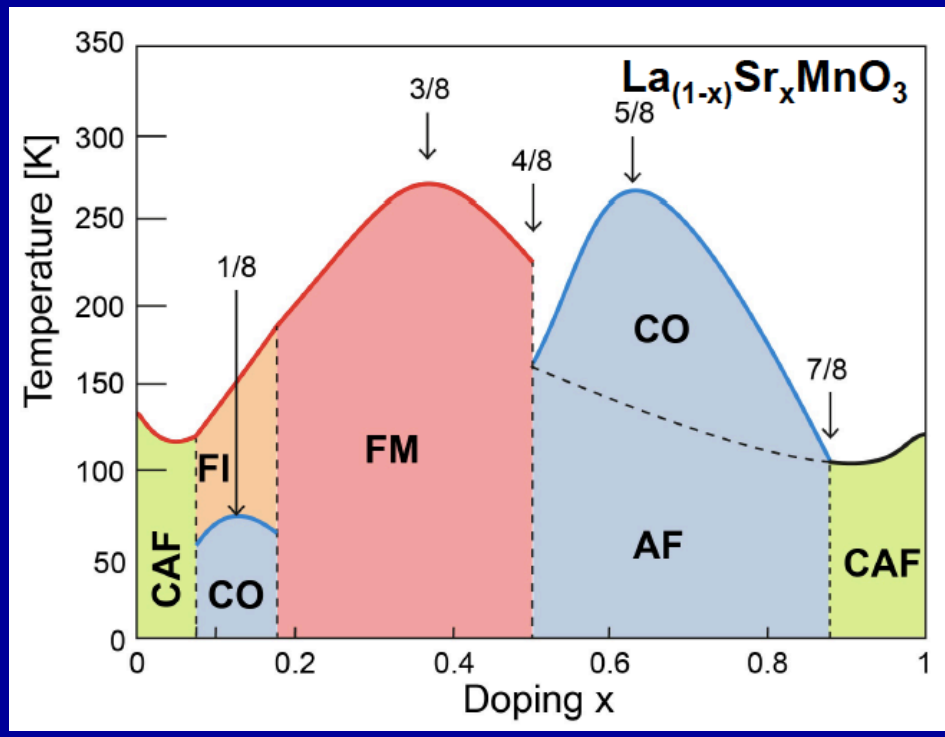
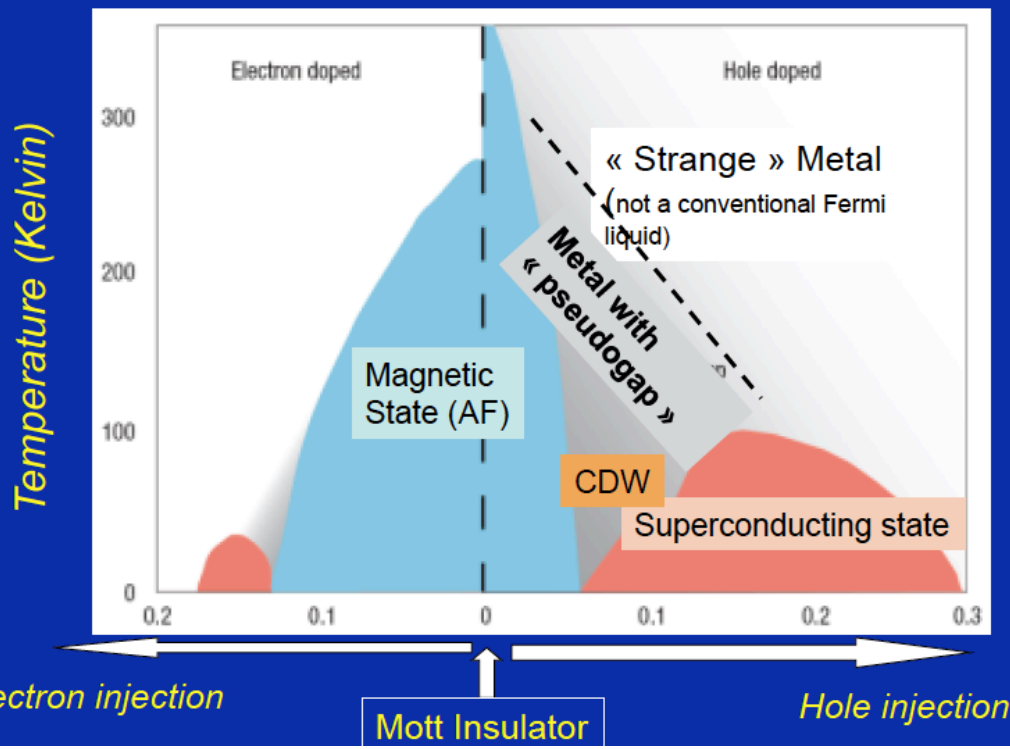


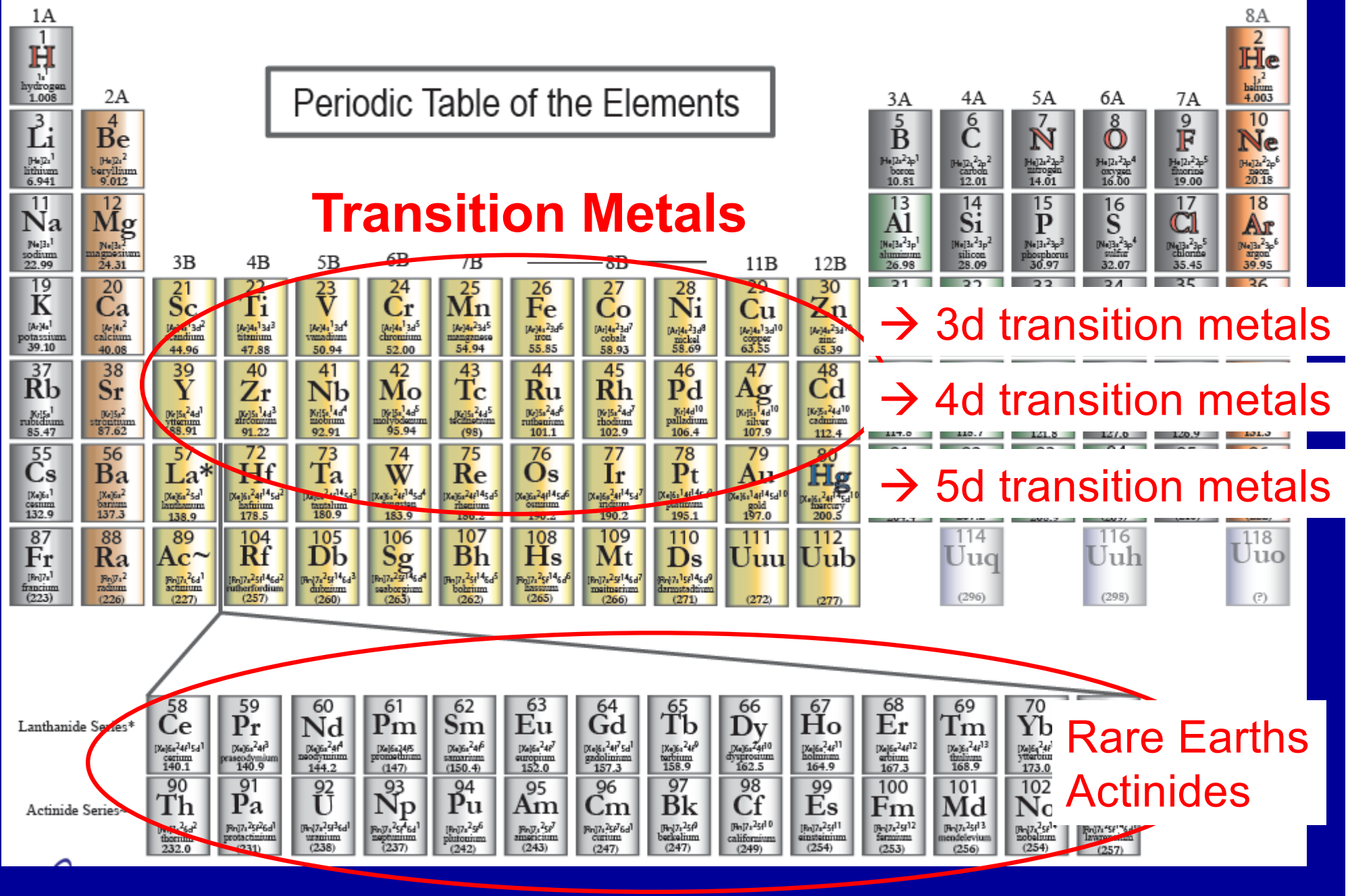
FIG. 70. Phase diagram for doped V_2O_3 systems, $(V_{1-x}Cr_x)_2O_3$ and $(V_{1-x}Ti_x)_2O_3$. From McWhan *et al.*, 1971, 1973.

