Dynamical Mean-Field Theory for Materials

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organization of the lecture

- the many-body problem
  - what are strong correlations
  - DFT and Kohn-Sham bands
  - Mott systems and the Hubbard model
- DMFT
  - Hubbard dimer
  - one-band Hubbard model
- DMFT for materials (LDA+DMFT)
  - multi-band Hubbard models
  - materials-specific models
  - examples
- conclusions

I. the many-body problem

strong correlations: what are they?

all of physics and chemistry is correlation

Born-Oppenheimer approximation, non-relativistic

kinetic energy | electron-electron interaction | potential energy | constant

$$\hat{H}_e = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$

why is it a *problem*?

simple interactions among many particles
lead to unexpected **emergent co-operative behavior**

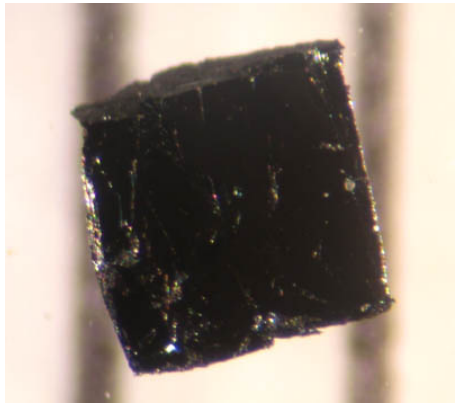
Philip Warren Anderson

4 August 1972, Volume 177, Number 4047

SCIENCE

more is different

emergence in solid-state systems

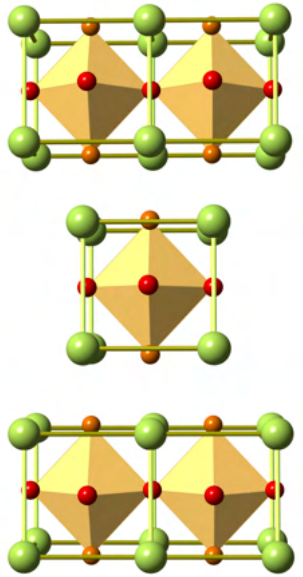


BSCCO-2223, photo from wikipedia

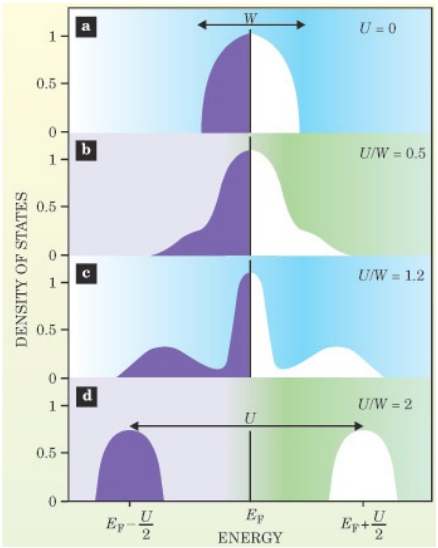
superconductivity

high-Tc superconductivity

non-conventional superconductivity

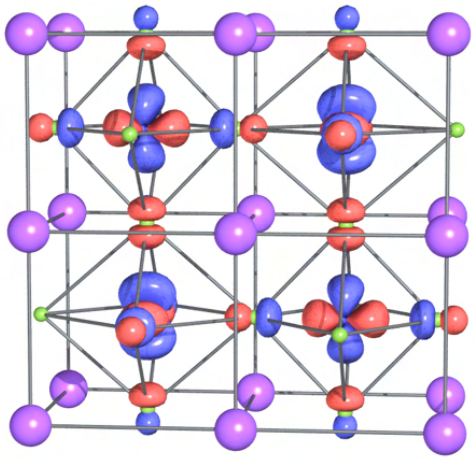


G. Zhang and E. Pavarini,
Rapid Research Letters **12**, 1800211 (2018)



Mott transition

G. Kotliar and D. Vollhardt, Physics Today **57,** 53 (2004)



orbital order

E. Pavarini, E. Koch, A.I. Lichtenstein, PRL **101**, 266405 (2008)

magnetism

photo from wikipedia

bad news: the exact solution is not an option

kinetic energy

potential energy

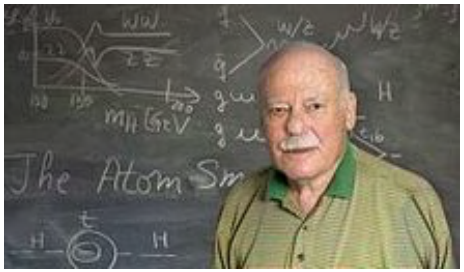
constant

$$\hat{H}_e = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$

electron-electron interaction

$$\hat{H}_e \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E_\alpha \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

good news: it would be anyway useless



H.J. Lipkin

On the other hand, the exact solution of a many-body problem is really irrelevant since it includes a large mass of information about the system which although measurable in principle is never measured in practice.

[..] An incomplete description of the system is considered to be sufficient if these measurable quantities and their behavior are described correctly.

what can be done then ?

$$\hat{H}_e \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E_\alpha \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

a way out: density-functional theory

1964

PHYSICAL REVIEW VOLUME 136, NUMBER 3B 9 NOVEMEBR 1964

Inhomogeneous Electron Gas*

P. HOHENBERG†
École Normale Superieure, Paris, France
AND
W. KOHN‡
École Normale Superieure, Paris, France and Faculté des Sciences, Orsay, France
and
University of California at San Diego, La Jolla, California
(Received 18 June 1964)

This paper deals with the ground state of an inter... proved that there exists a universal functional of the ... pression $E \equiv \int v(\mathbf{r})n(\mathbf{r})d\mathbf{r} + F[n(\mathbf{r})]$ has as its minimun... $v(\mathbf{r})$. The functional $F[n(\mathbf{r})]$ is then discussed for ... (2) $n(\mathbf{r}) = \varphi(\mathbf{r}/r_0)$ with φ arbitrary and $r_0 \to \infty$. In bot... relation energy and linear and higher order electronic ... also sheds some light on generalized Thomas-Fermi ... these methods are presented.

INTRODUCTION

DURING the last decade there has been considerable progress in understanding the properties of a homogeneous interacting electron gas.[1] The point of view has been, in general, to regard the electrons as similar to a collection of noninteracting particles with the important additional concept of collective excitations.

On the other hand, there has been in existence since the 1920's a different approach, represented by the Thomas-Fermi method[2] and its refinements, in which the electronic density $n(\mathbf{r})$ plays a central role and in which the system of electrons is pictured more like a classical liquid. This approach has been useful, up to now, for simple though crude descriptions of inhomogeneous systems like atoms and impurities in metals.

Lately there have been also some important advances along this second line of approach, such as the work of Kompaneets and Pavlovskii,[3] Kirzhnits,[4] Lewis,[5] Baraff and Borowitz,[6] Baraff,[7] and DuBois and Kivelson.[8] The present paper represents a contribution in the same area.

1965

PHYSICAL REVIEW VOLUME 140, NUMBER 4A 15 NOVEMBER 1965

Self-Consistent Equations Including Exchange and Correlation Effects*

W. KOHN AND L. J. SHAM
University of California, San Diego, La Jolla, California
(Received 21 June 1965)

From a theory of Hohenberg and Kohn, approximation methods for treating an inhomogeneous system of interacting electrons are developed. These methods are exact for systems of slowly varying or high density. For the ground state, they lead to self-consistent equations analogous to the Hartree and Hartree-Fock equations, respectively. In these equations the exchange and correlation portions of the chemical potential of a uniform electron gas appear as additional effective potentials. (The exchange portion of our effective potential differs from that due to Slater by a factor of $\frac{2}{3}$.) Electronic systems at finite temperatures and in magnetic fields are also treated by similar methods. An appendix deals with a further correction for systems with short-wavelength density oscillations.

I. INTRODUCTION

IN recent years a great deal of attention has been given to the problem of a homogeneous gas of interacting electrons and its properties have been established with a considerable degree of confidence over a wide range of densities. Of course, such a homogeneous gas represents only a mathematical model, since in all real systems (atoms, molecules, solids, etc.) the electronic density is nonuniform.

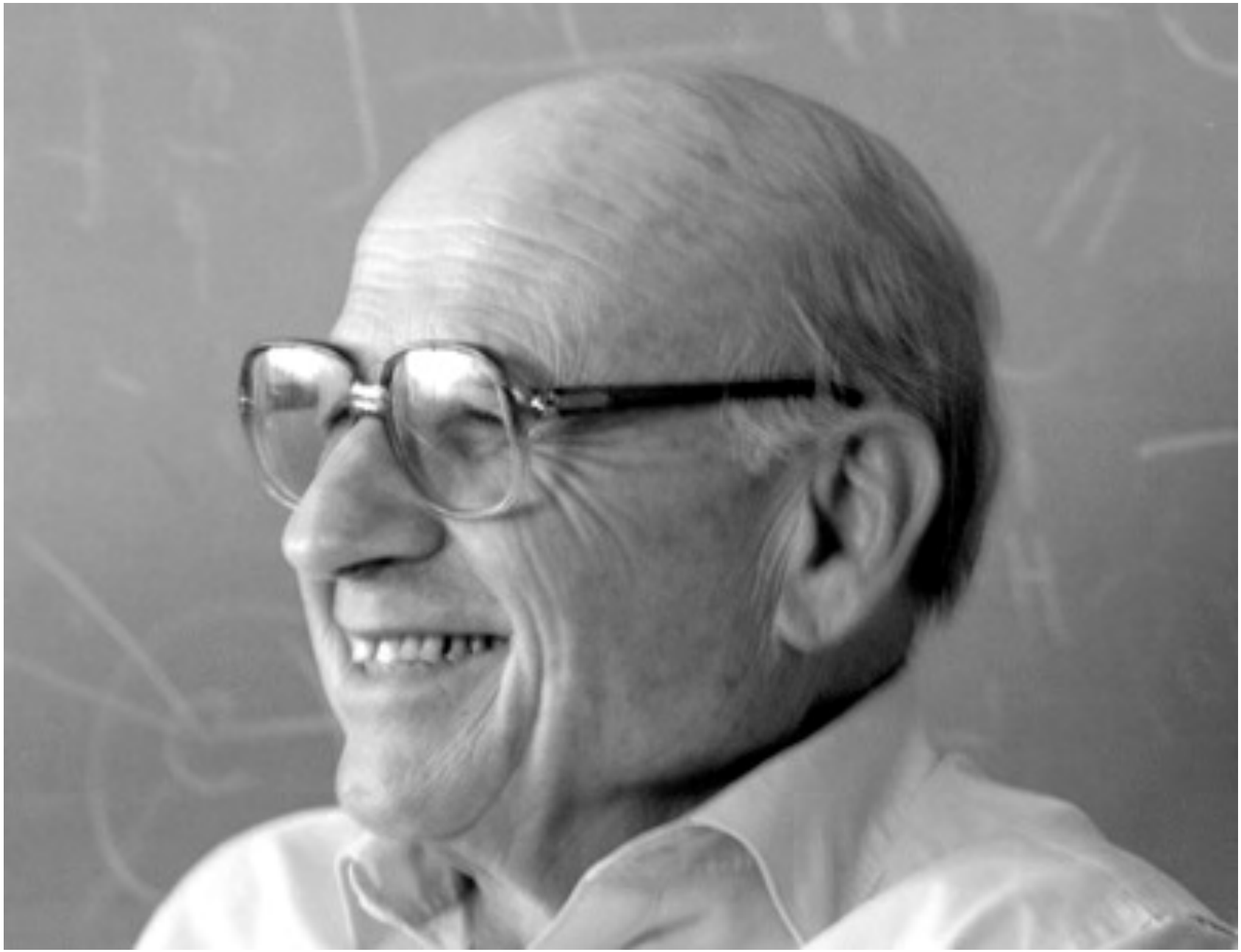
It is then a matter of interest to see how properties of the homogeneous gas can be utilized in theoretical

In Secs. III and IV, we describe the necessary modifications to deal with the finite-temperature properties and with the spin paramagnetism of an inhomogeneous electron gas.

Of course, the simple methods which are here proposed in general involve errors. These are of two general origins[4]: a too rapid variation of density and, for finite systems, boundary effects. Refinements aimed at reducing the first type of error are briefly discussed in Appendix II.

II. THE GROUND STATE

1998: Nobel Prize in Chemistry to Walter Kohn



the *standard model*: density-functional theory

$$\hat{H}_e \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E_\alpha \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

$$n_G(\mathbf{r}), \qquad E_G[n(\mathbf{r})], \qquad \ldots$$

1998: Nobel Prize in Chemistry to Walter Kohn

In my view DFT makes two kinds of contribution to the science of multi-particle quantum systems, including problems of electronic structure of molecules and of condensed matter:

The first is in the area of fundamental *understanding*. Theoretical chemists and physicists, following the path of the Schroedinger equation, have become accustomed to think in a truncated *Hilbert space of single particle orbitals*. The spectacular advances achieved in this way attest to the fruitfulness of this perspective. However, when high accuracy is required, so many Slater determinants are required (in some calculations up to ~ 10^{9}!) that *comprehension* becomes difficult. DFT provides a complementary perspective. It focuses on quantities in the real, 3-dimensional coordinate space, principally on the electron density $n(r)$ of the groundstate. Other quantities of great interest

(from the Nobel lecture)

the Kohn-Sham eigenvalues

$$\hat{H} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} - \sum_\alpha \frac{1}{2M_\alpha}\nabla_\alpha^2 + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$

from the ground-state wave-function to the electron density

Kohn-Sham auxiliary Hamiltonian

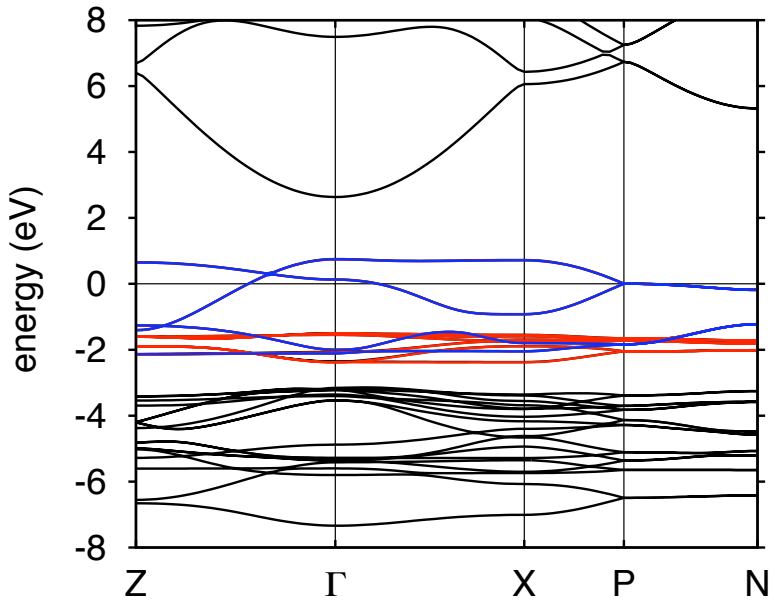
$$\hat{h}_e = \sum_i \left[-\frac{1}{2}\nabla_i^2 + v_R(\boldsymbol{r}_i)\right] = \sum_i \hat{h}_e(\boldsymbol{r}_i)$$

$$v_R(\boldsymbol{r}) = -\sum_\alpha \frac{Z_\alpha}{|\boldsymbol{r} - \boldsymbol{R}_\alpha|} + \int d\boldsymbol{r}' \frac{n(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} + \frac{\delta E_{\mathrm{xc}}[n]}{\delta n} = v_{en}(\boldsymbol{r}) + v_H(\boldsymbol{r}) + v_{xc}(\boldsymbol{r})$$

(in practice: LDA,GGA,…)

unexpected successes of DFT

Kohn-Sham eigenvalues as *elementary excitations!*



band structures, material trends, prediction

unexpected successes of DFT

Kohn-Sham eigenvalues as *elementary excitations!*

successes of the independent electron picture

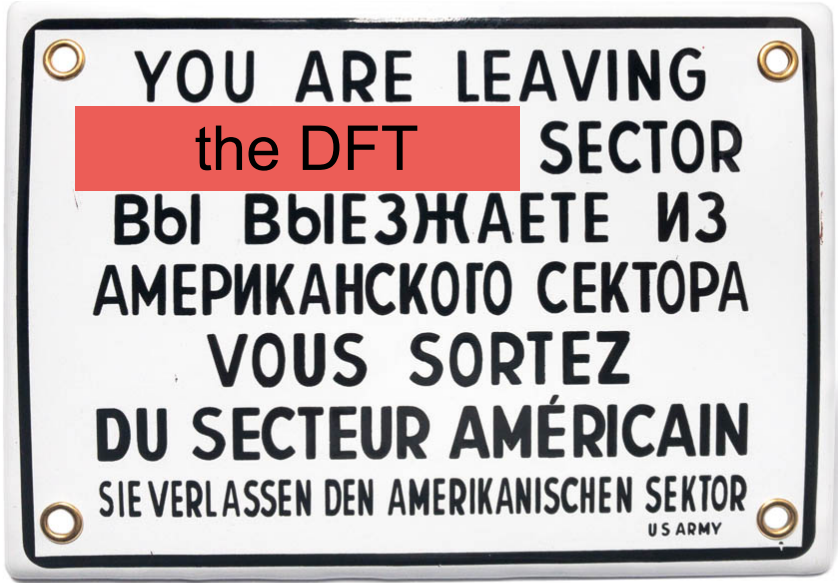
Kohn-Sham auxiliary Hamiltonian

$$\hat{h}_e = \sum_i \left[-\frac{1}{2}\nabla_i^2 + v_R(\boldsymbol{r}_i) \right] = \sum_i \hat{h}_e(\boldsymbol{r}_i)$$

mean-field-like Hamiltonian

mean-field-like Hamiltonian

… attention, this is going beyond DFT!



mean-field form

$$\hat{H}_e = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$

$$\hat{H}_e = \sum_i h(\mathbf{r}_i) + \frac{1}{2}\sum_{i,i'} u(\mathbf{r}_i, \mathbf{r}_{i'})$$

$$\hat{H}_e = \sum_i \tilde{h}(\mathbf{r}_i)$$

emergent behavior vs reductionism

Philip Warren Anderson

Nobel Prize in Physics 1977

The main fallacy in this kind of thinking is that the reductionist hypothesis does not by any means imply a "constructionist" one: The ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe. In fact, the more the ele-

(**1972**)

4 August 1972, Volume 177, Number 4047 **SCIENCE**

There is a school which essentially accepts the idea that **nothing further is to be learned in terms of genuine fundamentals** and all that is left for us to do is calculate. . . . [..] This is then the idea that I call "**The Great Solid State Physics Dream Machine**"…

. . . In other words the better the machinery, the more likely it is to conceal the workings of nature, in the sense that it simply gives you the experimental answer without telling you why the experimental answer is true **(1980)**

(R.O. Jones, *DFT for emergents*, Autumn School on Correlated Electrons 2013)

recognizing the successes

"the labours and controversies . . . in understanding the chemical binding in materials had finally come to a resolution in ***favour of 'LDA' and the modern computer" (1998)***

Philip Warren Anderson

… but "very deep problems" remain (1998)

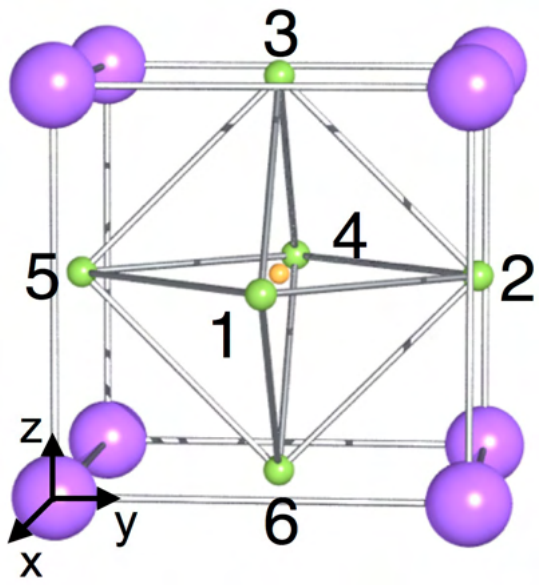
origin of failures: failure of one-electron picture

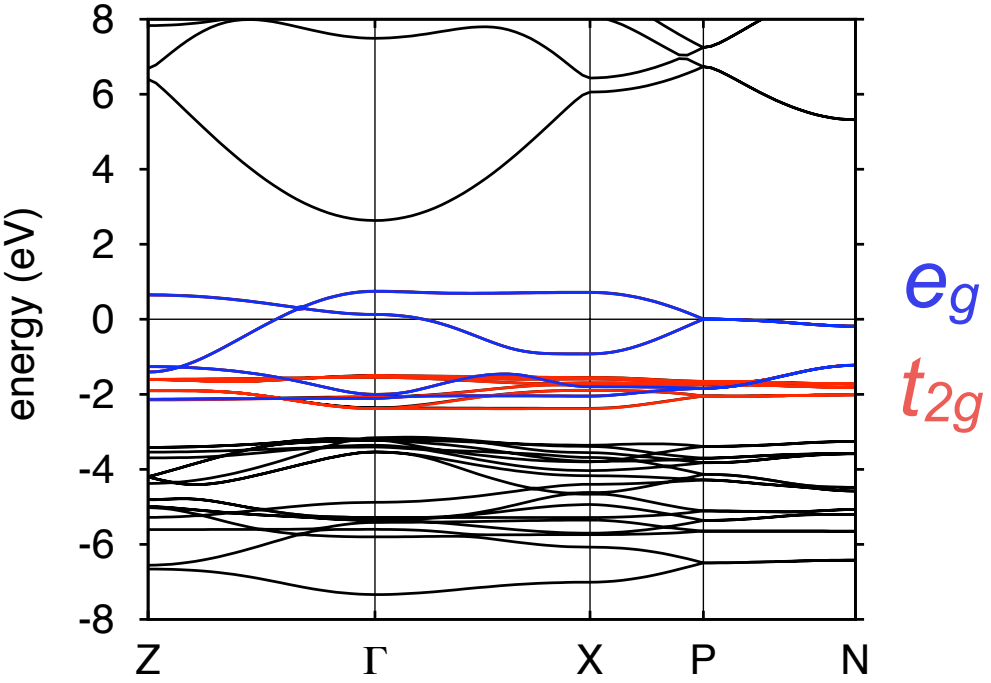
(R.O. Jones, *DFT for emergents*, Autumn School on Correlated Electrons 2013)

deep problems: Mott systems

$KCuF_3$

DFT (LDA): it is a metal!