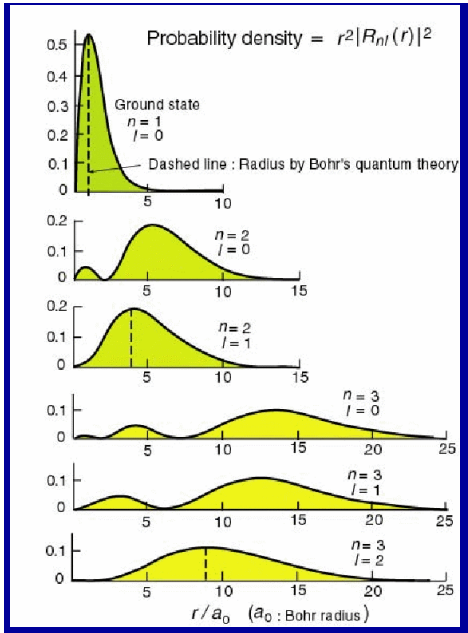




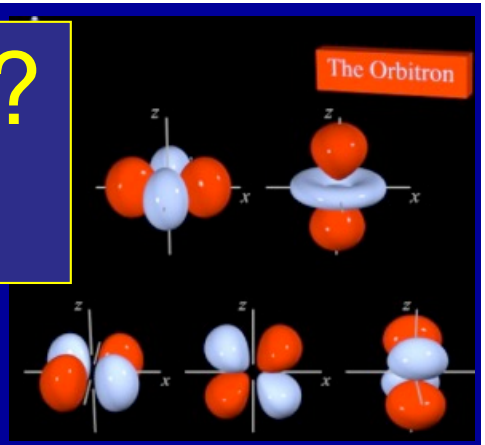
Remarkable Properties
Complex Phase Diagrams
Competing Phases

Which Materials display `Strong Electronic Correlations' ?


Periodic Table of the Elements
Transition Metals
→ 3d transition metals
→ 4d transition metals
→ 5d transition metals
Rare Earths
Actinides
Lanthanide Series*
Actinide Series~



Who are the suspects ? Localized orbitals !

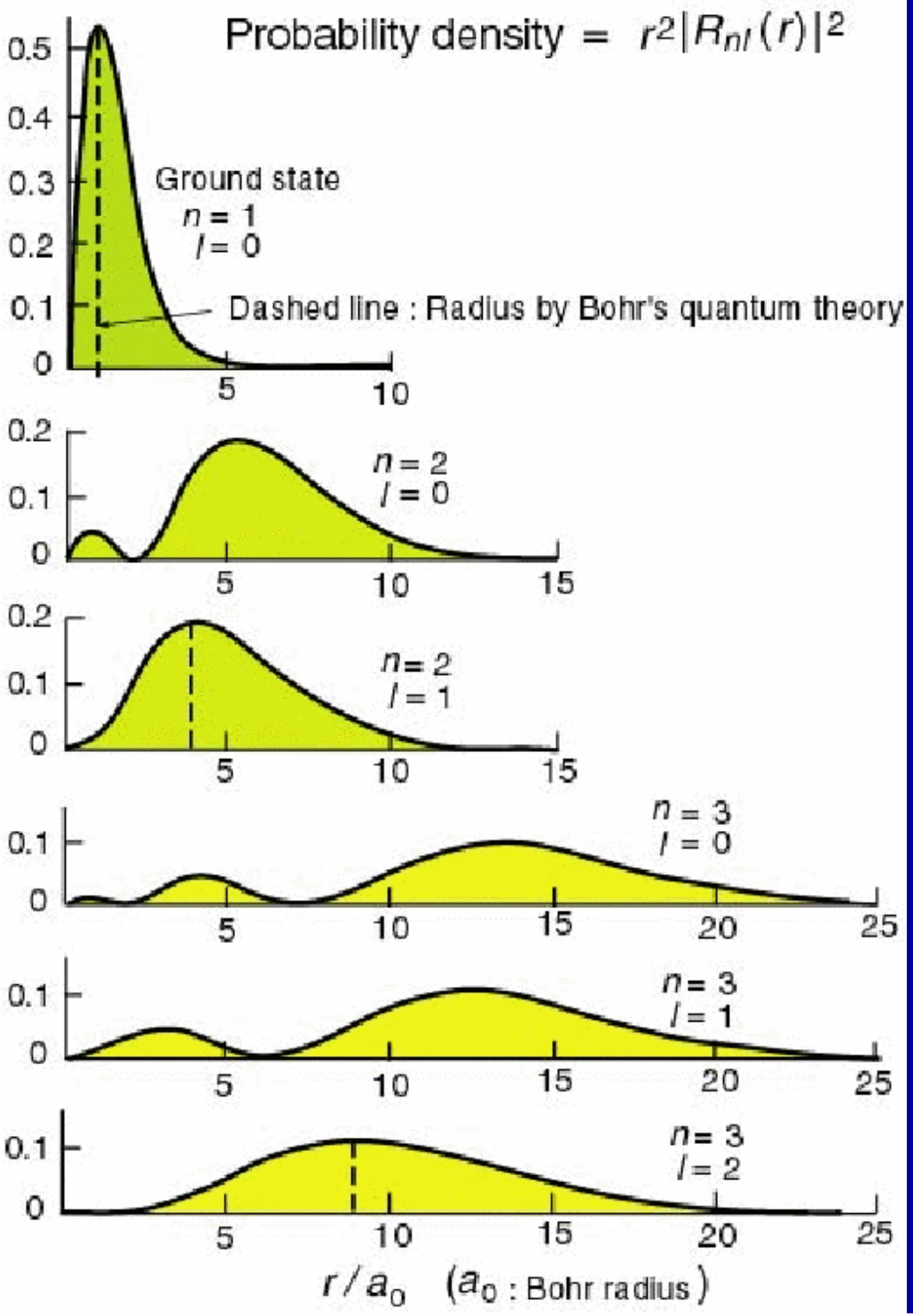


d- or f- orbitals are quite close to ions nuclei
(particularly 3d and 4f, for orthogonality reasons)

They do not behave as regular band-forming orbitals (e.g sp-bonding) and retain atomic-like aspects

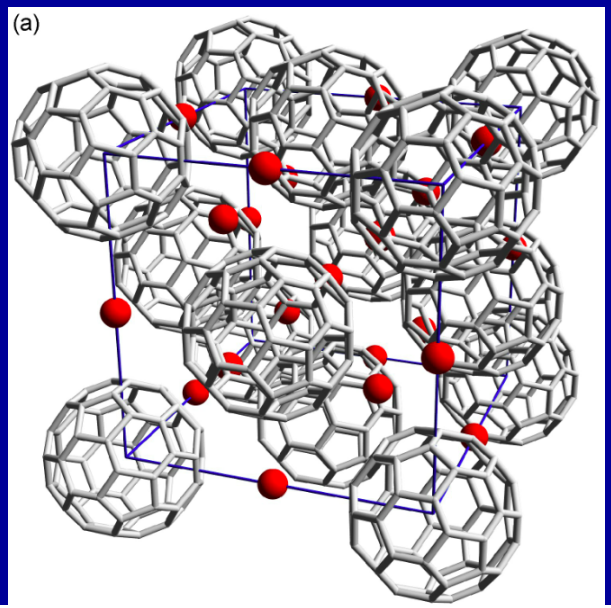
→ **Electrons "hesitate" between localized and itinerant behaviour !**