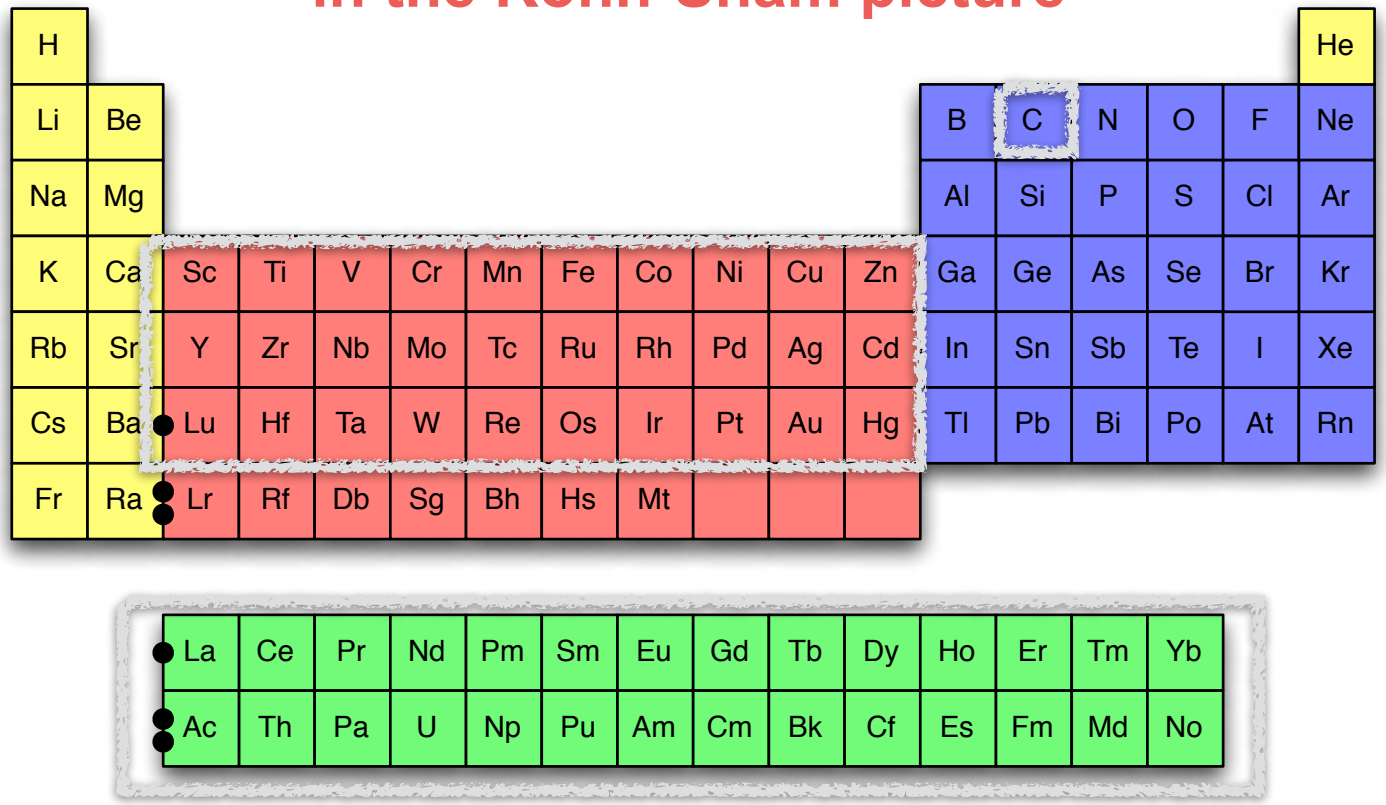




Experiments: insulator! Above 40 K a **paramagnetic** insulator

strongly correlated systems

paramagnetic Mott insulators are either metals or magnetically ordered insulators in the Kohn-Sham picture



Coulomb-induced metal-insulator transition
heavy-Fermions
unconventional superconductivity
spin-charge separation

why does the KS picture fail ?

we can understand it in a simple case

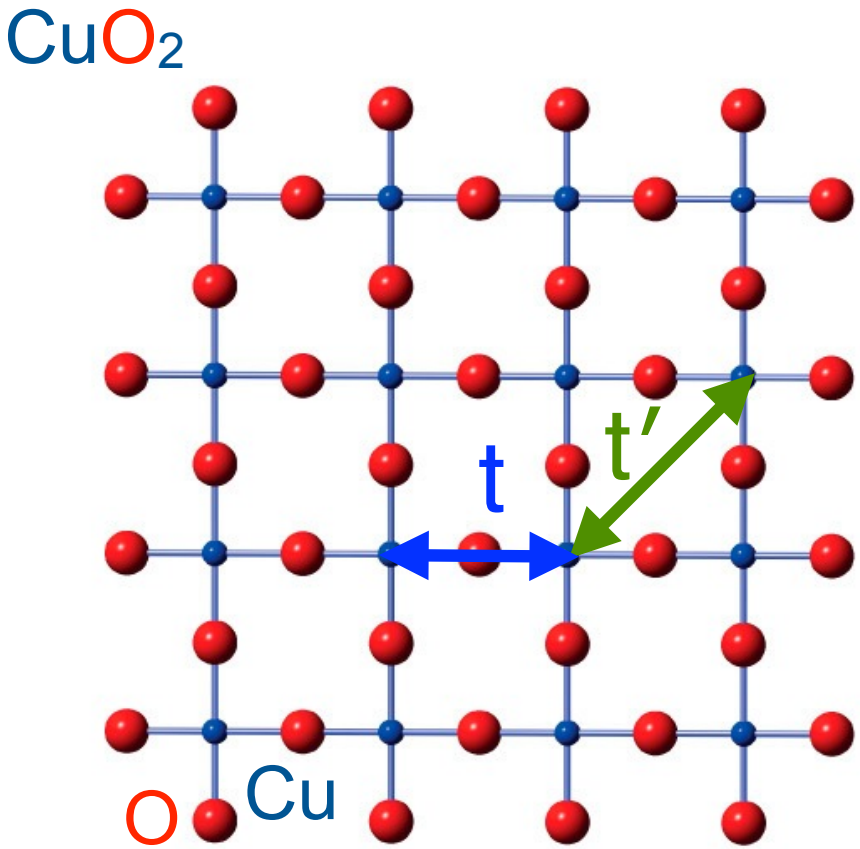
high-T_c superconducting cuprates

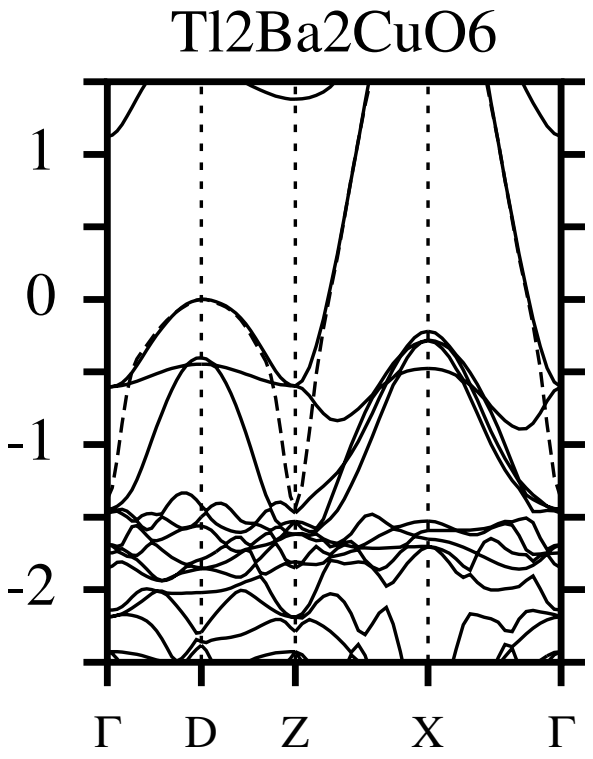
VOLUME 87, NUMBER 4 PHYSICAL REVIEW LETTERS 23 JULY 2001

Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_{c\,\max}$

E. Pavarini, I. Dasgupta,* T. Saha-Dasgupta,† O. Jepsen, and O. K. Andersen
Max-Planck-Institut für Festkörperforschung, D-70506 Stuttgart, Germany
(Received 4 December 2000; published 10 July 2001)

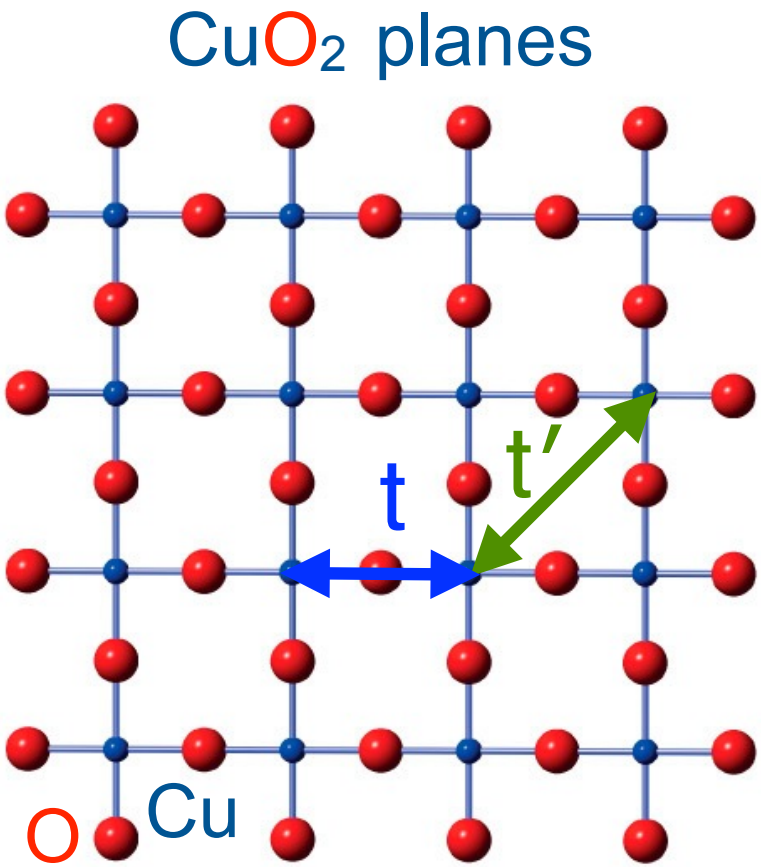
By calculation and analysis of the bare conduction bands in a large number of hole-doped high-temperature superconductors, we have identified the range of the intralayer hopping as the essential, material-dependent parameter. It is controlled by the energy of the axial orbital, a hybrid between Cu $4s$, apical-oxygen $2p_z$, and farther orbitals. Materials with higher $T_{c\,\max}$ have larger hopping ranges and axial orbitals more localized in the CuO_2 layers.

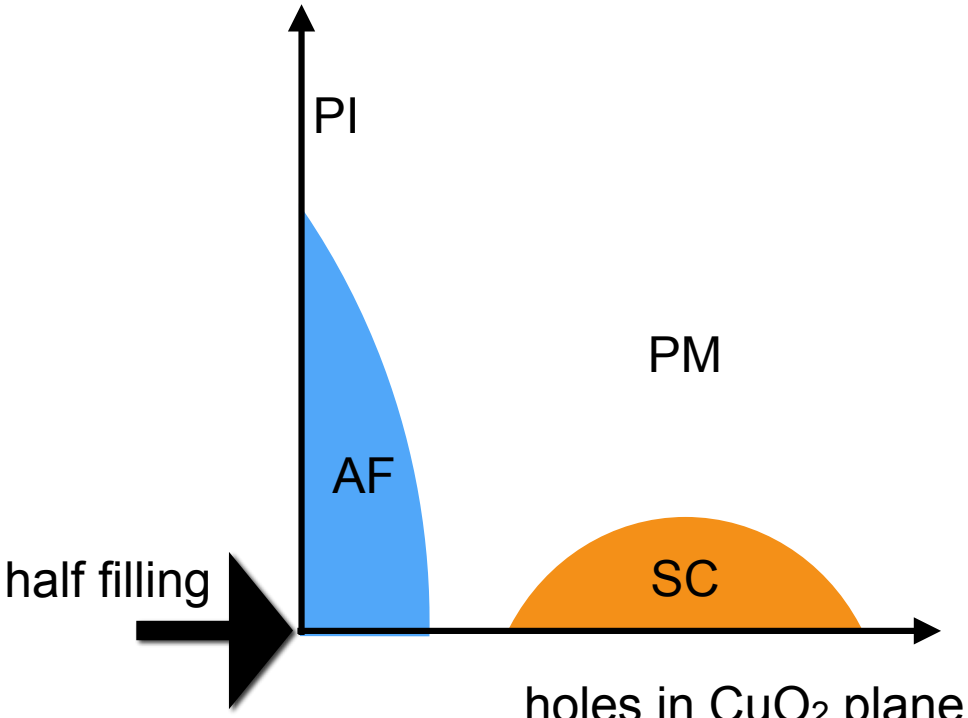




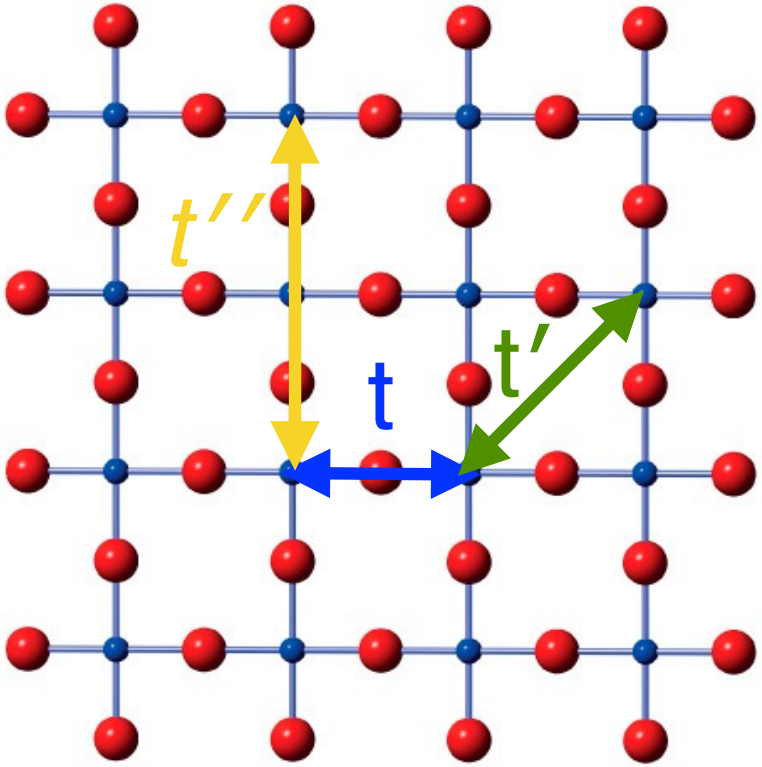
high-T_c superconducting cuprates

phase diagram



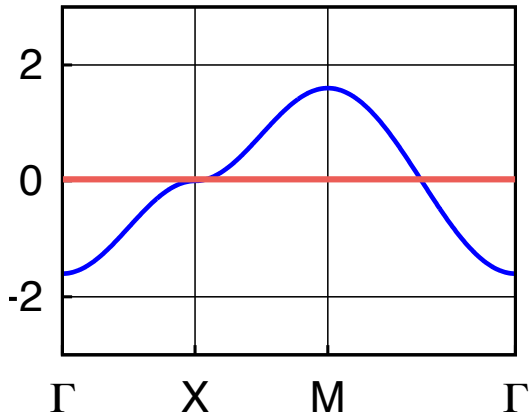


electron counting argument



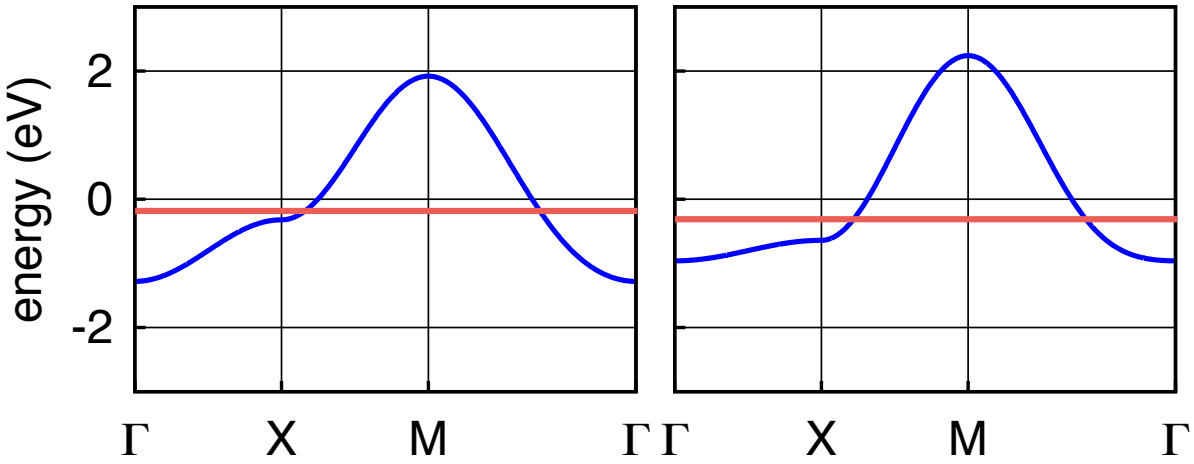
one electron per site

$$\varepsilon_{\boldsymbol{k}} = -2t[\cos k_x + \cos k_y]$$



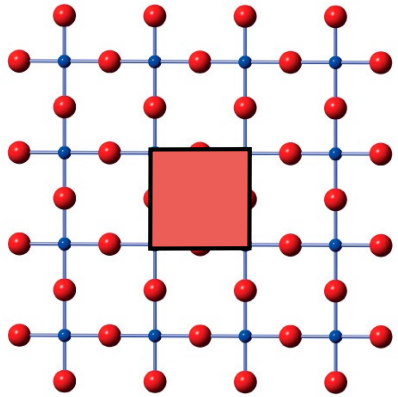
t′/t= =0.2

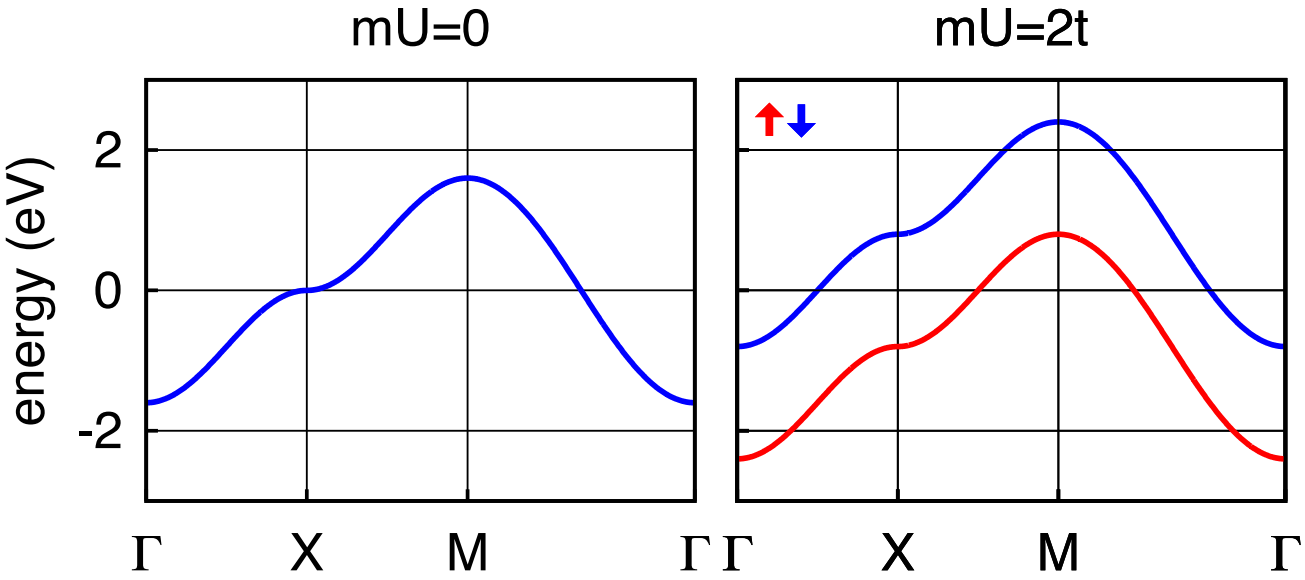
t′/t= =0.4



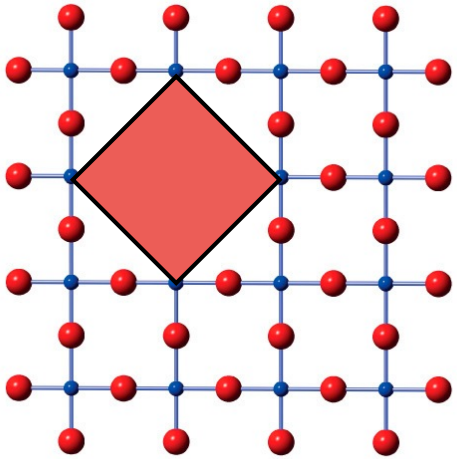
to open a gap we must lower the symmetry

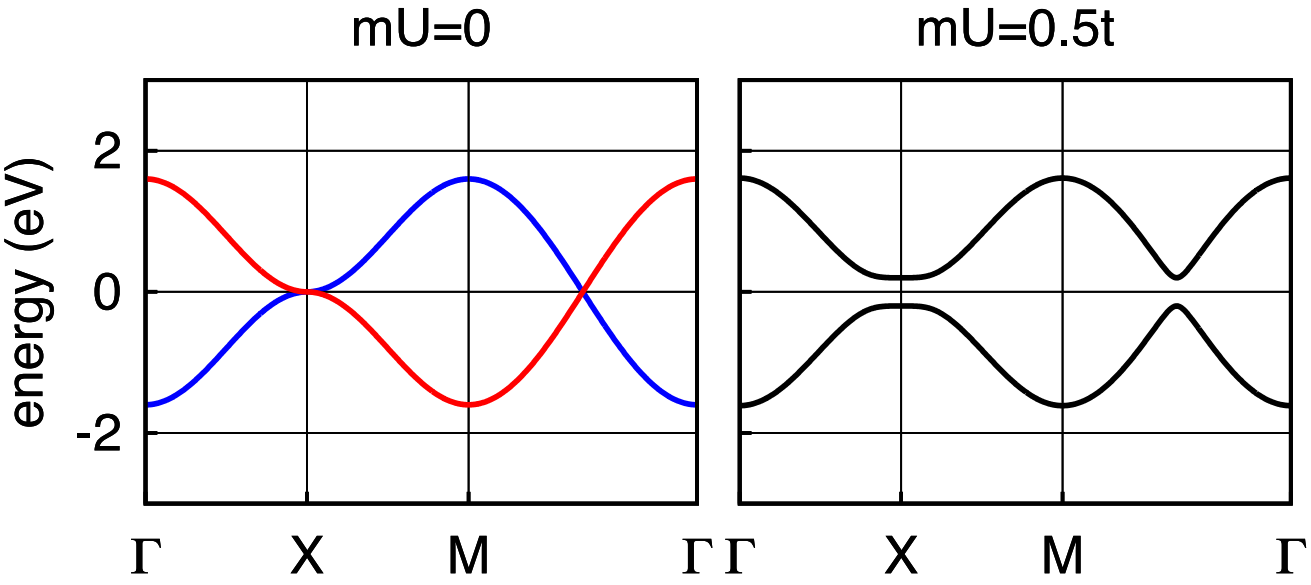
ferro





antiferro





to open a gap we must lower the symmetry

methods for lowering the symmetry

magnetic/orbital/charge order

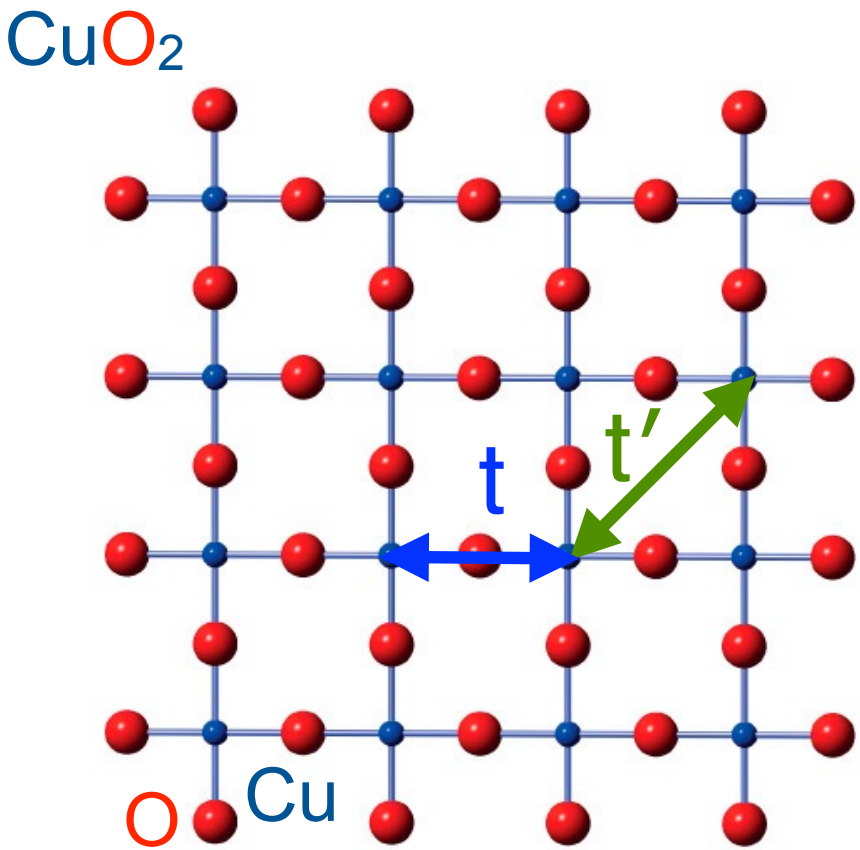
spin-glass-like

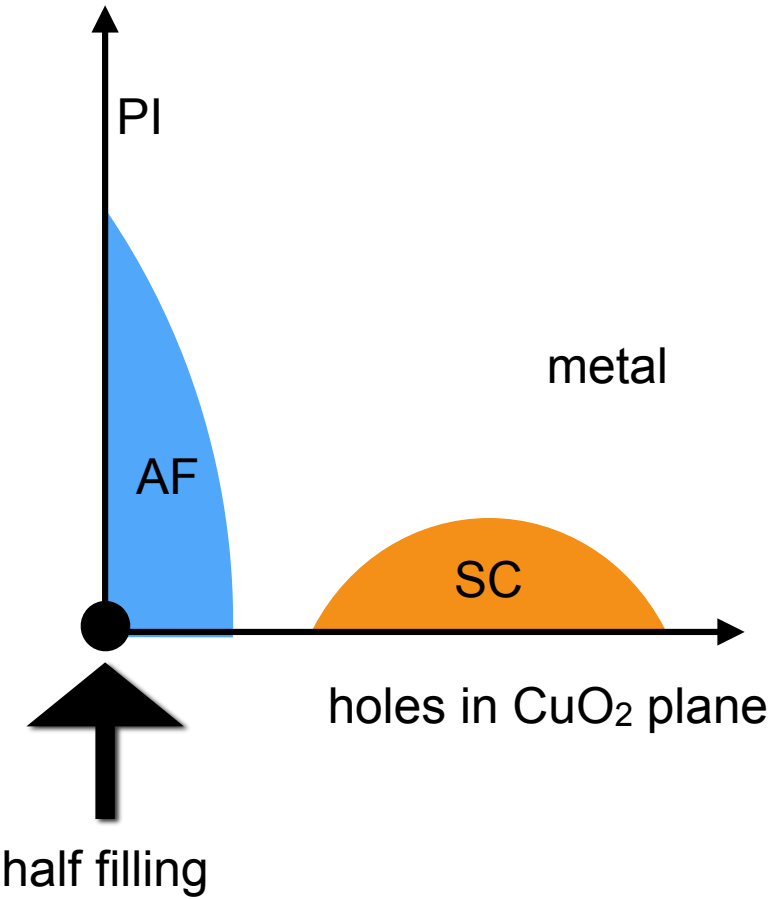
....

Slater insulator

high-T_c superconducting cuprates

phase diagram

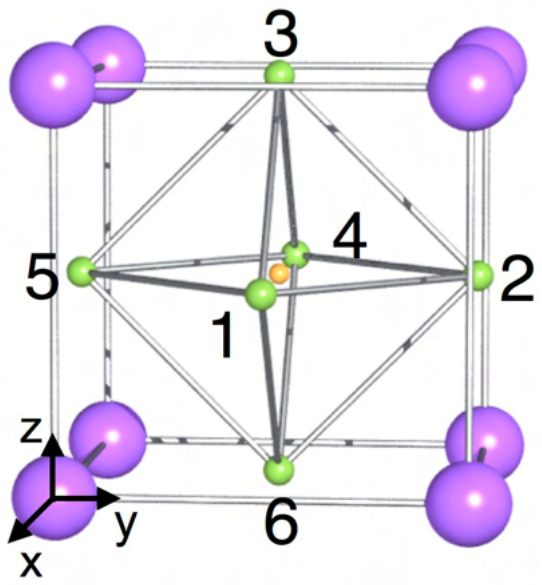


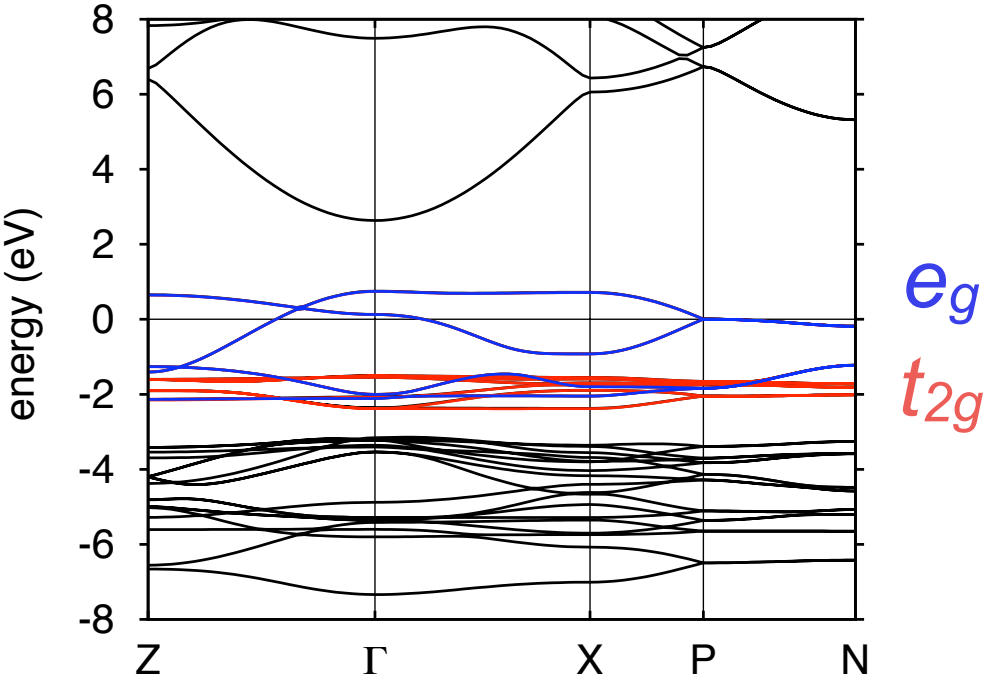


deep problems: Mott systems

$KCuF_3$

DFT (LDA): it is a metal!

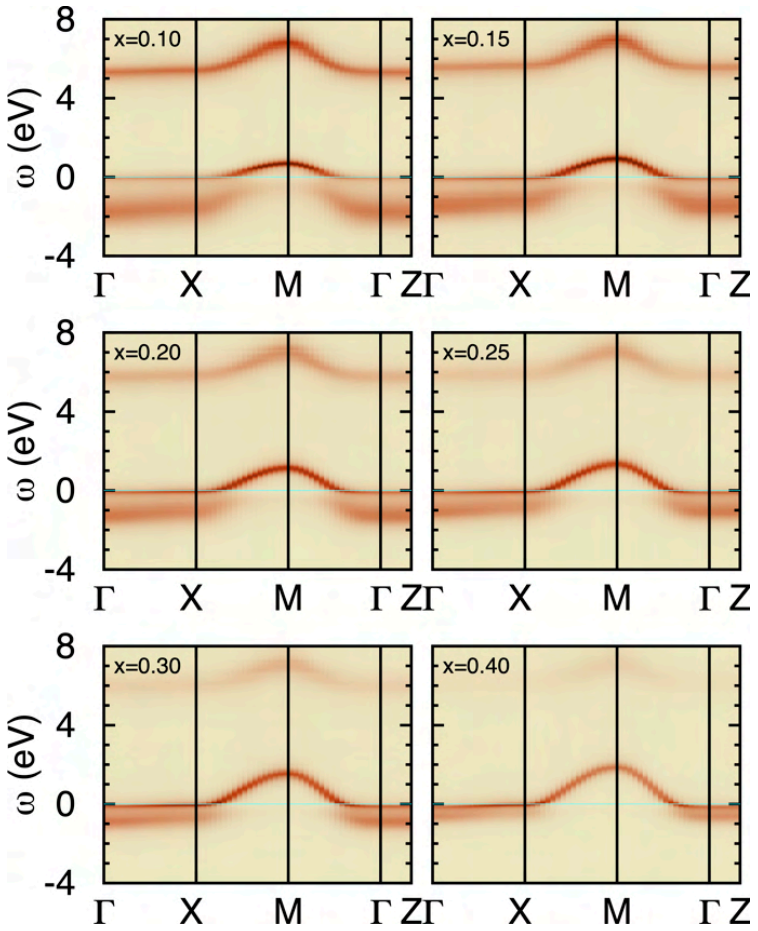




Experiments: insulator! and above 40 K a **paramagnetic** insulator

it is **not** only about the gap

coherent global picture not captured



Mott insulators have different properties than pure Slater insulators

Figure from E. Pavarini, La Rivista del Nuovo Cimento, https://doi.org/10.1007/s40766-021-00025-8

not a failure of DFT

within DFT, Kohn-Sham bands are merely auxiliary quantities to build the density

DFT with exact functional gives exact gap even if the Kohn-Sham description is wrong

(see lecture of Kieron Burke)

failure of *independent-electron* picture

Kohn-Sham eigenvalues as *elementary excitations*
only if the independent-electron picture works

some effects are **not** captured by the
independent- electron picture

when this happens, KS bands, while *ab-initio*,
remain a bad approximation

Mott transition

ab-initio Kohn-Sham approximation fails…

editorial

The Hubbard model at half a century

Models are abundant in virtually all branches of physics, with some achieving iconic status. The Hubbard model, celebrating its golden jubilee this year, continues to be one of the most popular contrivances of theoretical condensed-matter physics.

Capturing the essence of a phenomenon while being simple: the ingredients of a top model in physics. Since the early days of quantum mechanics, many models, Hamiltonians and theories aiming to provide a deeper understanding of various properties of condensed matter have been put forward — with varying degrees of success and fame. One truly legendary model is the Hubbard model, independently conceived by Martin Gutzwiller[1], Junjiro Kanamori[2] and, of course, John Hubbard[3] — their original papers all appearing in 1963. The refine his model. His 'Electron correlations in narrow energy bands' would eventually comprise six installments. 'Hubbard III'[4] became especially important as it showed that for one electron per lattice site — the Hubbard model at half filling — the Mott (or Mott–Hubbard) transition is reproduced. This is a type of metal–insulator transition that could not be understood in terms of conventional band theory (which predicts that a half-filled band always results in a conducting state).

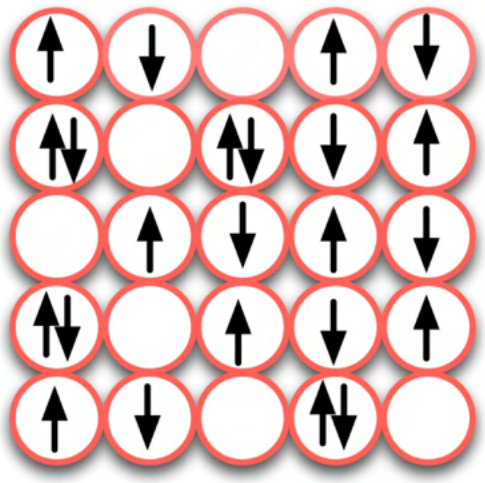
The simplicity of the Hubbard model, when written down, is deceptive. Not only when the field of cold-atom optical trapping had advanced so far that experimental realizations of the Hubbard model could be achieved. A landmark experiment demonstrated how a lattice of bosonic atoms displays a transition from a superfluid to a Mott insulator[5], a result accounted for by the Bose–Hubbard model (the Hubbard model for bosons). Many other variants of the Hubbard model, including the original model for fermions[6], have been experimentally realized by now, a development that nicely illustrates how a model can become the target of experiments

but it can be explained with simple models!