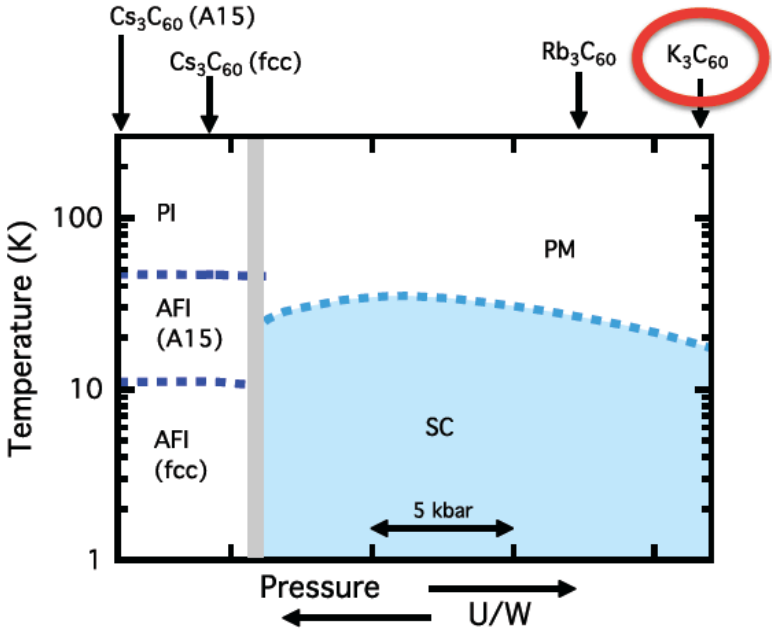
Materials: transition-metals and their oxides, rare-earth/actinides and their compounds, but also some organic materials


Probability density = $r^2|R_{nl}(r)|^2$
Ground state
$n = 1$
$l = 0$
Dashed line : Radius by Bohr's quantum theory
$n = 2$
$l = 0$
$n = 2$
$l = 1$
$n = 3$
$l = 0$
$n = 3$
$l = 1$
$n = 3$
$l = 2$
r / a_0 (a_0 : Bohr radius)