Hubbard model at half-filling

atomic hoppings atomic

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = \hat{H}_d + \hat{H}_T + \hat{H}_U$$

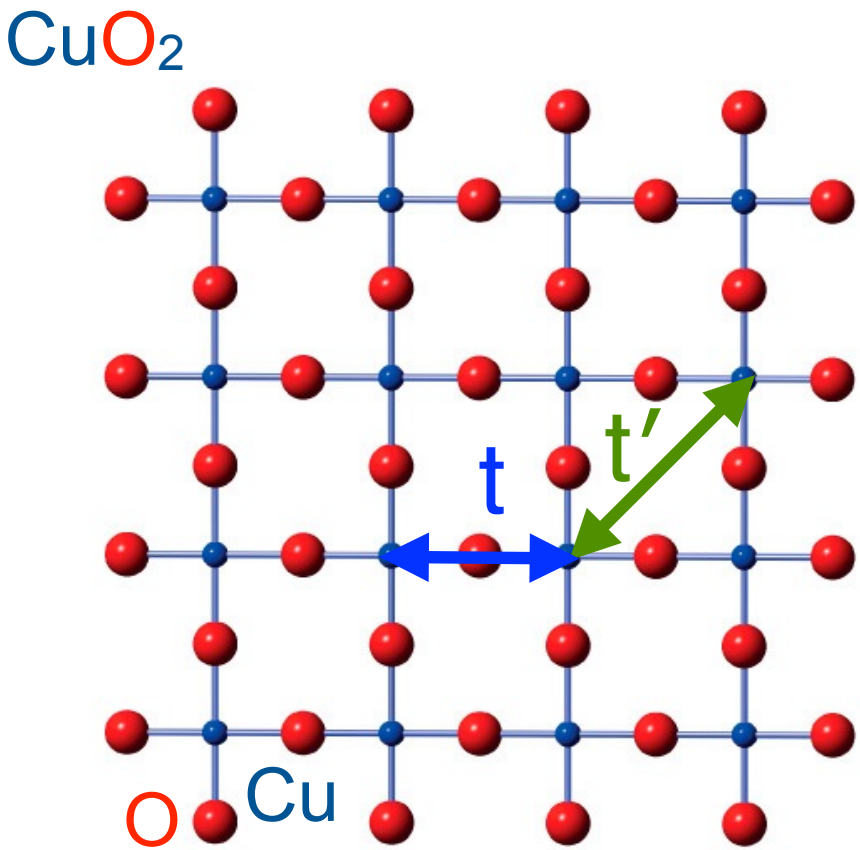


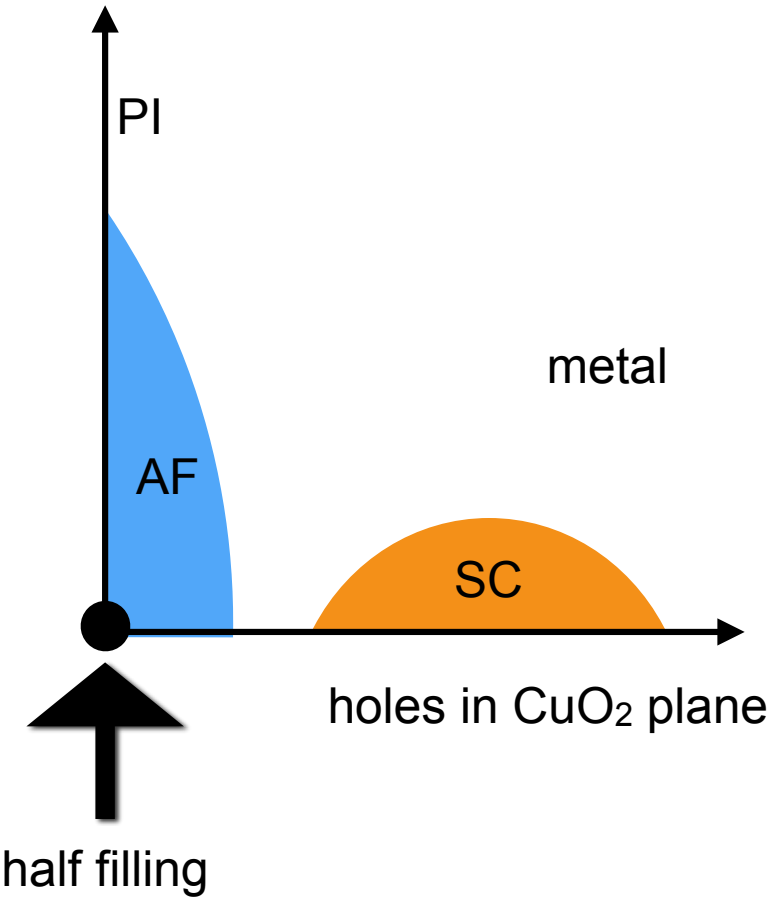
1. *t=0*: collection of atoms, **insulator**
2. *U=0*: half-filled band, **metal**

canonical model for Mott transition

high-T_c superconducting cuprates

phase diagram





1989-1992: dynamical mean-field theory

map LATTICE problem to QUANTUM IMPURITY problem

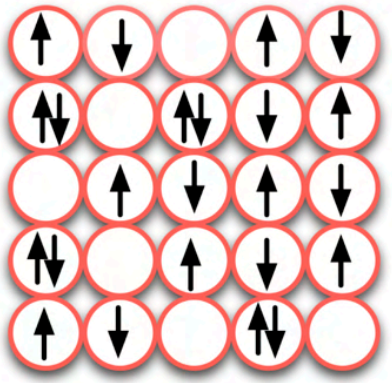
local self-energy approximation

- W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989)
- E. Müller-Hartmann, Z. Phys. B **74**, 507 (1989);
  Z. Phys. B **76**, 211 (1989); Int. J. Mod. Phys. B **3**, 2169 (1989)
- A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992)
- M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992)

1989-1992: dynamical mean-field theory

Hubbard model

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

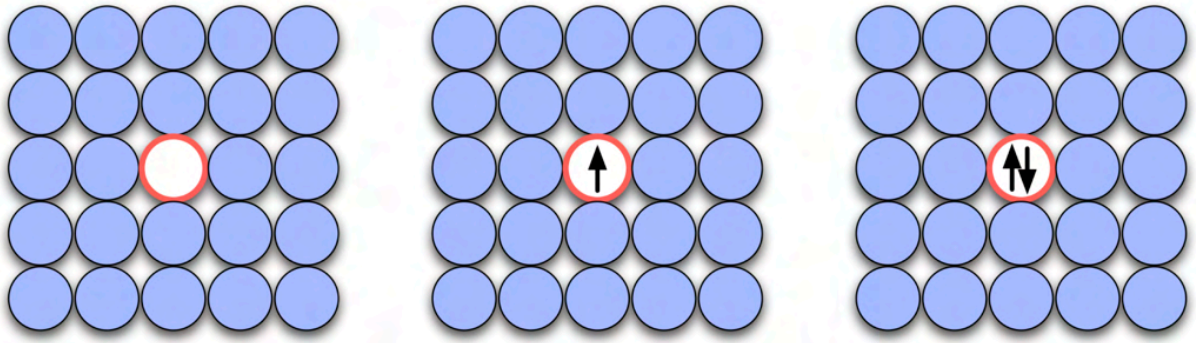


$G^{i,j}$

H^{LDA}

$U^{i,i}$

self-consistent
quantum-impurity model



$$\mathcal{G}^{-1} = G^{-1} + \Sigma$$

$$G = G^{i,i}$$

k-independent self-energy

exact in the infinite coordination number limit

Metzner and Vollhardt, PRL **62**, 324 (1989); Georges and Kotliar, PRB **45**, 6479 (1992).

dynamical mean-field theory

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

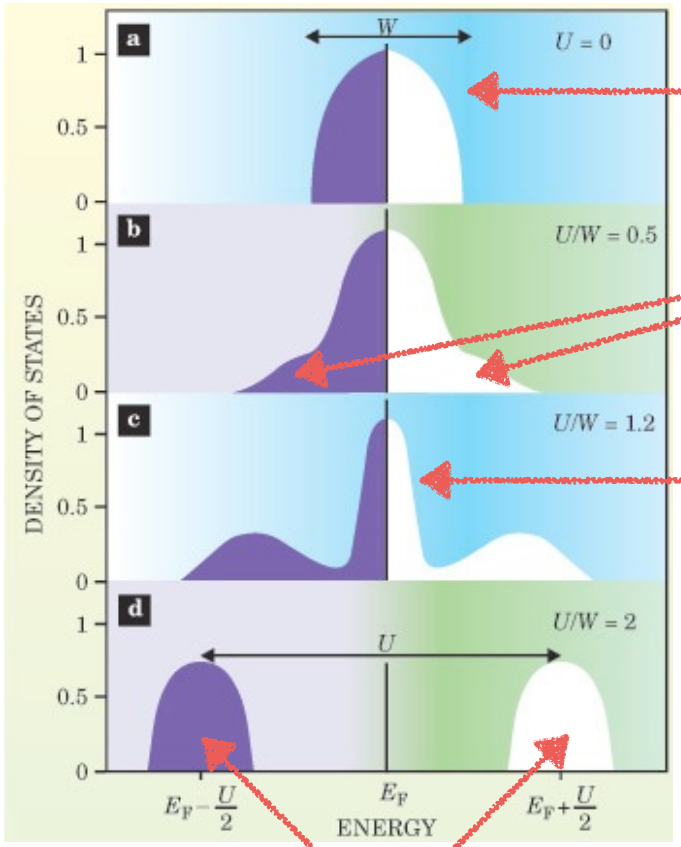
U=0

W: band width

Bethe Lattice

U~W

U>U_c



half-filled metal

spectral weight transfer

narrow quasi-particle peak

Hubbard bands

G. Kotliar and D. Vollhardt, Physics Today **57,** 53 (2004)

II: DMFT

DMFT for the Hubbard dimer

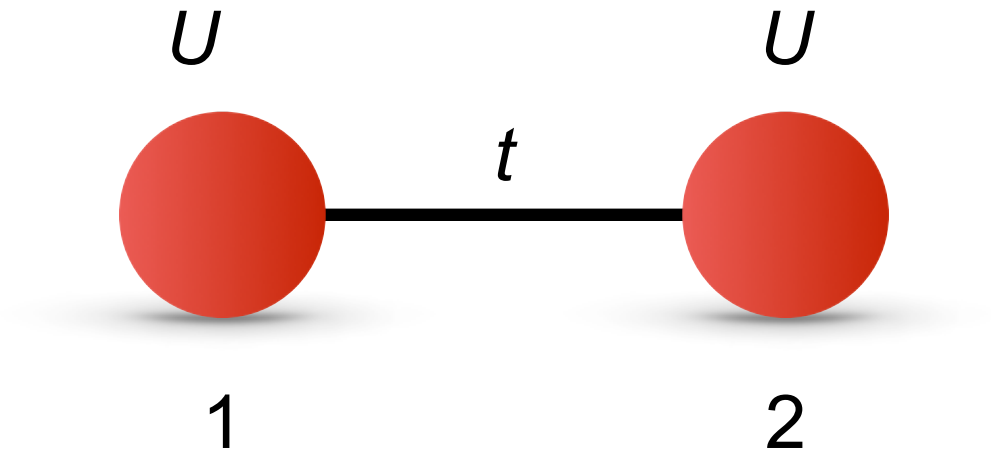
this is a **toy** model: coordination number is one

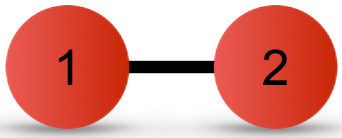
DMFT is exact for *t=0*, *U=0, for a single correlated site*
and in the **infinite dimension** limit

the Hubbard dimer

the Hubbard dimer

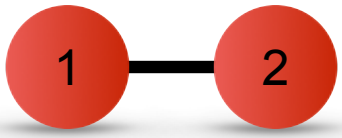
$$\hat{H} = \varepsilon_d \sum_{i\sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$





t=0: exact diagonalization

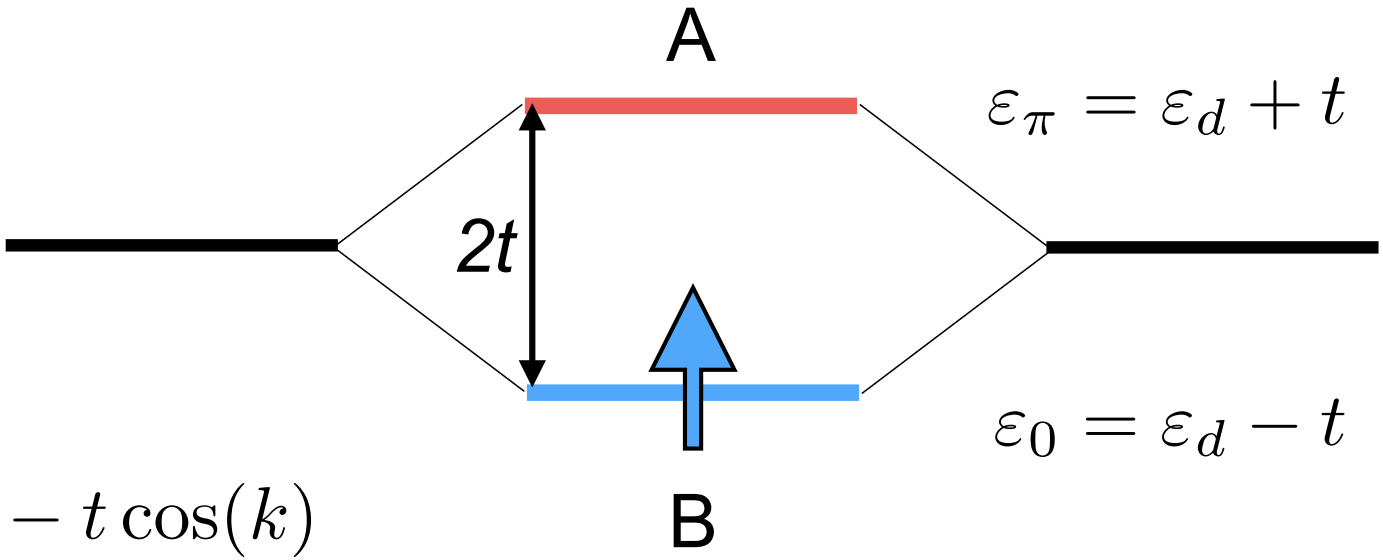
$\lvert N,S,S_z\rangle$			N	S	$E(N,S)$
$\lvert 0,0,0\rangle$	$=$	$\lvert 0\rangle$	0	0	0
$\lvert 1,1/2,\sigma\rangle_1$	$=$	$c^\dagger_{1\sigma}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 1,1/2,\sigma\rangle_2$	$=$	$c^\dagger_{2\sigma}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 2,1,1\rangle$	$=$	$c^\dagger_{2\uparrow}c^\dagger_{1\uparrow}\lvert 0\rangle$	2	1	$2\varepsilon_d$
$\lvert 2,1,-1\rangle$	$=$	$c^\dagger_{2\downarrow}c^\dagger_{1\downarrow}\lvert 0\rangle$	2	1	$2\varepsilon_d$
$\lvert 2,1,0\rangle$	$=$	$\frac{1}{\sqrt{2}}\left[c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}+c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\right]\lvert 0\rangle$	2	1	$2\varepsilon_d$
$\lvert 2,0,0\rangle_0$	$=$	$\frac{1}{\sqrt{2}}\left[c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}-c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\right]\lvert 0\rangle$	2	0	$2\varepsilon_d$
$\lvert 2,0,0\rangle_1$	$=$	$c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}\lvert 0\rangle$	2	0	$2\varepsilon_d+U$
$\lvert 2,0,0\rangle_2$	$=$	$c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\lvert 0\rangle$	2	0	$2\varepsilon_d+U$
$\lvert 3,1/2,\sigma\rangle_1$	$=$	$c^\dagger_{1\sigma}c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\lvert 0\rangle$	3	$1/2$	$3\varepsilon_d+U$
$\lvert 3,1/2,\sigma\rangle_2$	$=$	$c^\dagger_{2\sigma}c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}\lvert 0\rangle$	3	$1/2$	$3\varepsilon_d+U$
$\lvert 4,0,0\rangle$	$=$	$c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\lvert 0\rangle$	4	0	$4\varepsilon_d+2U$



finite *t*: exact diagonalization

N=1

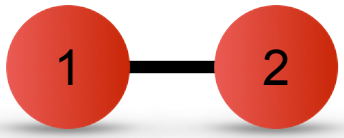
$\lvert 1, S, S_z\rangle_\alpha$	$E_\alpha(1,S)$	$d_\alpha(1,S)$
$\lvert 1,1/2,\sigma\rangle_+ = \frac{1}{\sqrt{2}}\left(\lvert 1,1/2,\sigma\rangle_1 - \lvert 1,1/2,\sigma\rangle_2\right)$	$\varepsilon_d + t$	2
$\lvert 1,1/2,\sigma\rangle_- = \frac{1}{\sqrt{2}}\left(\lvert 1,1/2,\sigma\rangle_1 + \lvert 1,1/2,\sigma\rangle_2\right)$	$\varepsilon_d - t$	2



$\varepsilon_\pi = \varepsilon_d + t$ **k=π**

$\varepsilon_0 = \varepsilon_d - t$ **k=0**

$\varepsilon_k = \varepsilon_d - t\cos(k)$

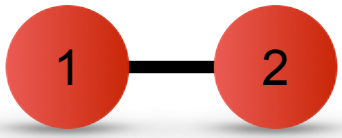


finite *t*: exact diagonalization

S=1 states S=0 states half filling (N=2)

$$\hat{H}_2(\varepsilon_d, U, t) = \begin{pmatrix} 2\varepsilon_d & 0 & 0 & 0 & 0 & 0 \\ 0 & 2\varepsilon_d & 0 & 0 & 0 & 0 \\ 0 & 0 & 2\varepsilon_d & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\varepsilon_d & -\sqrt{2}t & -\sqrt{2}t \\ 0 & 0 & 0 & -\sqrt{2}t & 2\varepsilon_d+U & 0 \\ 0 & 0 & 0 & -\sqrt{2}t & 0 & 2\varepsilon_d+U \end{pmatrix}$$

$\lvert 2,1,1\rangle$	$= c^\dagger_{2\uparrow}c^\dagger_{1\uparrow}\lvert 0\rangle$	2	1	$2\varepsilon_d$
$\lvert 2,1,-1\rangle$	$= c^\dagger_{2\downarrow}c^\dagger_{1\downarrow}\lvert 0\rangle$	2	1	$2\varepsilon_d$
$\lvert 2,1,0\rangle$	$= \frac{1}{\sqrt{2}}\left[c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} + c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\right]\lvert 0\rangle$	2	1	$2\varepsilon_d$
$\lvert 2,0,0\rangle_0$	$= \frac{1}{\sqrt{2}}\left[c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} - c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\right]\lvert 0\rangle$	2	0	$2\varepsilon_d$
$\lvert 2,0,0\rangle_1$	$= c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}\lvert 0\rangle$	2	0	$2\varepsilon_d + U$
$\lvert 2,0,0\rangle_2$	$= c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\lvert 0\rangle$	2	0	$2\varepsilon_d + U$

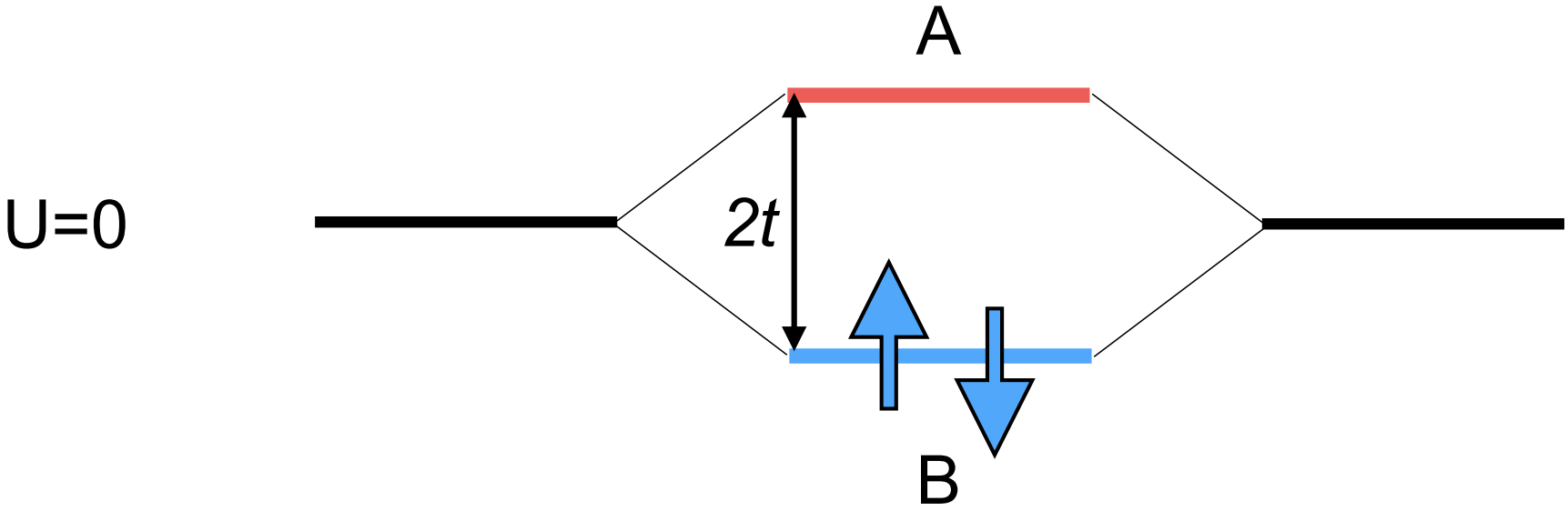


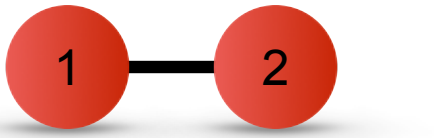
finite *t*: exact diagonalization

half filling (N=2)

$\lvert 2,S,S_z\rangle_\alpha$	$E_\alpha(2,S)$	$d_\alpha(2,S)$
$\lvert 2,0,0\rangle_+ = a_1\lvert 2,0,0\rangle_0 - \frac{a_2}{\sqrt{2}}\left(\lvert 2,0,0\rangle_1 + \lvert 2,0,0\rangle_2\right)$	$2\varepsilon_d + \frac{1}{2}\left(U+\Delta(t,U)\right)$	1
$\lvert 2,0,0\rangle_o = \frac{1}{\sqrt{2}}\left(\lvert 2,0,0\rangle_1 - \lvert 2,0,0\rangle_2\right)$	$2\varepsilon_d + U$	1
$\lvert 2,1,m\rangle_o = \lvert 2,1,m\rangle$	$2\varepsilon_d$	3
$\lvert 2,0,0\rangle_- = a_2\lvert 2,0,0\rangle_0 + \frac{a_1}{\sqrt{2}}\left(\lvert 2,0,0\rangle_1 + \lvert 2,0,0\rangle_2\right)$	$2\varepsilon_d + \frac{1}{2}\left(U-\Delta(t,U)\right)$	1

$$\Delta(t,U) = \sqrt{U^2+16t^2}$$





the ground state

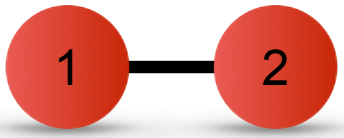
$$|G\rangle_H = \frac{a_2(t,U)}{\sqrt{2}}\left(c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} - c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\right)|0\rangle + \frac{a_1(t,U)}{\sqrt{2}}\left(c^\dagger_{1\uparrow}c^\dagger_{1\downarrow} + c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\right)|0\rangle$$

$$a_1^2(t,U) = \frac{1}{\Delta(t,U)}\frac{\Delta(t,U)-U}{2}, \qquad a_2^2(t,U) = \frac{4t^2}{\Delta(t,U)}\frac{2}{\Delta(t,U)-U},$$

$$\Delta(t,U) = \sqrt{U^2+16t^2}$$

$$E_0(2) = 2\varepsilon_d + \frac{1}{2}\left(U - \Delta(t,U)\right)$$

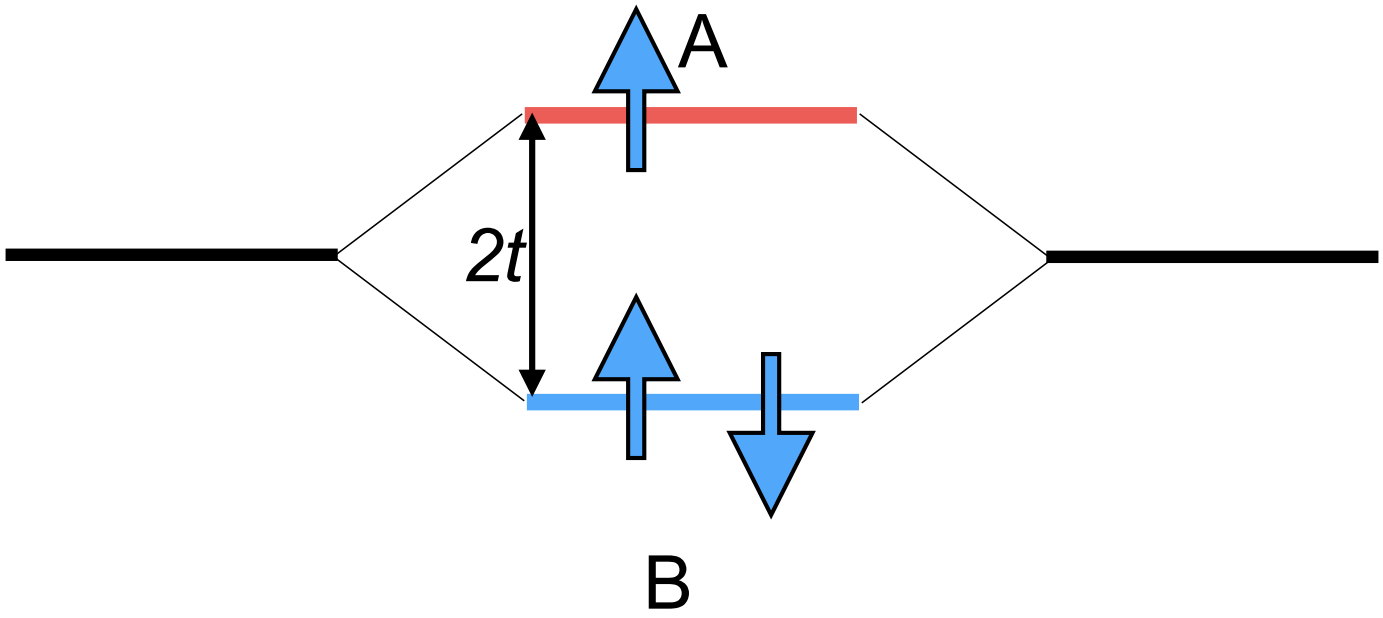
mix three Slater determinants



finite *t*: exact diagonalization

N=3

$\lvert 3, S, S_z\rangle_\alpha$		$E_\alpha(3)$	$d_\alpha(3,S)$
$\lvert 3, 1/2, \sigma\rangle_+$	$= \frac{1}{\sqrt{2}}\left(\lvert 1, 1/2, \sigma\rangle_1 + \lvert 1, 1/2, \sigma\rangle_2\right)$	$3\varepsilon_d + U + t$	2
$\lvert 3, 1/2, \sigma\rangle_-$	$= \frac{1}{\sqrt{2}}\left(\lvert 1, 1/2, \sigma\rangle_1 - \lvert 1, 1/2, \sigma\rangle_2\right)$	$3\varepsilon_d + U - t$	2

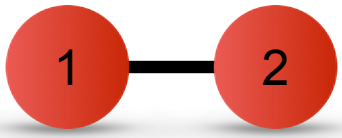


Lehmann representation

$$G^{\sigma}_{i,i}(i\nu_n) = -\int_0^{\beta} d\tau\, e^{i\nu_n \tau} \left\langle \mathcal{T} c_{i\sigma}(\tau) c^{\dagger}_{i\sigma}(0) \right\rangle,$$

$$G^{\sigma}_{i,i}(i\nu_n) = \frac{1}{Z} \sum_{ll'NN'} \frac{e^{-\Delta E_{l'}(N')\beta} + e^{-\Delta E_{l}(N)\beta}}{i\nu_n + \Delta E_l(N) - \Delta E_{l'}(N')} \left| \langle N'_{l'} | c^{\dagger}_{i\sigma} | N_l \rangle \right|^2.$$

$$\Delta E_l(N) = E_l(N) - \mu N$$



the local Green function

Lehmann representation

$d^1 \rightarrow d^0$

$$|\langle 1|c_\sigma|2\rangle|^2$$

$$\mu = \varepsilon_d + \frac{U}{2}$$

$$G^{\sigma}_{i,i}(i\nu_n) = \frac{1}{4}\left(\frac{1 + w(t,U)}{i\nu_n - (E_0(2) - \varepsilon_d + t - \mu)} + \frac{1 - w(t,U)}{i\nu_n - (E_0(2) - \varepsilon_d - t - \mu)} \right.$$

E(2)-E(1)

$$|\langle 3|c^\dagger_\sigma|2\rangle|^2$$

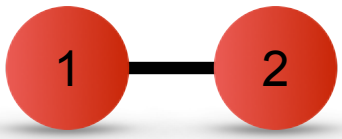
$$\left. + \frac{1 - w(t,U)}{i\nu_n - (-E_0(2) + U + 3\varepsilon_d + t - \mu)} + \frac{1 + w(t,U)}{i\nu_n - (-E_0(2) + U + 3\varepsilon_d - t - \mu)} \right)$$

E(3)-E(2)

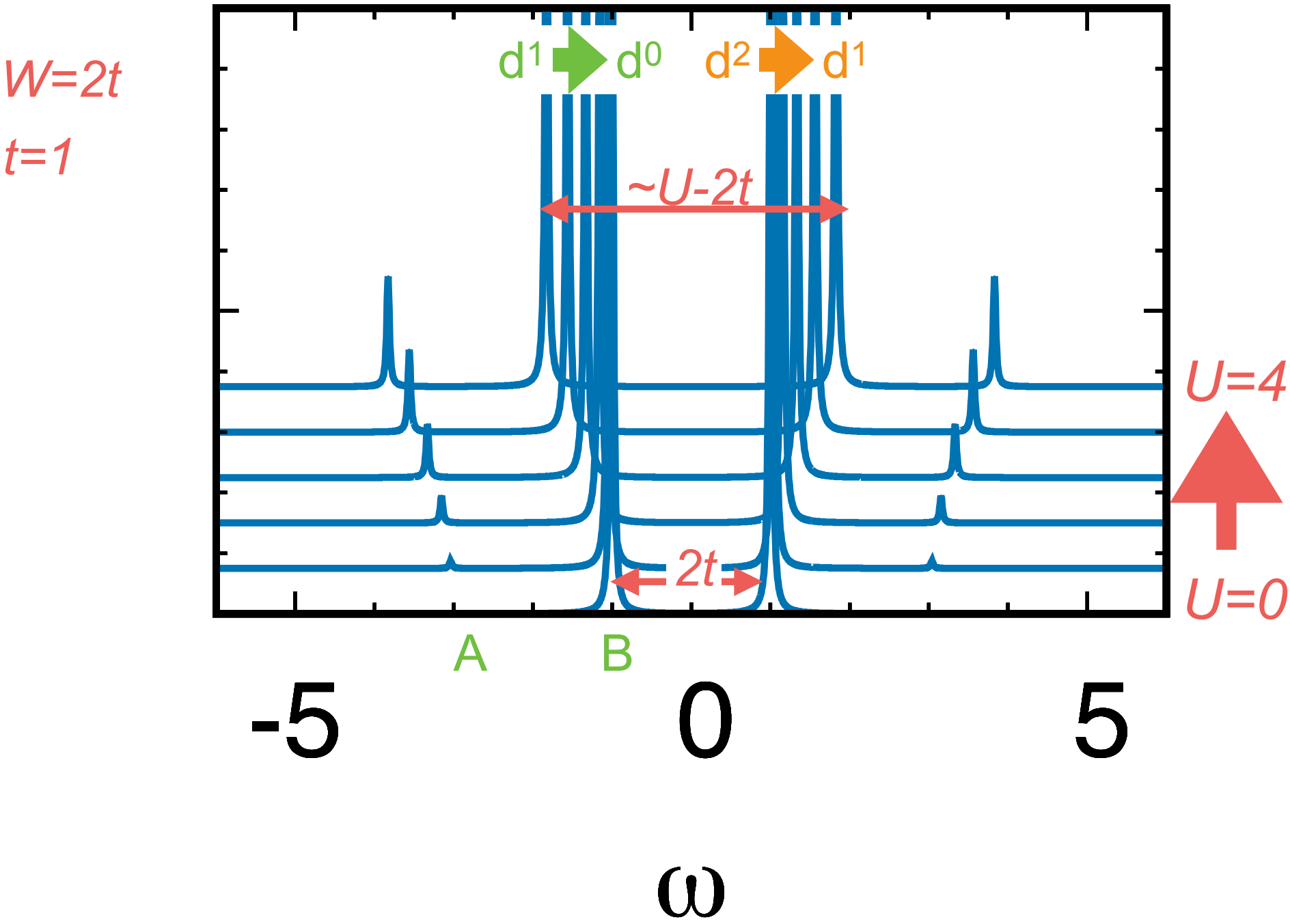
$d^2 \rightarrow d^1$

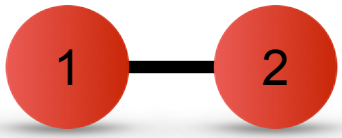
U=0: $E(2) = 2\varepsilon_d - 2t$

t=0: $E(2) = 2\varepsilon_d$



the local spectral function





the local Green function

Lehmann representation

$d^1 \rightarrow d^0$

$$|\langle 1|c_\sigma|2\rangle|^2$$

$$G^{\sigma}_{i,i}(i\nu_n) = \frac{1}{4}\left(\frac{1+w(t,U)}{i\nu_n - (E_0(2) - \varepsilon_d + t - \mu)} + \frac{1-w(t,U)}{i\nu_n - (E_0(2) - \varepsilon_d - t - \mu)} \right.$$

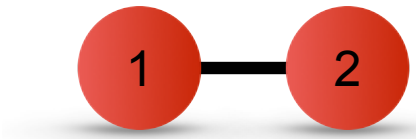
E(2)-E(1)

$$|\langle 3|c^\dagger_\sigma|2\rangle|^2$$

$$\left. + \frac{1-w(t,U)}{i\nu_n - (-E_0(2) + U + 3\varepsilon_d + t - \mu)} + \frac{1+w(t,U)}{i\nu_n - (-E_0(2) + U + 3\varepsilon_d - t - \mu)} \right)$$

E(3)-E(2)

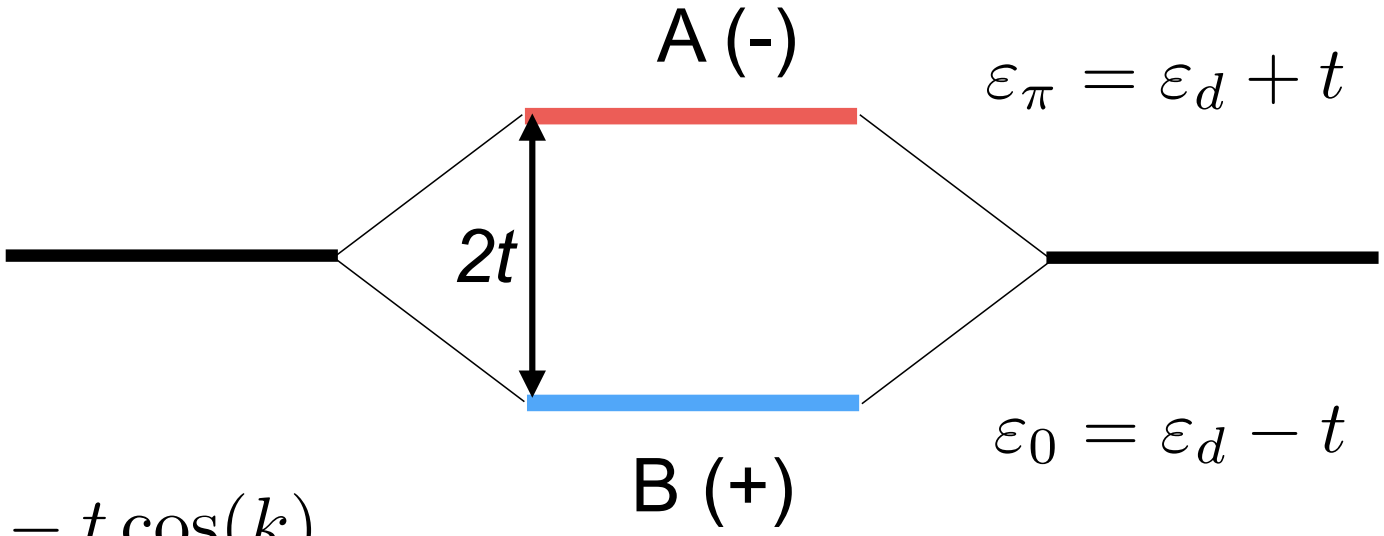
$d^2 \rightarrow d^1$



the local Green function

change from **site** to ***k*** representation

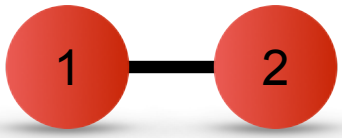
$$c_{k\sigma} = \frac{1}{\sqrt{2}}\left(c_{1\uparrow} \mp c_{2\uparrow}\right)$$



$\varepsilon_\pi = \varepsilon_d + t$ ***k*=π**

$\varepsilon_0 = \varepsilon_d - t$ ***k*=0**

$\varepsilon_k = \varepsilon_d - t\cos(k)$



the local Green function

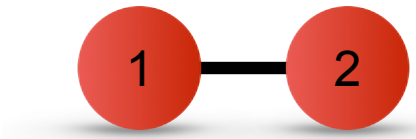
change from **site** to ***k*** representation

$$c_{k\sigma} = \frac{1}{\sqrt{2}}\left(c_{1\uparrow} \mp c_{2\uparrow}\right)$$

$$G^{\sigma}_{i,i}(i\nu_n) = \frac{1}{2}\left(\underbrace{\frac{1}{i\nu_n + \mu - \varepsilon_d + t - \Sigma^{\sigma}(0, i\nu_n)}}_{G^{\sigma}(0,i\nu_n)} + \underbrace{\frac{1}{i\nu_n + \mu - \varepsilon_d - t - \Sigma^{\sigma}(\pi, i\nu_n)}}_{G^{\sigma}(\pi,i\nu_n)} \right)$$