Molecular Materials

κ-$(ET)_2Cu[N(CN)_2]Cl$





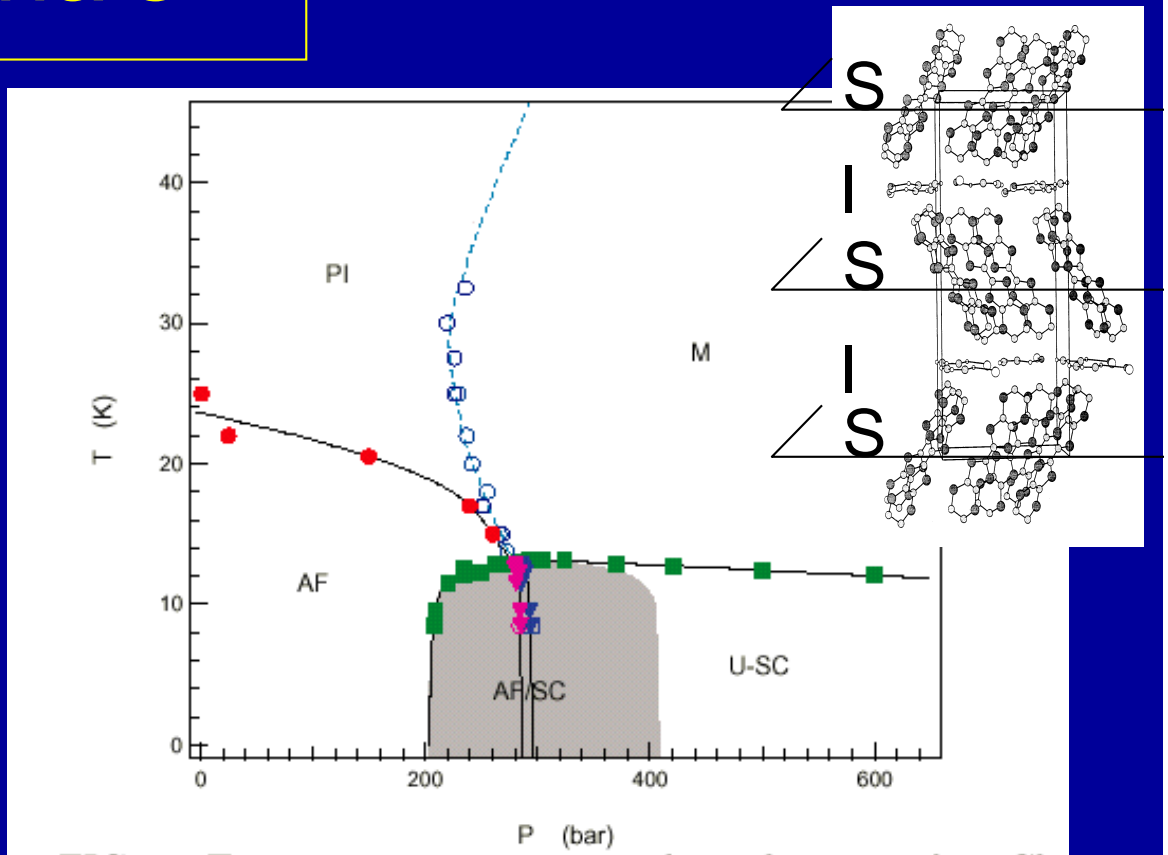
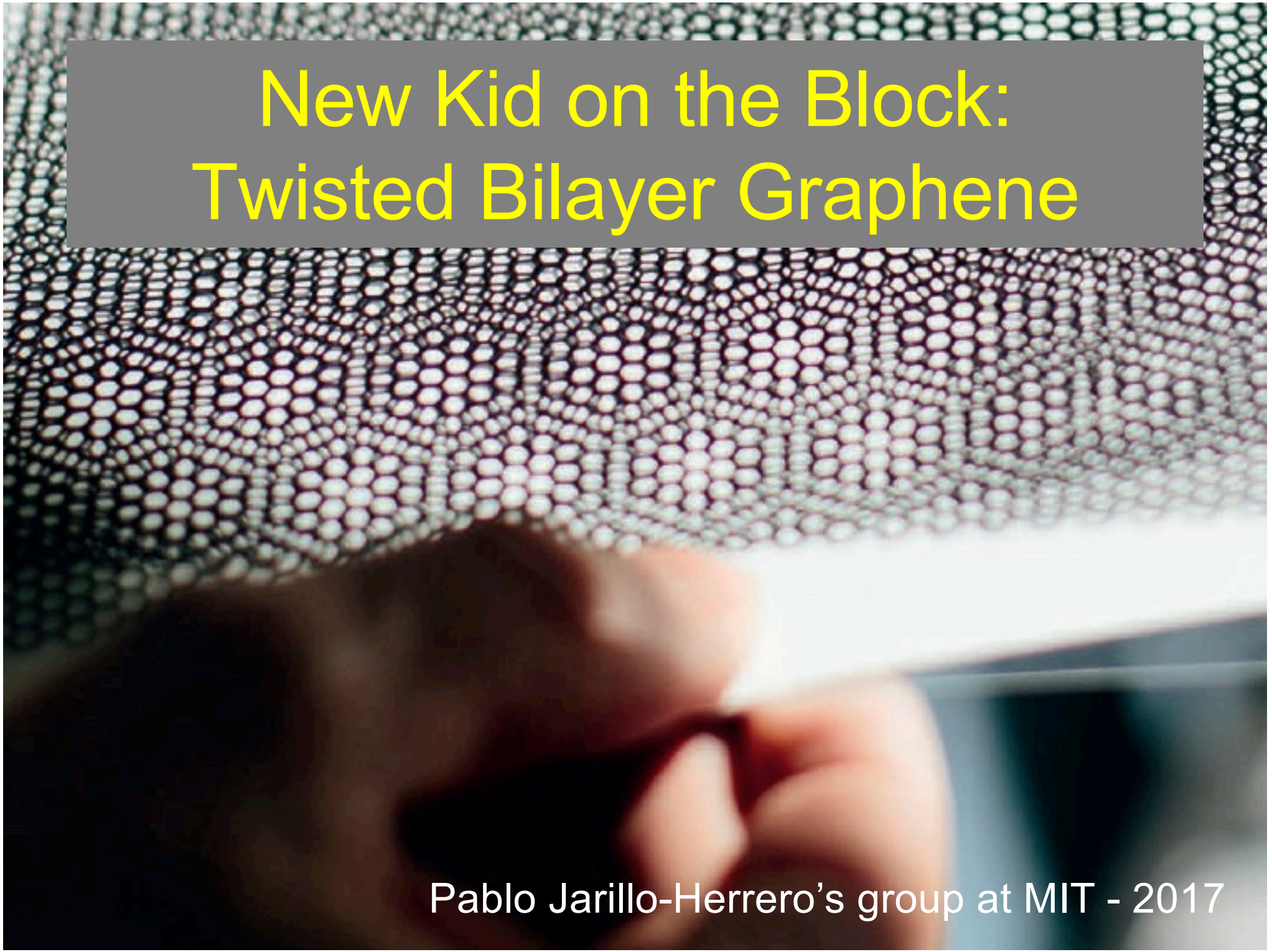
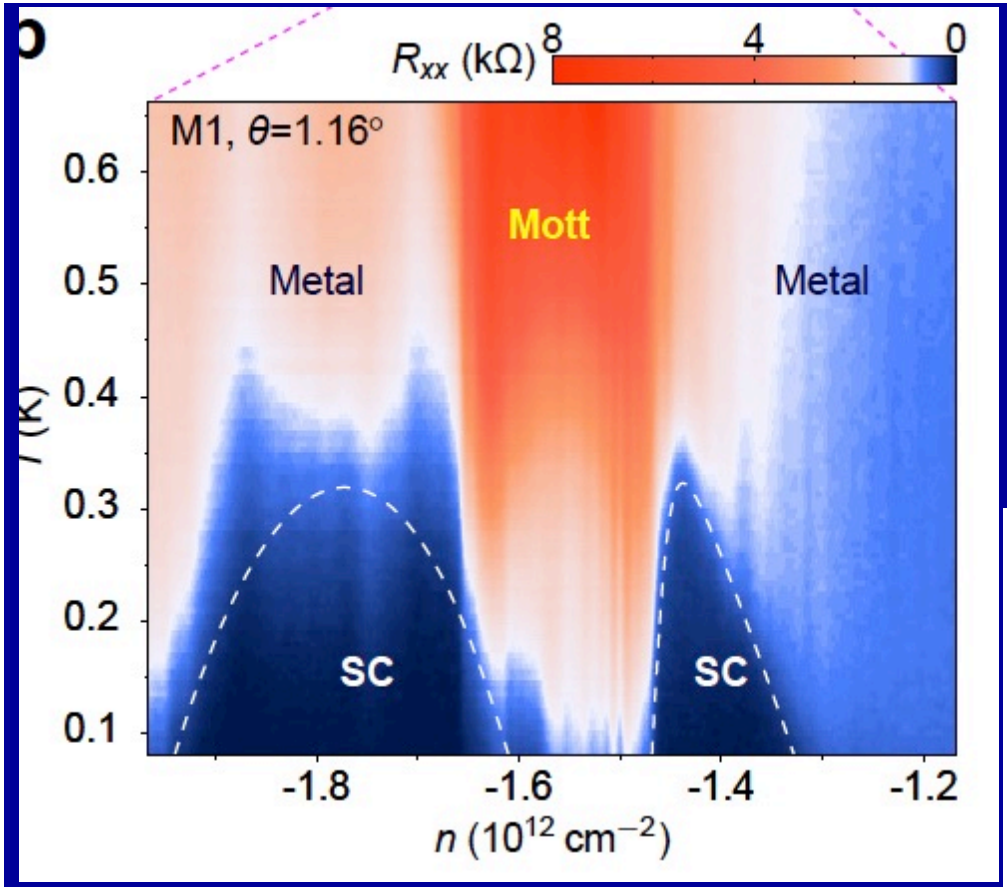
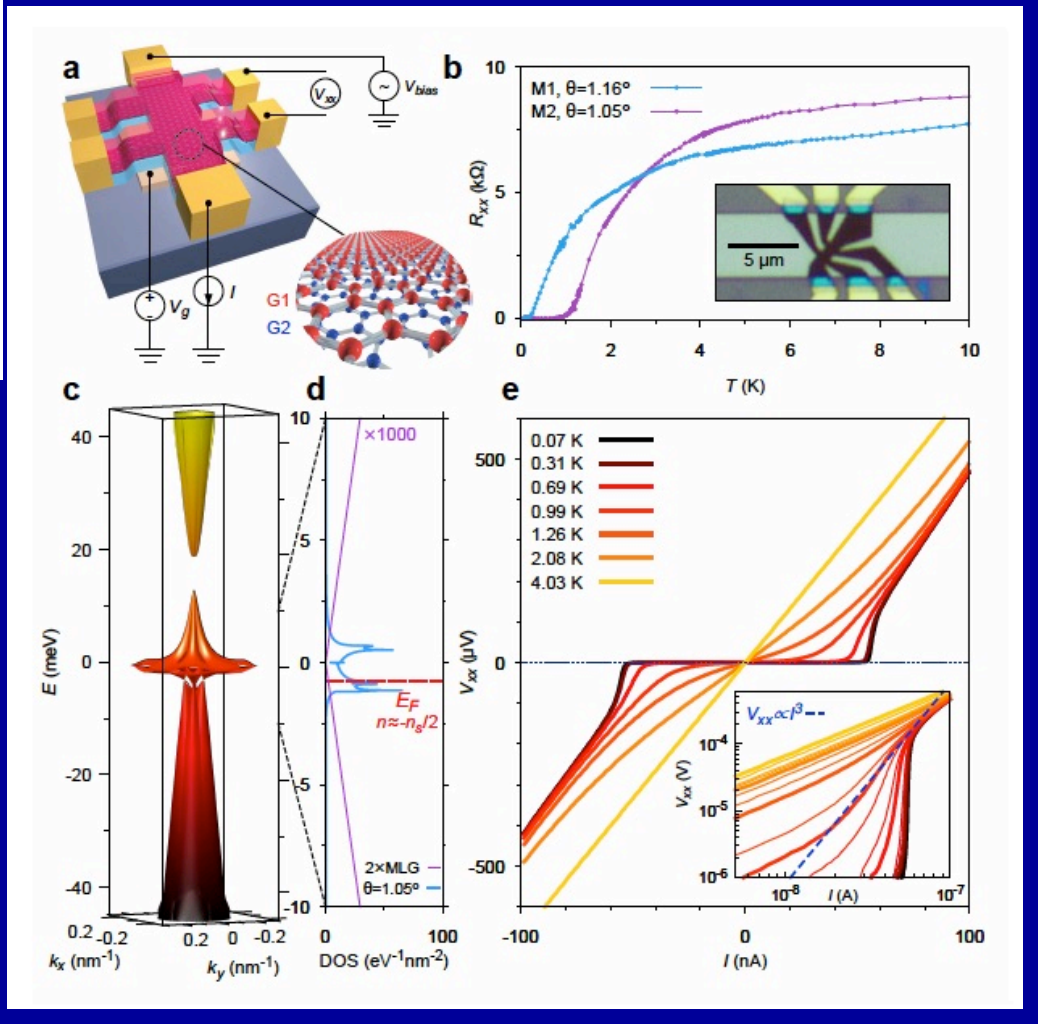


FIG. 1. Temperature *vs* pressure phase diagram of $\kappa-$Cl. The antiferromagnetic (AF) critical line $T_N(P)$ (dark circles) was determined from NMR relaxation rate while $T_c(P)$ for unconventional superconductivity (U-SC: squares) and the metal-insulator $T_{MI}(P)$ (MI: open circles) lines were obtained from the AC susceptibility. The AF-SC boundary (double dashed line) is determined from the inflexion point of $\chi'(P)$ and, for 8.5K, from sublattice magnetization. This boundary line separates two regions of inhomogeneous phase coexistence (shaded area).