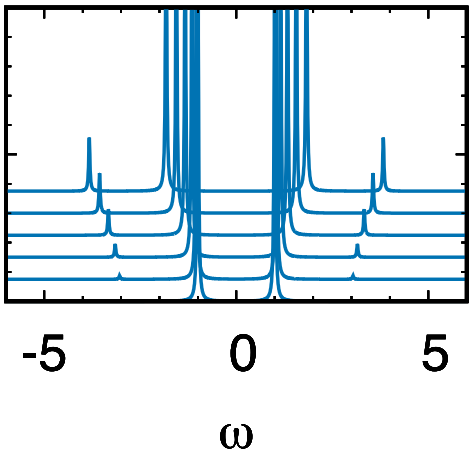
$$\Sigma^{\sigma}(k, i\nu_n) = \frac{U}{2} + \frac{U^2}{4}\,\frac{1}{i\nu_n + \mu - \varepsilon_d - \frac{U}{2} - \; e^{ik}\,3t}.$$

$$\varepsilon_k = -t\cos(k)$$

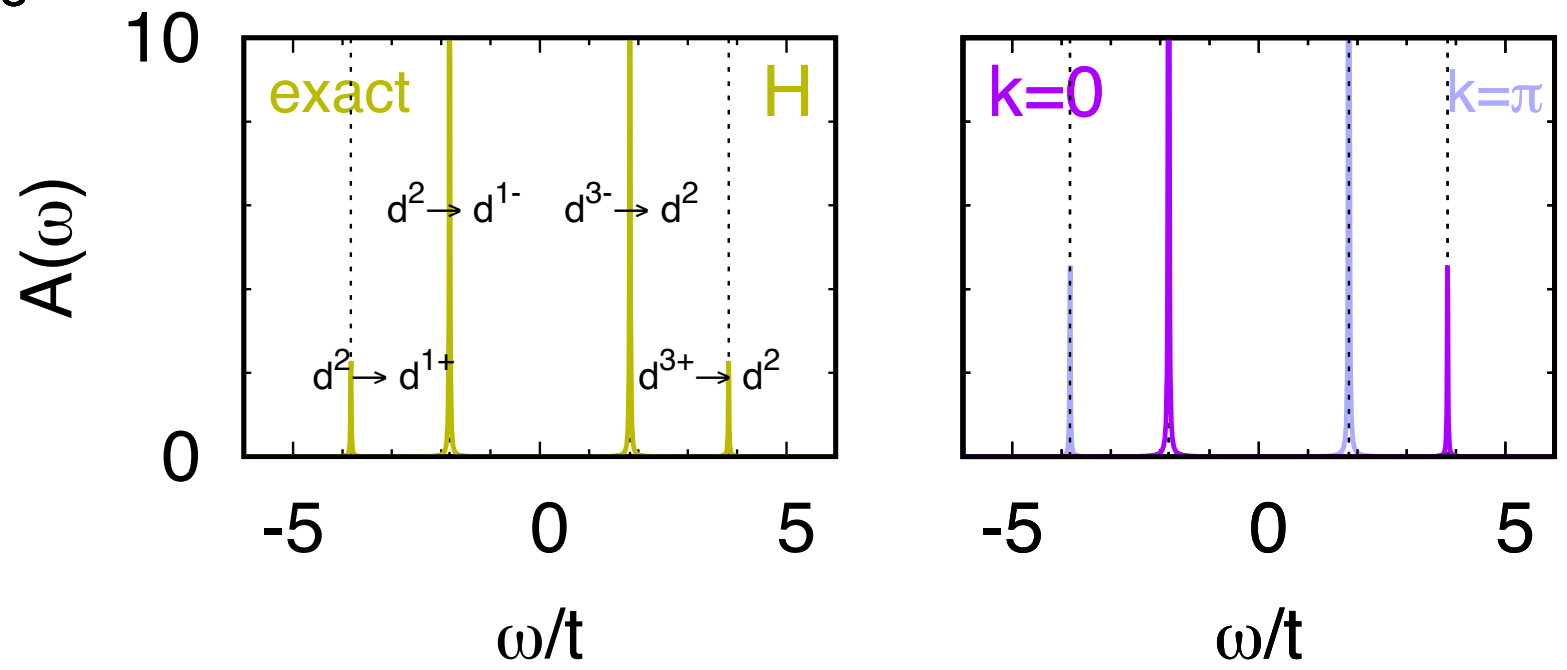


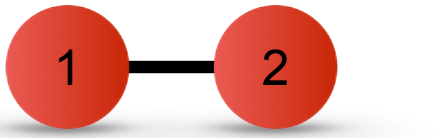
the local Green function

change from **site** to ***k*** representation



$$c_{k\sigma} = \frac{1}{\sqrt{2}} \left(c_{1\uparrow} \mp c_{2\uparrow} \right)$$





local Green function

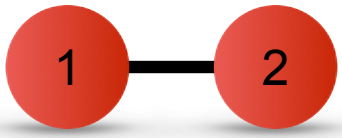
U=0 vs finite *U*

$$G_{11}^{0\sigma}(i\nu_n) = \frac{1}{2}\sum_k \frac{1}{i\nu_n - (\varepsilon_k - \mu)} = \frac{1}{i\nu_n - (\varepsilon_d + F^0(i\nu_n) - \mu)},$$

$$G_{11}^{\sigma}(i\nu_n) = \frac{1}{2}\sum_k \frac{1}{i\nu_n - (\varepsilon_k + \Sigma^\sigma(k, i\nu_n) - \mu)} = \frac{1}{i\nu_n - (\varepsilon_d + \Sigma_l^\sigma(i\nu_n) + F^\sigma(i\nu_n) - \mu)}$$

$$\varepsilon_k = \varepsilon_d - t\cos(k)$$

local self-energy plus modified hybridization function



the local Green function

energy level

$$\varepsilon_d$$

modified energy level

$$\varepsilon_d + \Sigma_l^\sigma(i\nu_n)$$

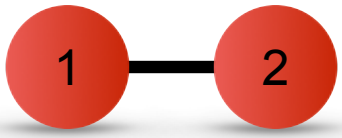
local self-energy

$$\Sigma_l^\sigma(i\nu_n) = \frac{1}{2}\left(\Sigma^\sigma(\pi, i\nu_n) + \Sigma^\sigma(0, i\nu_n)\right) = \frac{U}{2} + \frac{U^2}{4}\,\frac{i\nu_n + \mu - \varepsilon_d - \frac{U}{2}}{(i\nu_n + \mu - \varepsilon_d - \frac{U}{2})^2 - (3t)^2}$$

second order in U!

it is a function!

more poles



the local Green function

hybridization function

$$F^0(i\nu_n) = \frac{t^2}{i\nu_n - (\varepsilon_d - \mu)}$$

modified **hybridization function**

$$F^\sigma(i\nu_n) = \frac{(t + \Delta\Sigma_l(i\nu_n))^2}{i\nu_n - (\varepsilon_d - \mu + \Sigma_l^\sigma(i\nu_n))}$$

non-local self-energy

$$\Delta\Sigma_l^\sigma(i\nu_n) = \frac{1}{2}\Big(\Sigma^\sigma(\pi, i\nu_n) - \Sigma^\sigma(0, i\nu_n)\Big) = \frac{U^2}{4}\,\frac{3t}{(i\nu_n + \mu - \varepsilon_d - \frac{U}{2})^2 - (3t)^2}$$

local Dyson equation

$$\Sigma_l^\sigma(i\nu_n) = \frac{1}{\mathfrak{G}_{i,i}^\sigma(i\nu_n)} - \frac{1}{G_{i,i}^\sigma(i\nu_n)},$$

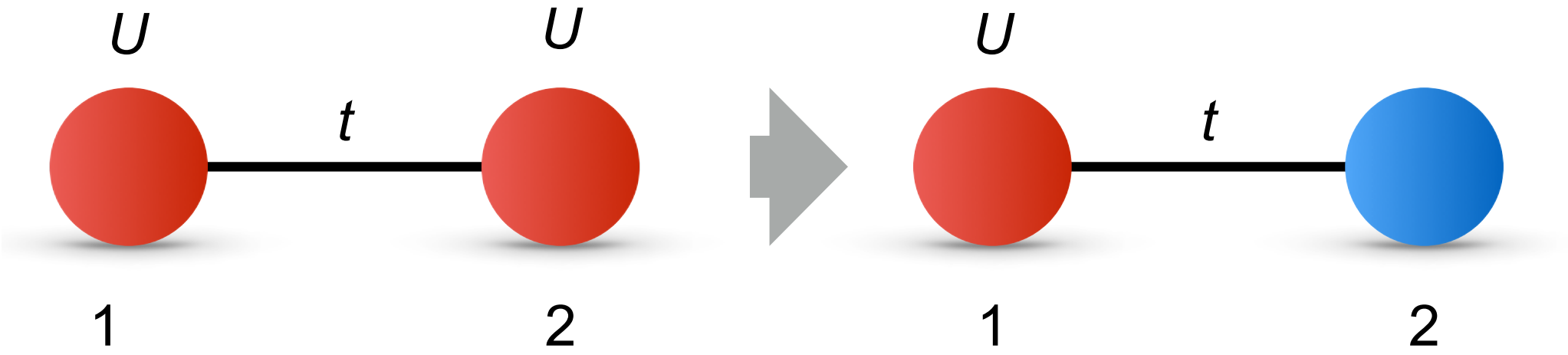
$$\mathfrak{G}_{i,i}^\sigma(i\nu_n) = \frac{1}{i\nu_n + \mu - \varepsilon_d - F^\sigma(i\nu_n)}.$$

similar to quantum impurity

$$\Sigma_A^\sigma(i\nu_n) = \frac{1}{G_{d,d}^{0\sigma}(i\nu_n)} - \frac{1}{G_{d,d}^\sigma(i\nu_n)}$$

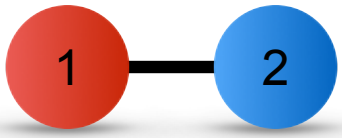
map to a quantum impurity model ?

the Anderson molecule



$$\hat{H}^{\mathrm{A}} = \varepsilon_s \sum_{\sigma} \hat{n}_{s\sigma} - t \sum_{\sigma} \left(c^{\dagger}_{d\sigma} c_{s\sigma} + c^{\dagger}_{s\sigma} c_{d\sigma} \right) + \varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$

~ same local self-energy and Green-function?



self-consistency

half filling: N=2

$$\hat{H}_2(\varepsilon_d, U, t) = \begin{pmatrix} 2\varepsilon_d & 0 & 0 & 0 & 0 & 0 \\ 0 & 2\varepsilon_d & 0 & 0 & 0 & 0 \\ 0 & 0 & 2\varepsilon_d & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\varepsilon_d & -\sqrt{2}t & -\sqrt{2}t \\ 0 & 0 & 0 & -\sqrt{2}t & 2\varepsilon_d+U & 0 \\ 0 & 0 & 0 & -\sqrt{2}t & 0 & 2\varepsilon_d+U \end{pmatrix}$$

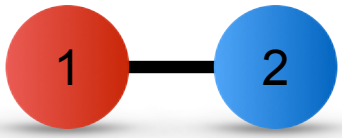
Hubbard

$$\hat{H}_2^A(\varepsilon_d, U, t; \varepsilon_s) = \begin{pmatrix} \varepsilon_d+\varepsilon_s & 0 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_d+\varepsilon_s & 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_d+\varepsilon_s & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_d+\varepsilon_s & -\sqrt{2}t & -\sqrt{2}t \\ 0 & 0 & 0 & -\sqrt{2}t & 2\varepsilon_d+U & 0 \\ 0 & 0 & 0 & -\sqrt{2}t & 0 & 2\varepsilon_s \end{pmatrix}$$

Anderson

same occupations of Hubbard dimer

$\varepsilon_s=\varepsilon_d+U/2=\mu$



solution: Hubbard vs Anderson

Anderson molecule

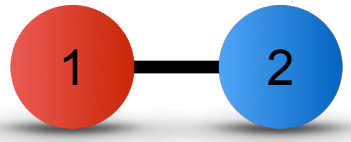
$$G^{\sigma}_{dd}(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma^{\sigma}_{l}(i\nu_n) + F^{\sigma}_{0}(i\nu_n))}$$

Hubbard dimer

$$G^{\sigma}_{11}(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma^{\sigma}_{l}(i\nu_n) + F^{\sigma}(i\nu_n))}$$

the local self-energies are identical!

let us neglect the **non-local** self-energy in Hubbard model



solution: Hubbard vs Anderson

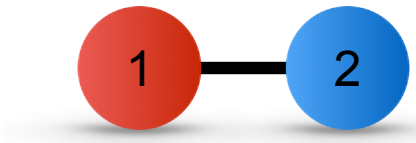
hybridization function

$$F^0(i\nu_n) = \frac{t^2}{i\nu_n - (\varepsilon_d - \mu)},$$

modified **hybridization function**

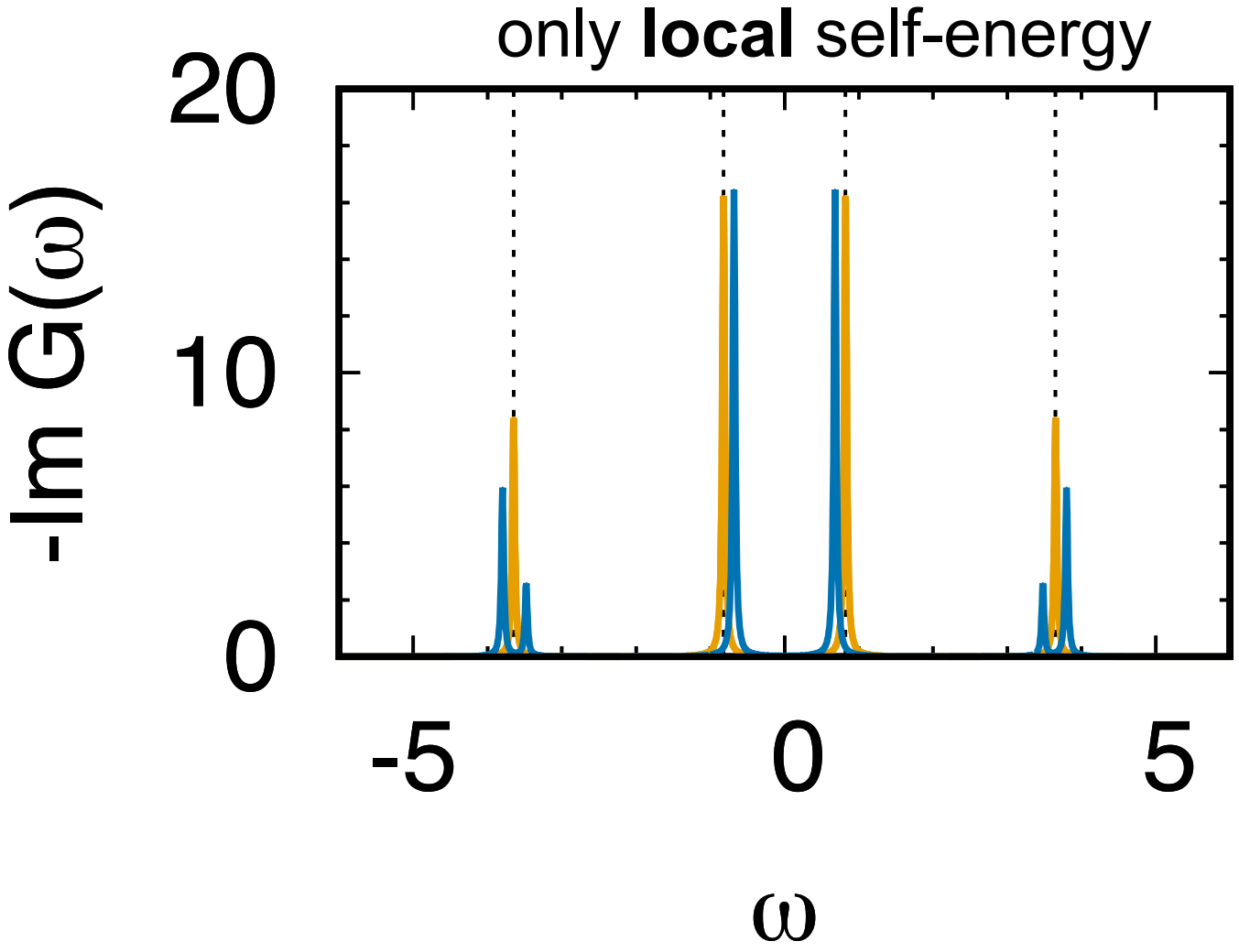
$$F^\sigma(i\nu_n) = \frac{(t + \Delta\Sigma_l(i\nu_n))^2}{i\nu_n - (\varepsilon_d - \mu + \Sigma_l^\sigma(i\nu_n))}.$$

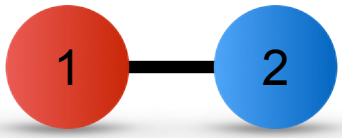
local self-energy approximation



Green function *U=4t*

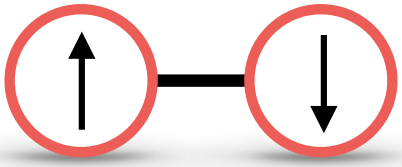
Anderson vs Hubbard (local self-ene approx)





DMFT for the dimer

$$\hat{H} = \varepsilon_d \sum_{i\sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

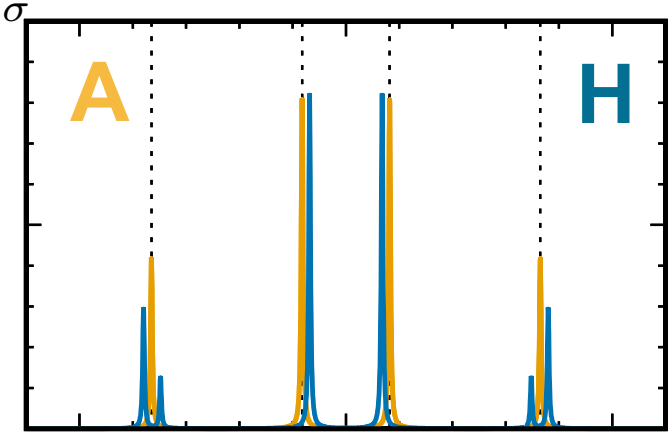


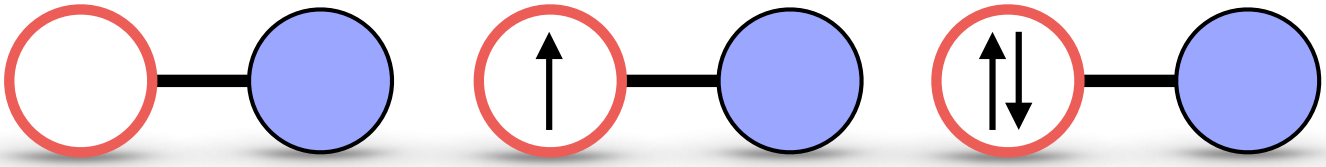
map to quantum impurity model (QIM) in local self-energy approximation

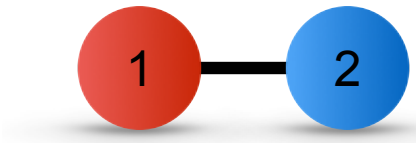
$$\hat{H}^{\mathrm{A}} = \varepsilon_s \sum_{\sigma} \hat{n}_{s\sigma} - t \sum_{\sigma} \left(c^{\dagger}_{d\sigma} c_{s\sigma} + c^{\dagger}_{s\sigma} c_{d\sigma} \right) + \varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$

QIM solver

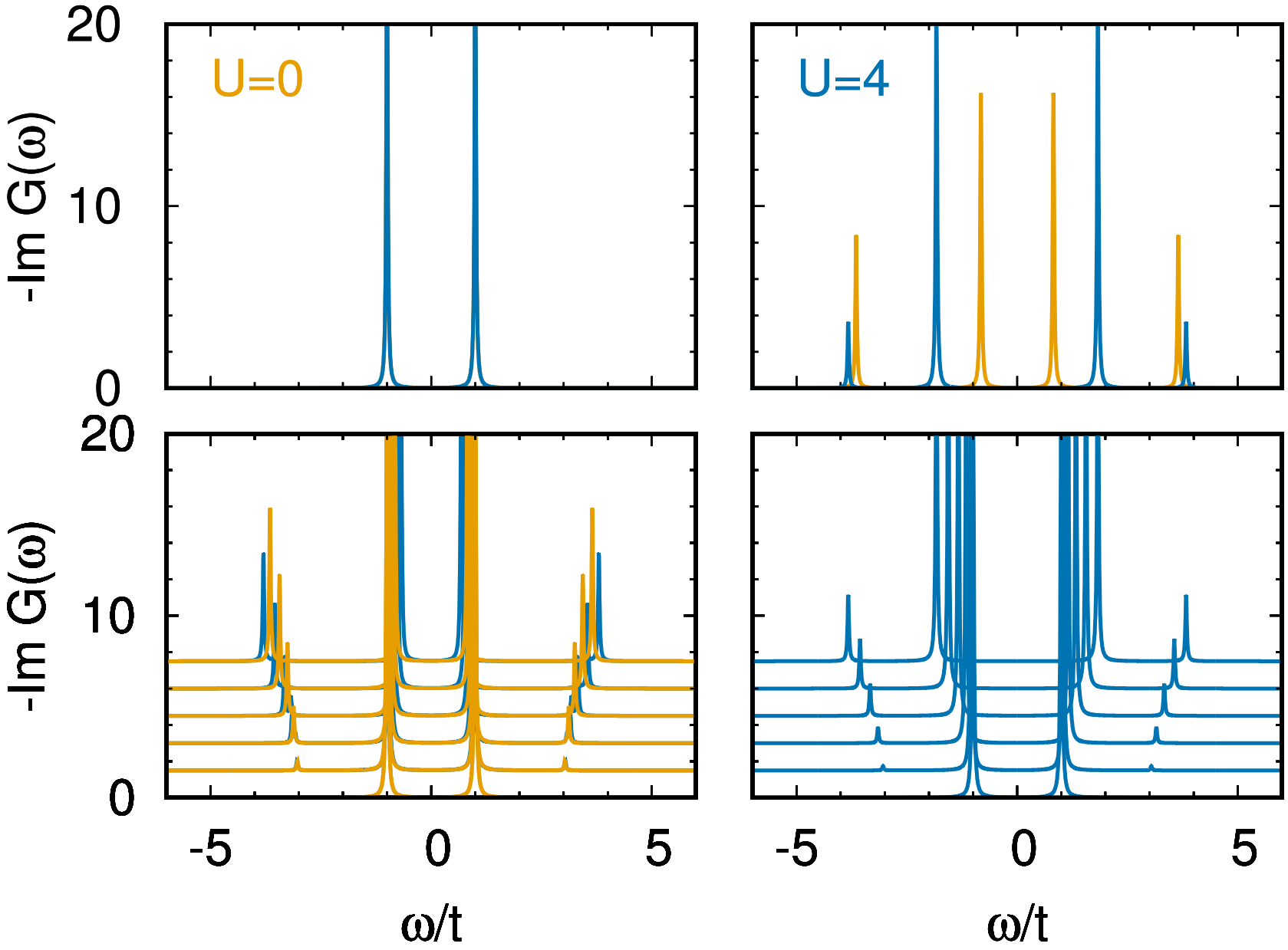
self-consistency loop







DMFT for the Hubbard dimer



DMFT is exact in the following cases

- U=0
- t=0
- quantum impurity limit
- infinite co-ordination number limit

$$\Sigma(\mathbf{k},\omega) \longrightarrow \Sigma(\omega)$$

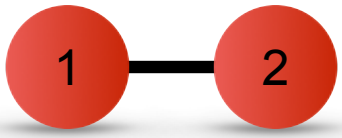
why only a local U?

$$\Sigma(\mathbf{k},\omega) \longrightarrow \Sigma_d(\omega)$$

non-local self-energy terms

vs non-local interaction

$$U_{ijij}$$

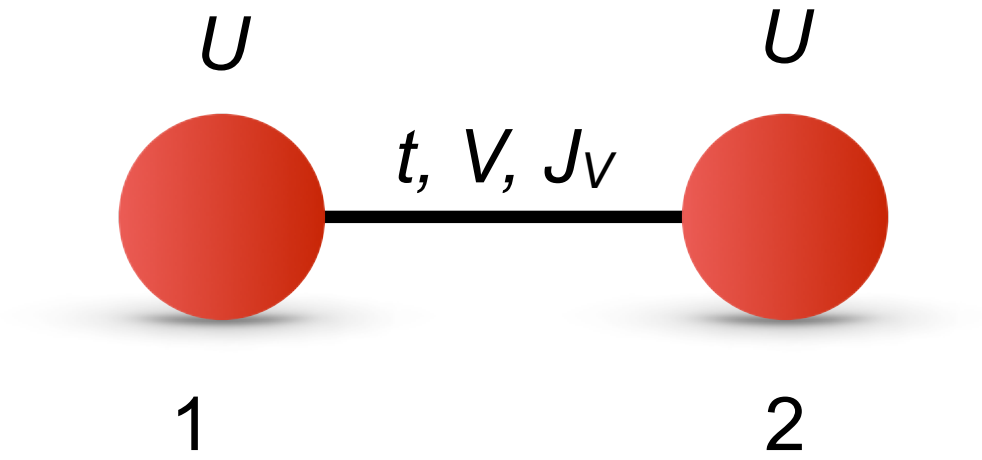


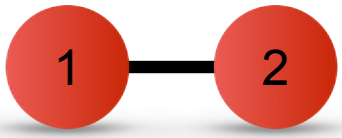
non-local Coulomb terms

how important are they ?

$$\hat{H} = \varepsilon_d \sum_{i\sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right) + U \sum_{i=1,2} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$+ \sum_{\sigma\sigma'} \left(V - 2J_V - J_V \, \delta_{\sigma\sigma'} \right) \hat{n}_{1\sigma} \hat{n}_{2\sigma'} - J_V \sum_{i \neq i'} \left(c^{\dagger}_{i\uparrow} c_{i\downarrow} c^{\dagger}_{i'\downarrow} c_{i'\uparrow} + c^{\dagger}_{i'\uparrow} c^{\dagger}_{i'\downarrow} c_{i\uparrow} c_{i\downarrow} \right)$$





non-local Coulomb terms

N=2 half filling

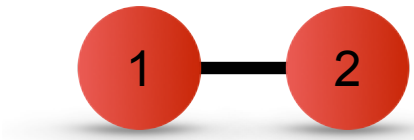
Hubbard

$$\hat{H}_2(\varepsilon_d, U, t) = \begin{pmatrix} 2\varepsilon_d & 0 & 0 & 0 & 0 & 0 \\ 0 & 2\varepsilon_d & 0 & 0 & 0 & 0 \\ 0 & 0 & 2\varepsilon_d & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\varepsilon_d & -\sqrt{2}t & -\sqrt{2}t \\ 0 & 0 & 0 & -\sqrt{2}t & 2\varepsilon_d+U & 0 \\ 0 & 0 & 0 & -\sqrt{2}t & 0 & 2\varepsilon_d+U \end{pmatrix}$$

Hubbard
+non-local

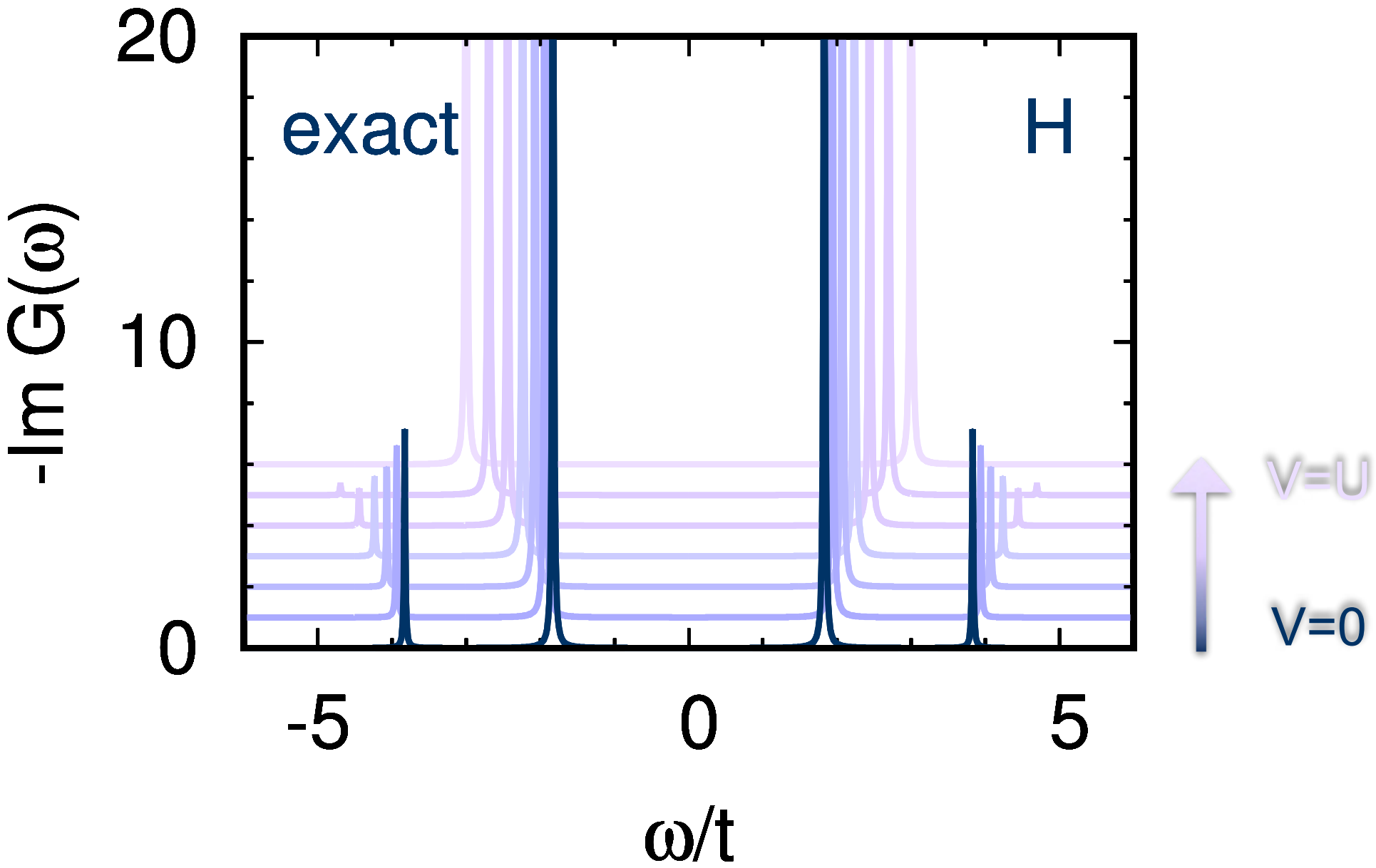
$$\hat{H}_2^{\mathrm{NL}} = \begin{pmatrix} 2\varepsilon_d + V - 3J_V & 0 & 0 & 0 & 0 & 0 \\ 0 & 2\varepsilon_d + V - 3J_V & 0 & 0 & 0 & 0 \\ 0 & 0 & 2\varepsilon_d + V - 3J_V & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\varepsilon_d + V - J_V & -\sqrt{2}t & -\sqrt{2}t \\ 0 & 0 & 0 & -\sqrt{2}t & 2\varepsilon_d + U & -J_V \\ 0 & 0 & 0 & -\sqrt{2}t & -J_V & 2\varepsilon_d + U \end{pmatrix}$$

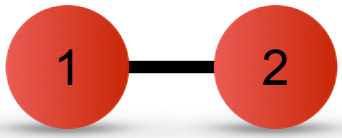
Setting for simplicity $J_V = 0$, we can notice that $\hat{H}_2^{\mathrm{NL}}$ equals $\hat{H}_2(\varepsilon'_d, U', t)$, the Hamiltonian of the $J_V = V = 0$ Hubbard dimer, with parameters $\varepsilon'_d = \varepsilon_d + V/2$ and $U' = U - V$.



non-local Coulomb terms

N=2 half filling and J_V=0





non-local Coulomb terms

U=*V*: *N*=2, effective non-correlated dimer

Strong-correlation effects when local electron-electron repulsion dominates over non-local terms

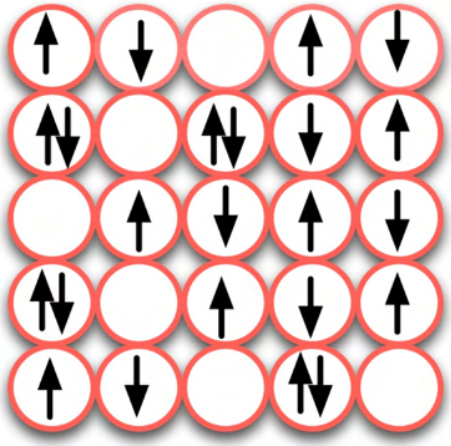
If Coulomb interaction independent on site distance

effective weakly-correlated model

DMFT for the one-band Hubbard model

$$H = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

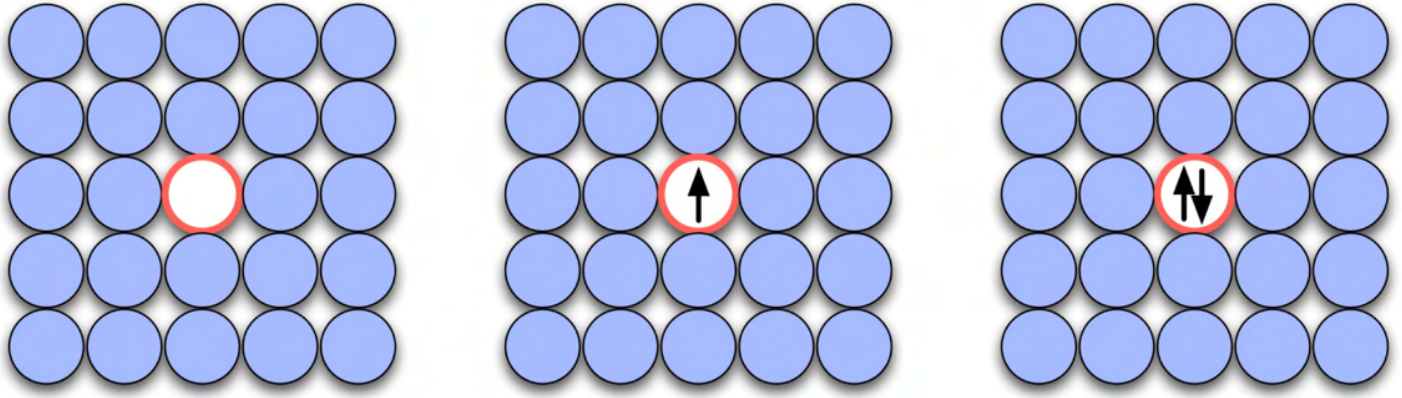
dynamical mean-field theory



$G^{i,j}$

H^{LDA}

$U^{i,i}$



$$\mathcal{G}^{-1} = G^{-1} + \Sigma$$

$$G = G^{i,i}$$

Metzner and Vollhardt, PRL **62**, 324 (1989); Georges and Kotliar, PRB **45,** 6479 (1992)

self-consistency loop

$$H = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

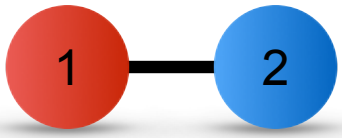
quantum impurity model (QIM)

$$\hat{H}^A = \underbrace{\sum_{\boldsymbol{k}\sigma} \varepsilon^s_{\boldsymbol{k}} \hat{n}_{\boldsymbol{k}\sigma}}_{\hat{H}_{\rm bath}} + \underbrace{\sum_{\boldsymbol{k}\sigma} \left(V^s_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{d\sigma} + \text{h.c.} \right)}_{\hat{H}_{\rm hyb}} + \underbrace{\varepsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}}_{\hat{H}_{\rm imp}}$$

QIM solver: **QMC**, ED, NRG, DMRG,…

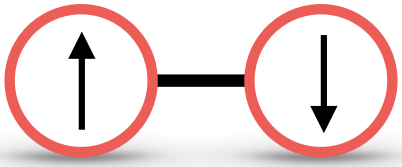
self-consistency loop $G_{dd}=G_{ii}$

quantum-impurity solvers



DMFT for the dimer

$$\hat{H} = \varepsilon_d \sum_{i\sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

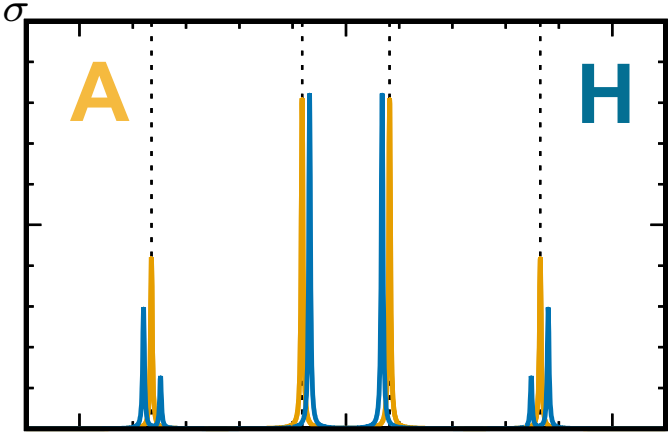


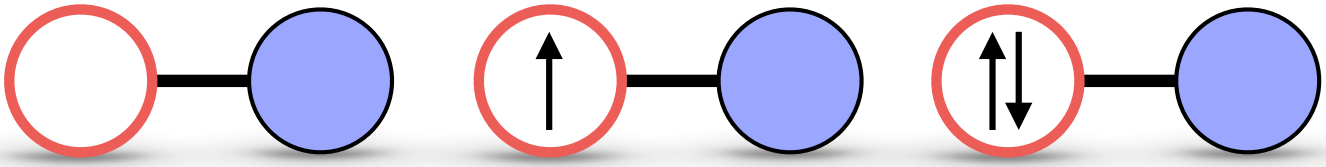
map to quantum impurity model (QIM) in local self-energy approximation

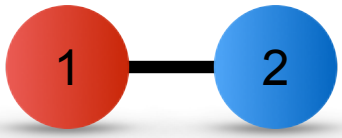
$$\hat{H}^{\mathrm{A}} = \varepsilon_s \sum_{\sigma} \hat{n}_{s\sigma} - t \sum_{\sigma} \left(c^{\dagger}_{d\sigma} c_{s\sigma} + c^{\dagger}_{s\sigma} c_{d\sigma} \right) + \varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$

QIM solver

self-consistency loop



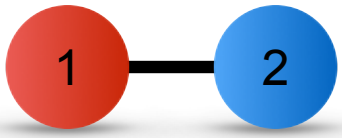




quantum-impurity solver

$$\hat{H}^{\mathrm{A}} = \underbrace{\varepsilon_s \sum_{\sigma} \hat{n}_{s\sigma}}_{\hat{H}_{\mathrm{bath}}} \underbrace{-t \sum_{\sigma} \left(c^{\dagger}_{d\sigma} c_{s\sigma} + c^{\dagger}_{s\sigma} c_{d\sigma} \right)}_{\hat{H}_{\mathrm{hyb}}} + \underbrace{\varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}}_{\hat{H}_{\mathrm{loc}}}$$

hybridization-expansion CT-QMC



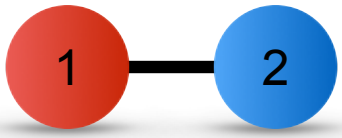
quantum-impurity solver

hybridization expansion

$$Z = \mathrm{Tr}\left(e^{-\beta(\hat{H}_0-\mu\hat{N})}\hat{V}(\beta)\right)$$

$$\hat{V}(\beta) = e^{\beta(\hat{H}_0-\mu\hat{N})}e^{-\beta(\hat{H}_0+\hat{H}_{\mathrm{hyb}}-\mu\hat{N})} = \sum_m \underbrace{\int_0^\beta d\tau_1 \cdots \int_{\tau_{m-1}}^\beta d\tau_m}_{\int d\boldsymbol{\tau}^m} \underbrace{(-1)^m \prod_{l=m}^1 \hat{H}_{\mathrm{hyb}}(\tau_l)}_{\hat{O}^m(\boldsymbol{\tau})}$$

only even orders survive (m=2k)



quantum-impurity solver

bath-impurity decoupling

$$\frac{Z}{Z_{\text{bath}}} = \sum_k \int^k d\boldsymbol{\tau} \int^k d\bar{\boldsymbol{\tau}} \sum_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}} d^k_{\bar{\boldsymbol{\sigma}},\boldsymbol{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})\, t^k_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})$$

(d_c over $d^k_{\bar{\boldsymbol{\sigma}},\boldsymbol{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})$, t_c over $t^k_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})$)

$$w_c = d\boldsymbol{\tau}_c\, d_c\, t_c$$

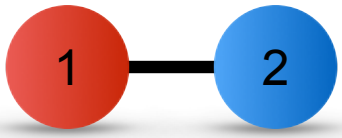
d_c

$$d^k_{\bar{\boldsymbol{\sigma}},\boldsymbol{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}}) = \det\left(F^k_{\bar{\boldsymbol{\sigma}},\boldsymbol{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})\right)$$

non-interacting hybridization function

t_c

the difficult part: local trace $\quad t^k_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})$