New Kid on the Block:
Twisted Bilayer Graphene
Pablo Jarillo-Herrero's group at MIT - 2017



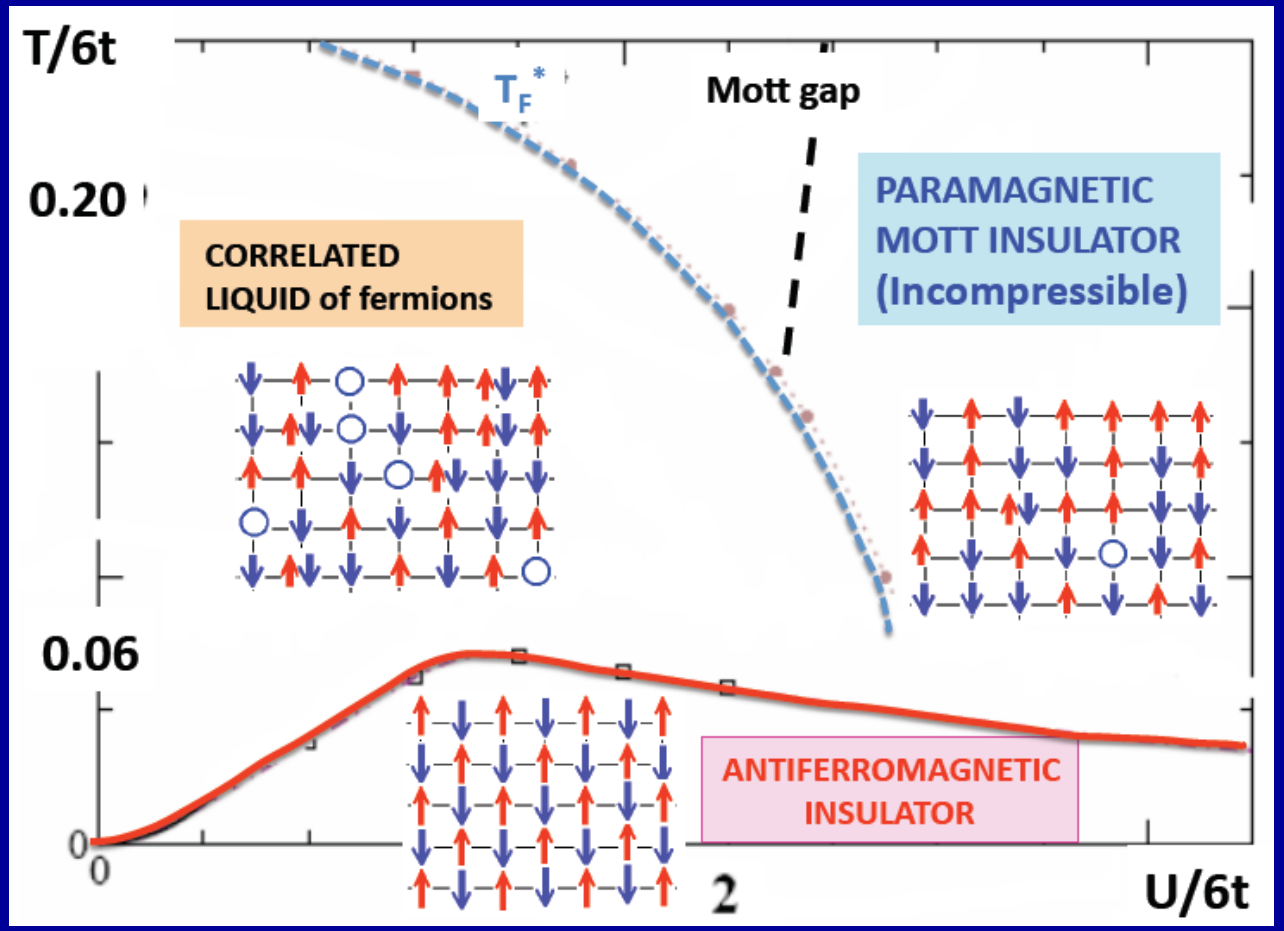
Cao et al.
Nature 556 (2018)
pages 43 and 80



Why do we need to go beyond (effective) one-particle descriptions ?

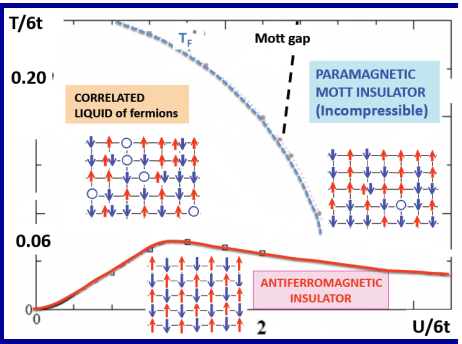
Why DMFT ?

Illustrate this on a simple case:
½ filled Hubbard model on cubic lattice



From: A.G. DMFT@25 book;
Crossover lines are indicative (not quantitative)

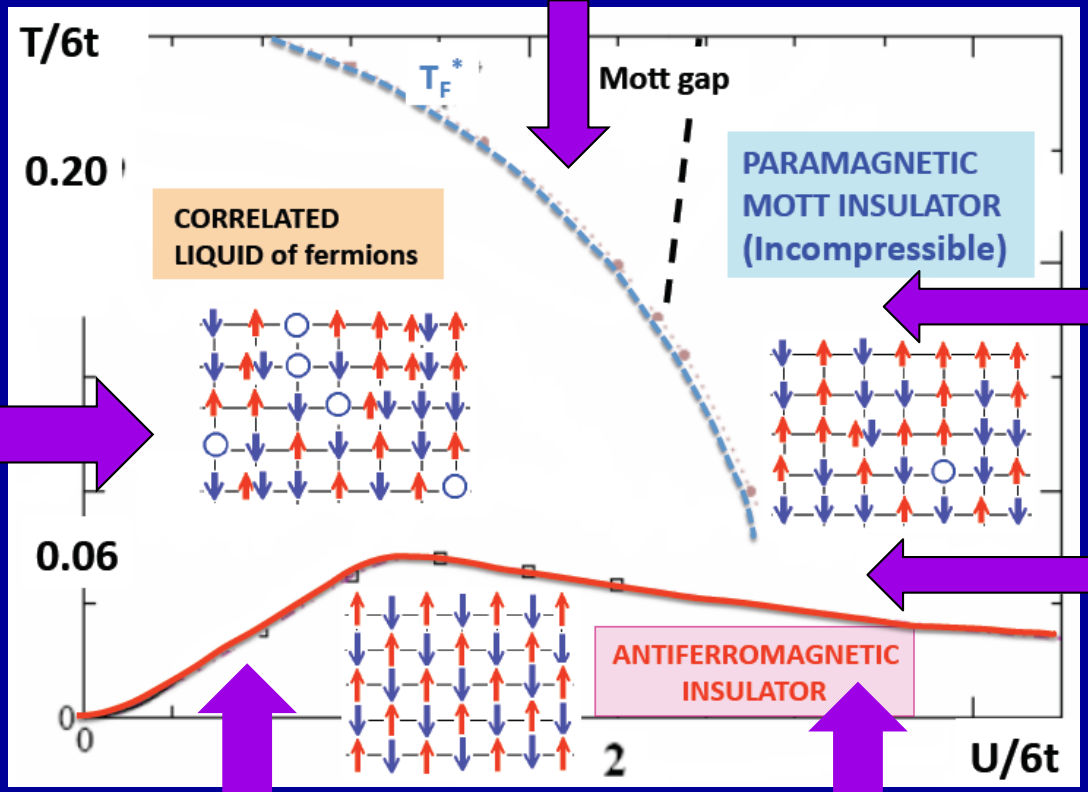
Please note:



- Ordered phase: Crossover from Slater-like antiferromagnet to localized Heisenberg AF
- Phase w/out long-range order:
- Weak-coupling: Crossover corresponding to the formation of coherent quasiparticles
- Strong coupling - Two crossovers:
- - Opening of Mott gap ~ U
- - Onset of magnetic correlations ~ $J=4t^2/U$
- At strong coupling, the onset of Mott insulating regime (incompressible w/ local moments) has nothing to do with magnetism

Hence, 6 distinct regimes:

Incoherent Soup



Mott Insulating Paramagnet (Fluctuating Local Moments)

~ Fermi Liquid

Mott Insulator with short-range AF correlations

~ Slater AF

~ Heisenberg AF Ordered Mott Insulator

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, $YTiO_3$, cuprates etc…

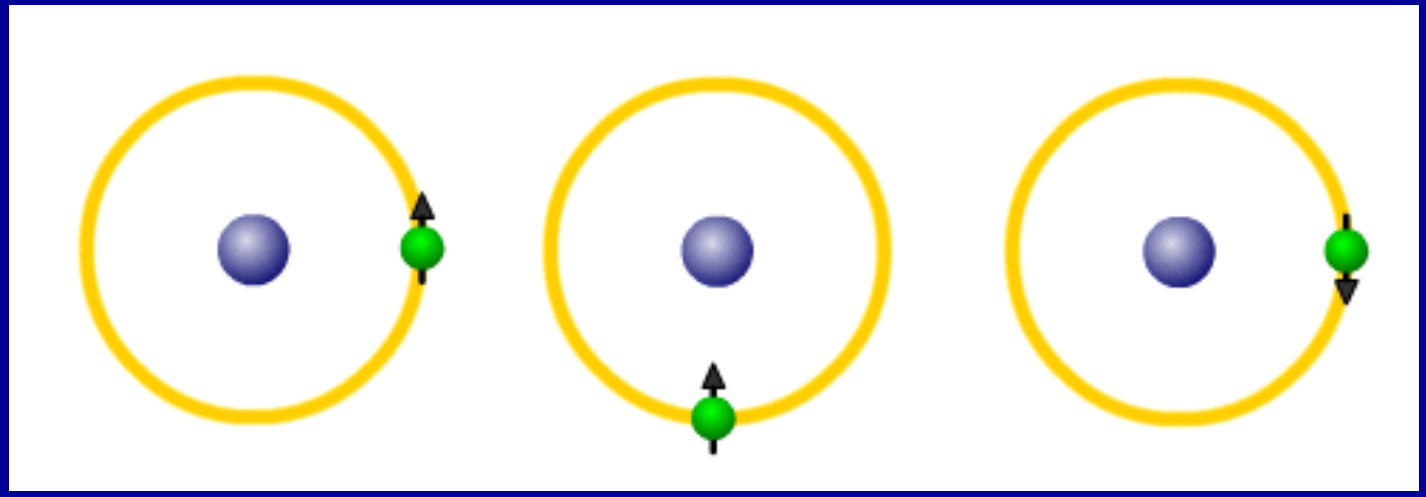
In contrast, LDA+U needs to assume ordering to describe the insulator

OBSERVABLES

- Since we want to also understand crossovers, we cant just rely on (static) order parameters
- Need to address nature of excited states (especially low-energy)
- Green's function
- Spectral Function
- Relation to photoemission experiments
- Two-particle response functions: charge, spin, current, etc…

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

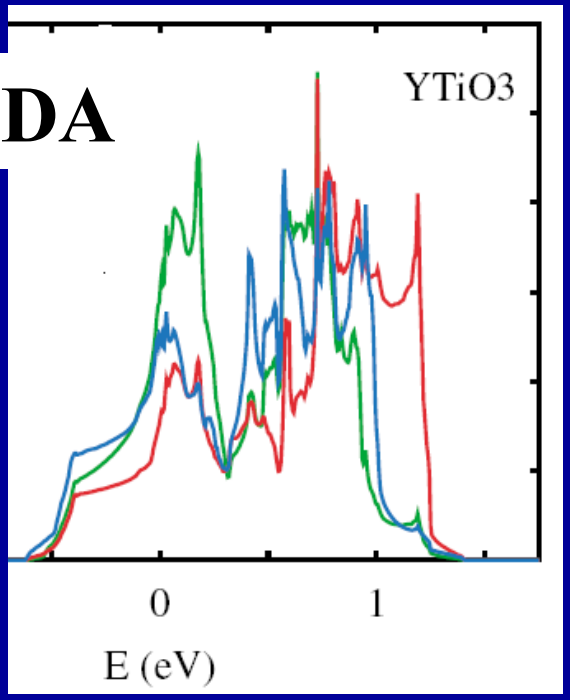


We see this from spectroscopy…

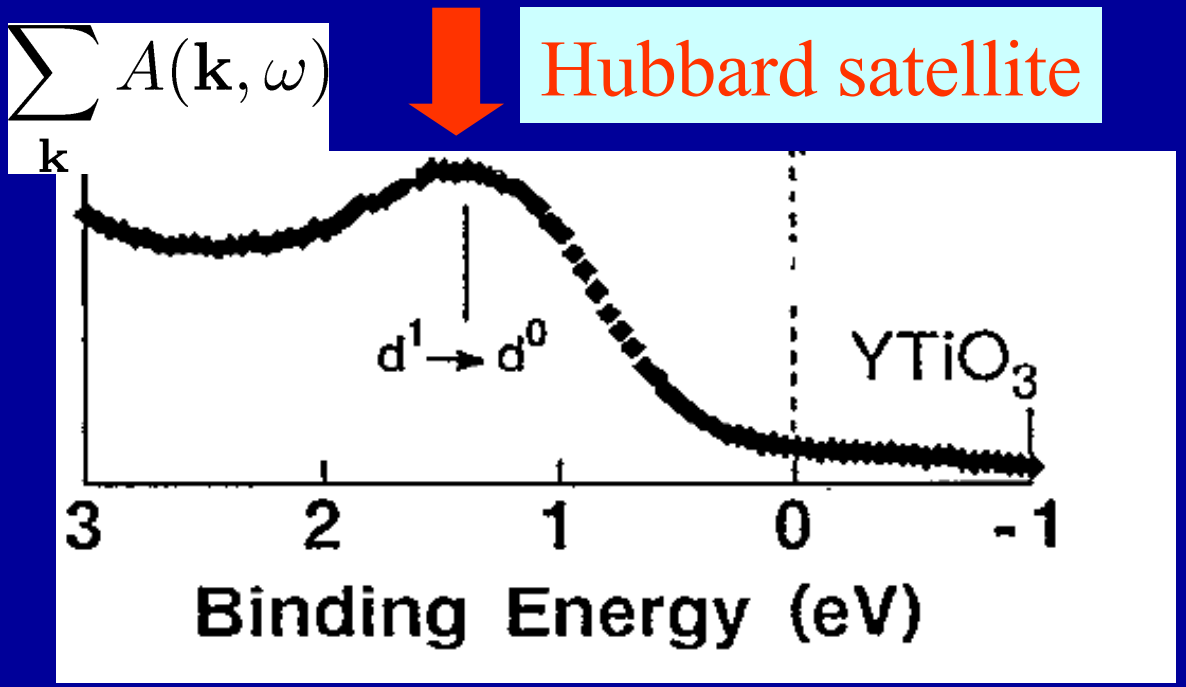
Mott insulators :

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 !

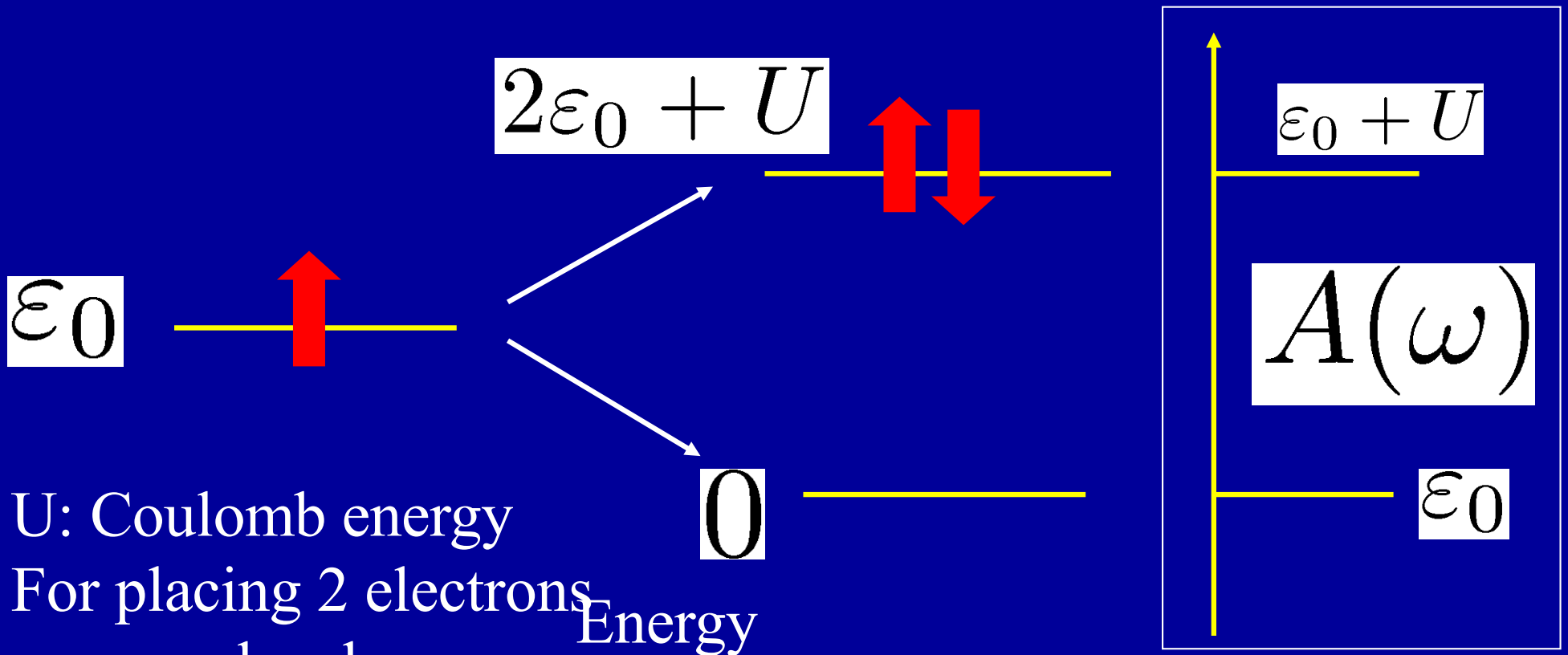


Photoemission: Fujimori et al., PRL 1992

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

(broadened by the solid-state environment)

Imagine a simplified atom with a single atomic level

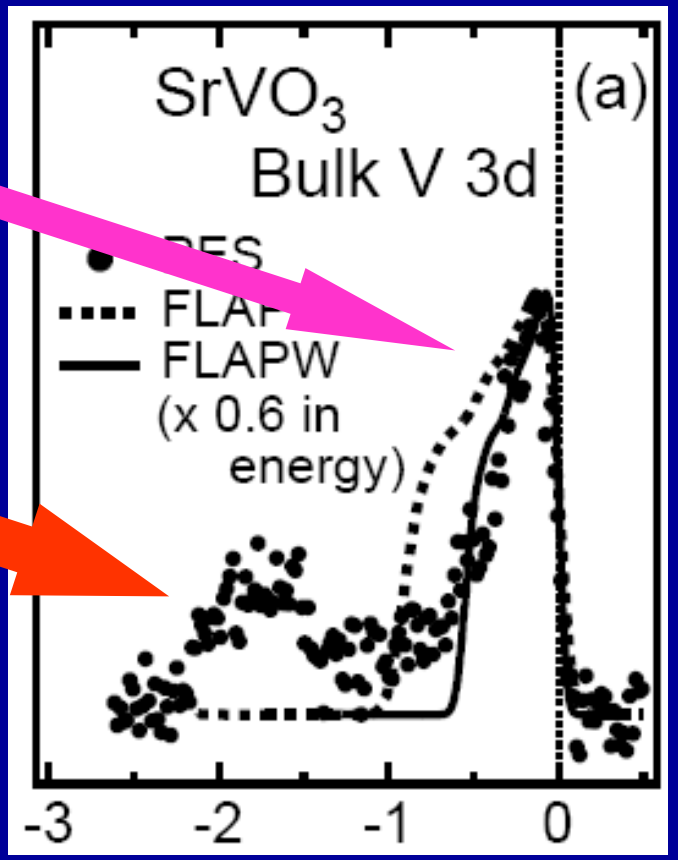


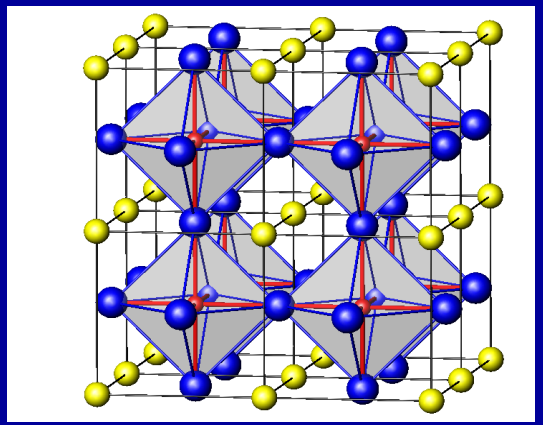
U: Coulomb energy
For placing 2 electrons on same level

Note: Energetics of the Mott gap requires an accurate description of the many-body eigenstates of single atoms (`multiplets'; $U, J_H, \ldots$)

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)





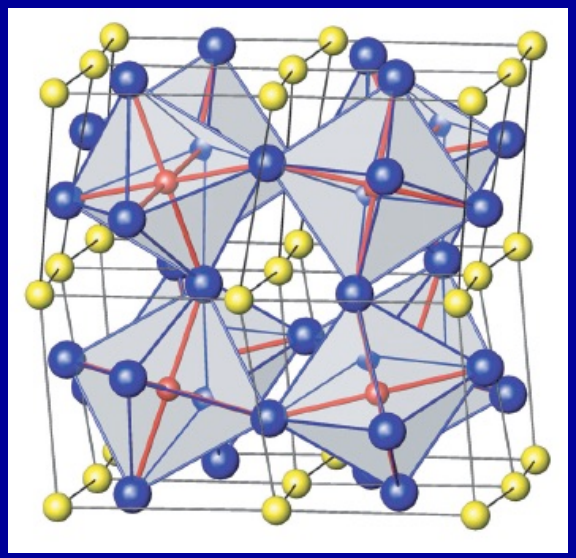
Dashed line:
Spectrum obtained from Conventional band-structure methods (DFT-LDA)

$SrVO_3$

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 ?



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

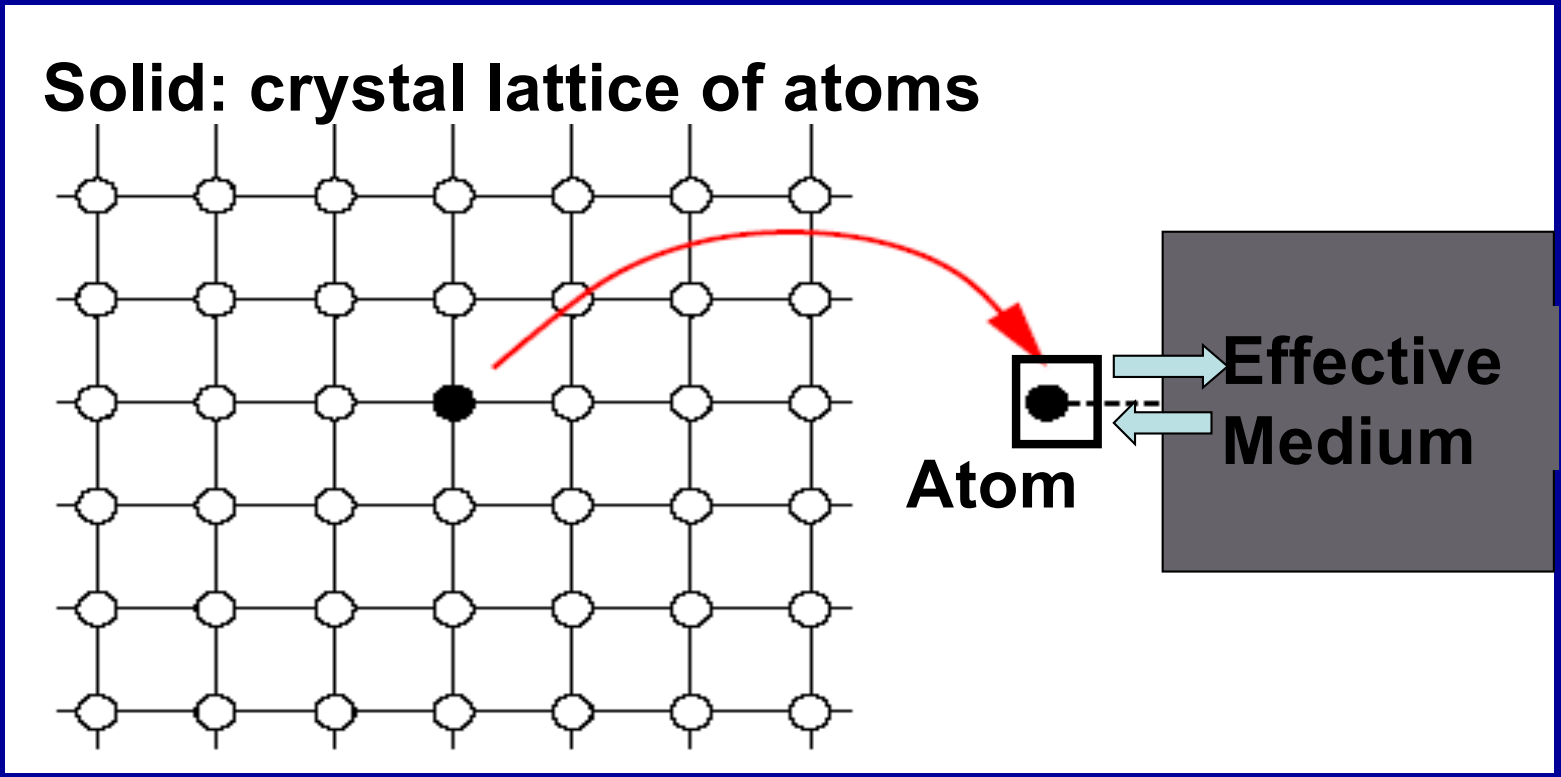
Dynamical Mean-Field Theory:
A.G. & G.Kotliar, PRB 45, 6479 (1992)
Correlated electrons in large dimensions:
W.Metzner & D.Vollhardt, PRL 62, 324 (1989)

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)

Dynamical Mean-Field Theory:

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



Correlated electrons in large dimensions: W.Metzner & D.Vollhardt, 1989

Dynamical Mean-Field Theory: A.G. & G.Kotliar, 1992

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

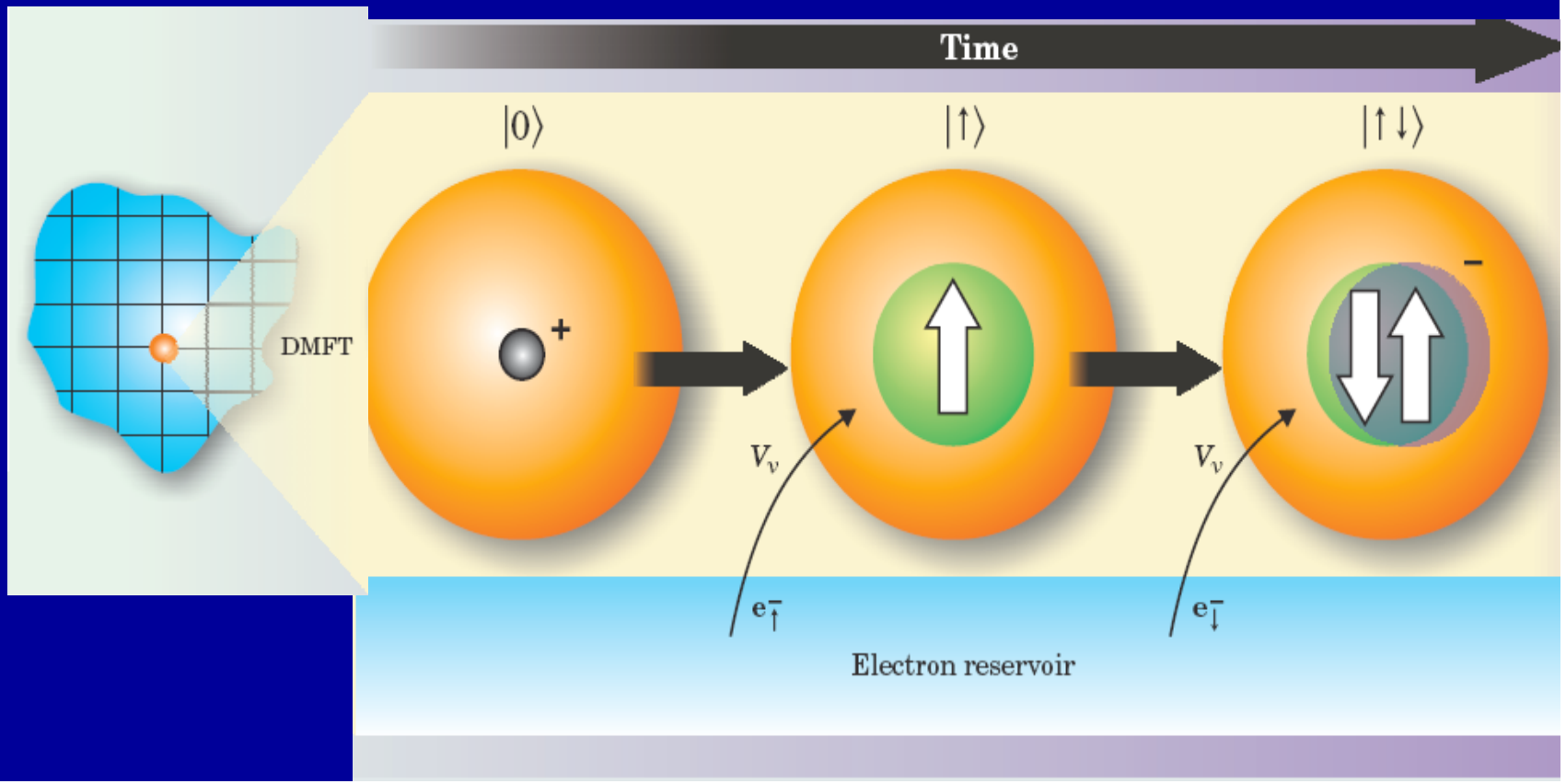
$$H = -\sum_{\mathbf{R}\mathbf{R}'} t_{\mathbf{R}\mathbf{R}'} d^{\dagger}_{\mathbf{R}\sigma} d_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} H^{\mathbf{R}}_{atom}$$

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

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

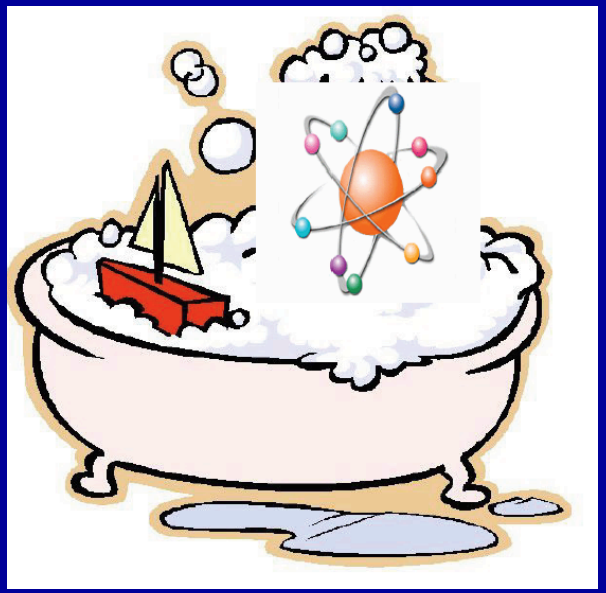
$$H_c = \sum_{l\sigma} E_l a^+_{l\sigma} a_{l\sigma}$$

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

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''



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

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 self-consistency condition:

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

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:

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