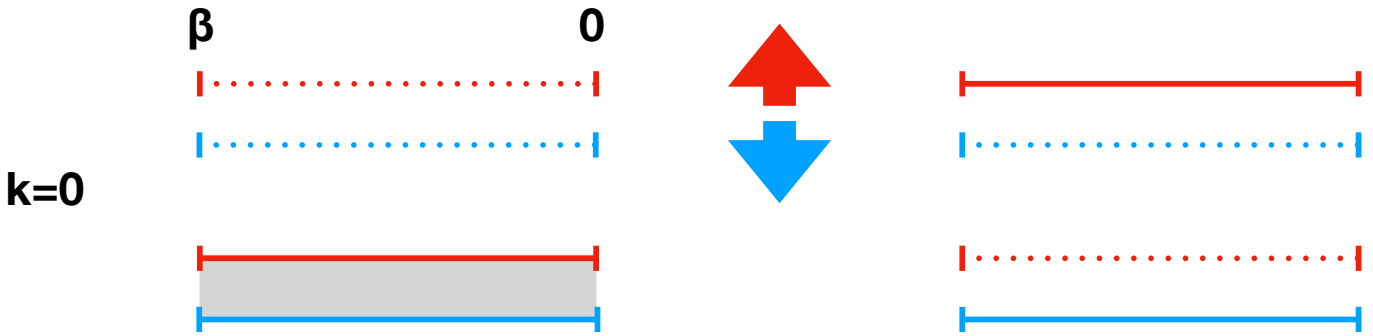


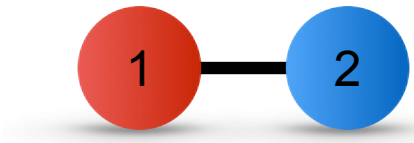
quantum-impurity solver

local trace: segment solver

$$t^{k}_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}}) = \mathrm{Tr}_{\mathrm{loc}}\left(e^{-\beta(\hat{H}_{\mathrm{loc}}-\mu\hat{N}_d)}\mathcal{T}\Pi^{1}_{i=k}c_{d\sigma_i}(\tau_i)c^{\dagger}_{d\bar{\sigma}_i}(\bar{\tau}_i)\right),$$

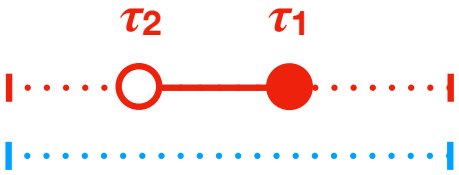
order (k) gives number of creators/annhilators

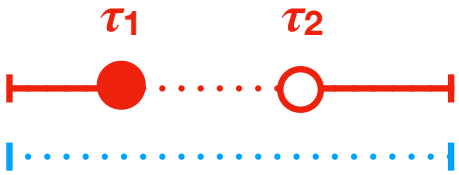


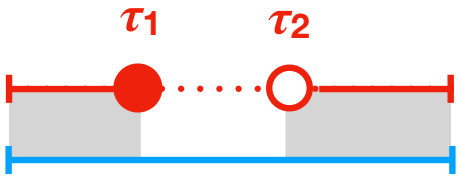


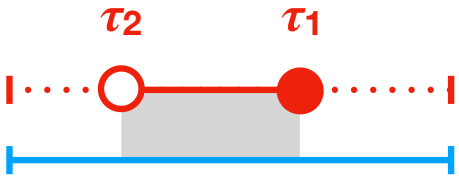
analytic expression k=1

k=1

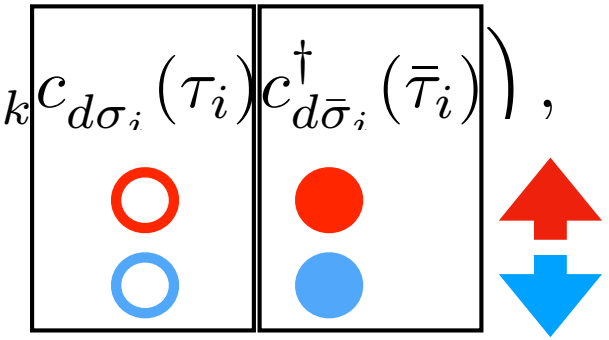




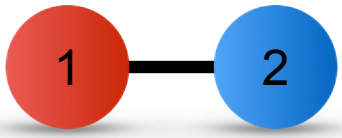




$$t^k_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}}) = \mathrm{Tr}_{\mathrm{loc}}\left(e^{-\beta(\hat{H}_{\mathrm{loc}}-\mu\hat{N}_d)}\mathcal{T}\Pi^1_{i=k} c_{d\sigma_i}(\tau_i)c^\dagger_{d\bar{\sigma}_i}(\bar{\tau}_i)\right),$$



$$t^k_{\sigma,\bar{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}}) = \left(\prod_\sigma s^{k_\sigma}_\sigma\right) e^{-\sum_{\sigma\sigma'}((\varepsilon_d-\mu)\delta_{\sigma\sigma'}+\frac{U}{2}(1-\delta_{\sigma,\sigma'}))l_{\sigma,\sigma'}}$$



quantum-impurity solver

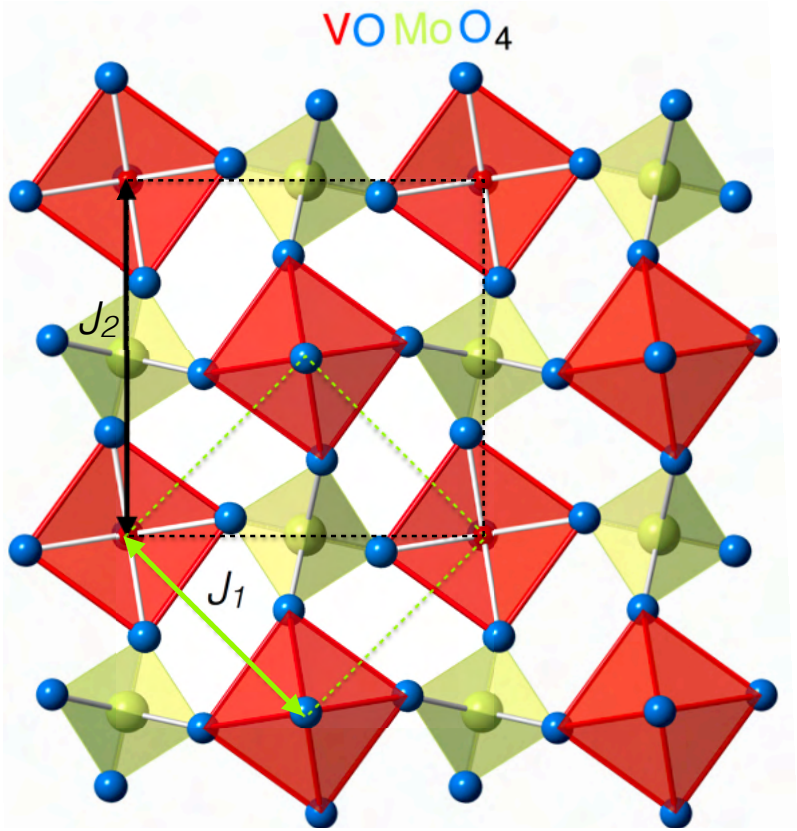
$$Z = \sum_c w_c = \sum_c |w_c| \ \mathrm{sign}\ w_c$$

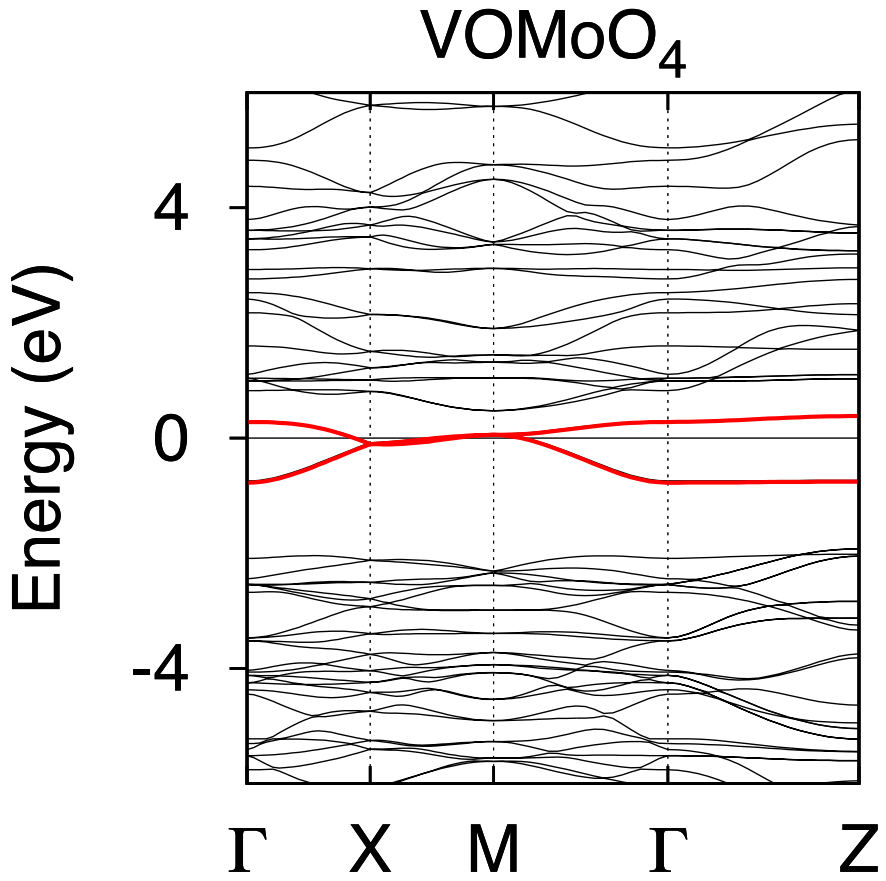
$$w_c = d\boldsymbol{\tau}_c \ d_c \ t_c$$

configuration *c*: expansion order & segments

moves: addition & removal of segments, antisegments, or complete lines

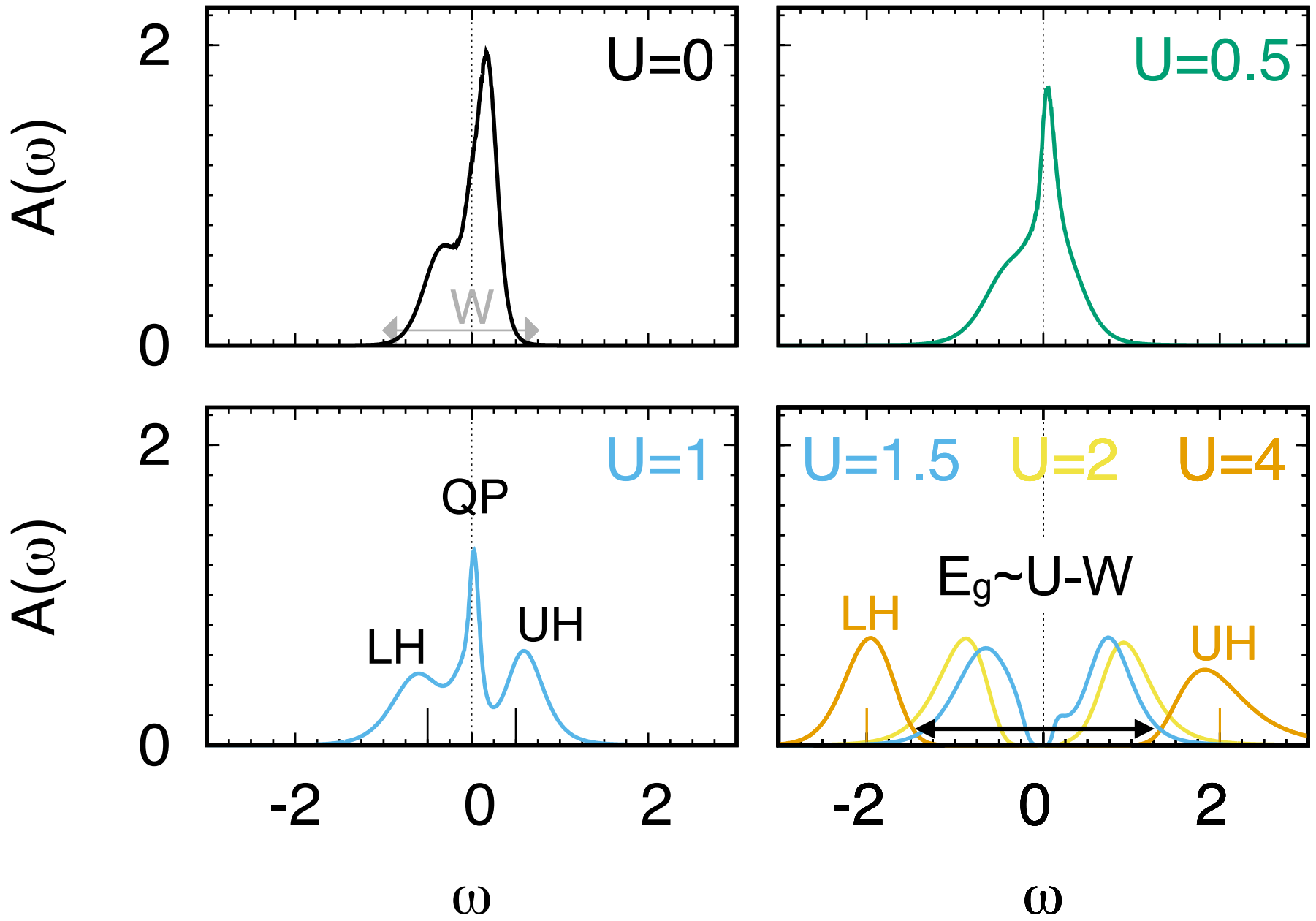
a real-system case: $VOMoO_4$





Amin Kiani and Eva Pavarini, Phys. Rev. B **94**, 075112 (2016)

a real-system: $VOMoO_4$



why not
with static mean-field methods?

comparison to Hartree-Fock (LDA+*U*)

Hartree-Fock Hamiltonian and bands

$$U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \longrightarrow U\left(\bar{n}_{i\uparrow}\hat{n}_{i\downarrow} + \hat{n}_{i\uparrow}\bar{n}_{i\downarrow} - \bar{n}_{i\uparrow}\bar{n}_{i\downarrow}\right)$$

ferromagnetic Hartree-Fock

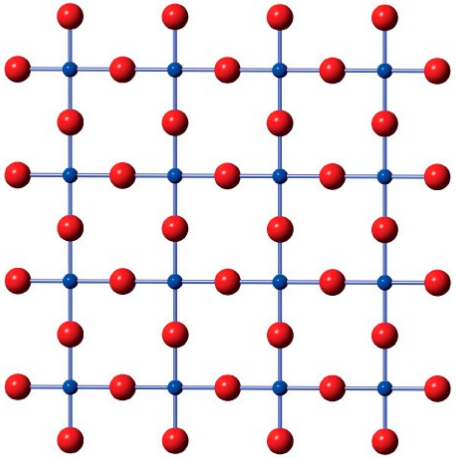
$$\hat{H}_{\mathrm{MF}} = \sum_{\boldsymbol{k}\sigma}\left[\varepsilon_{\boldsymbol{k}} + U\left(\frac{1}{2} - \sigma m\right)\right]\hat{n}_{\boldsymbol{k}\sigma}$$

self-energy

m: magnetization

ferromagnetic Hartree-Fock

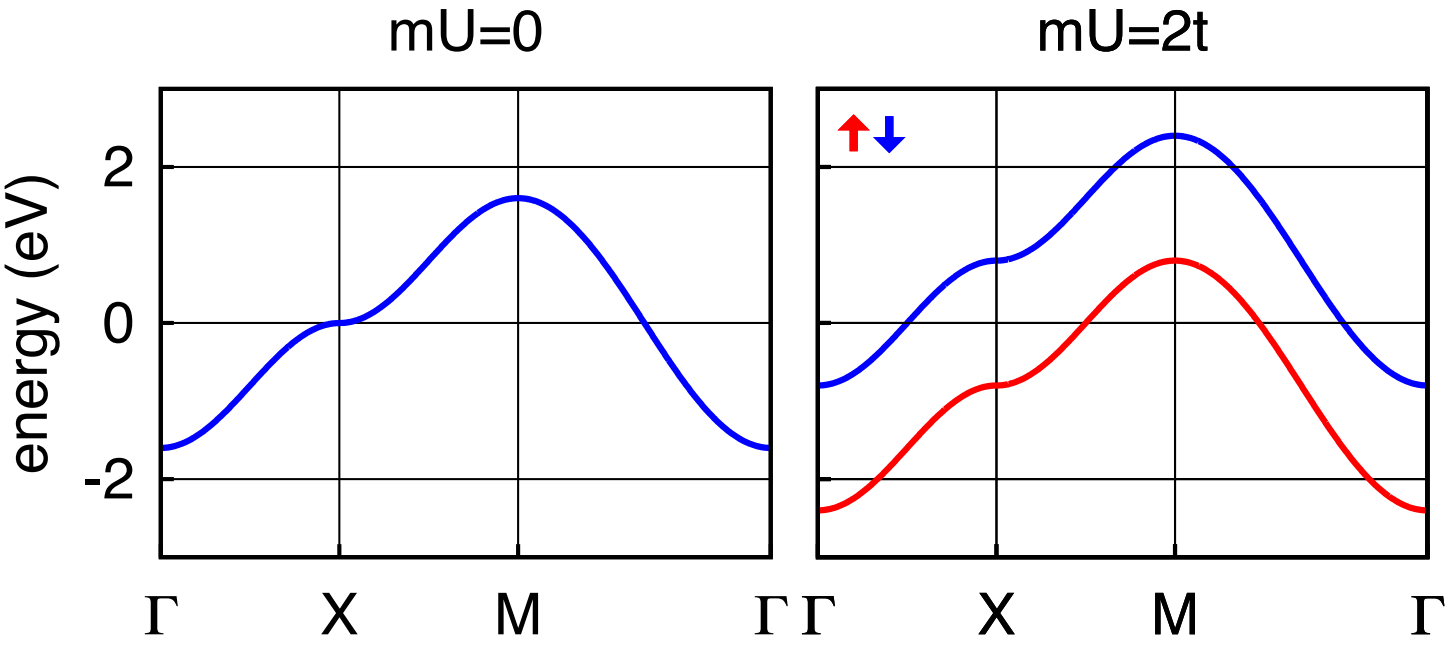
CuO_2



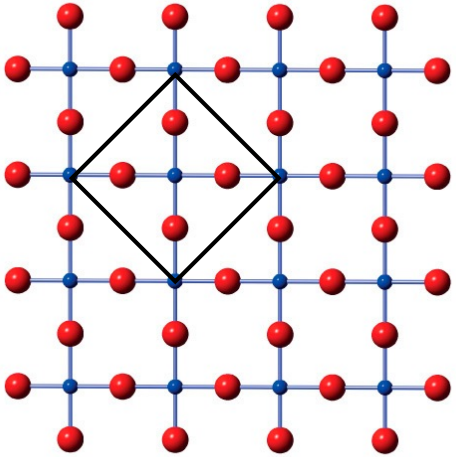
2d-tight binding model

$$\varepsilon_{\boldsymbol{k}} = -2t[\cos k_x + \cos k_y]$$

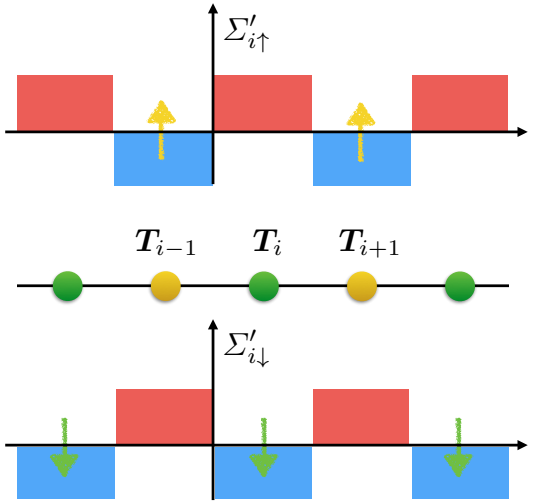
$$\Sigma^{\sigma}(k, i\nu_n) = U\left(\frac{1}{2} - \sigma m\right)$$

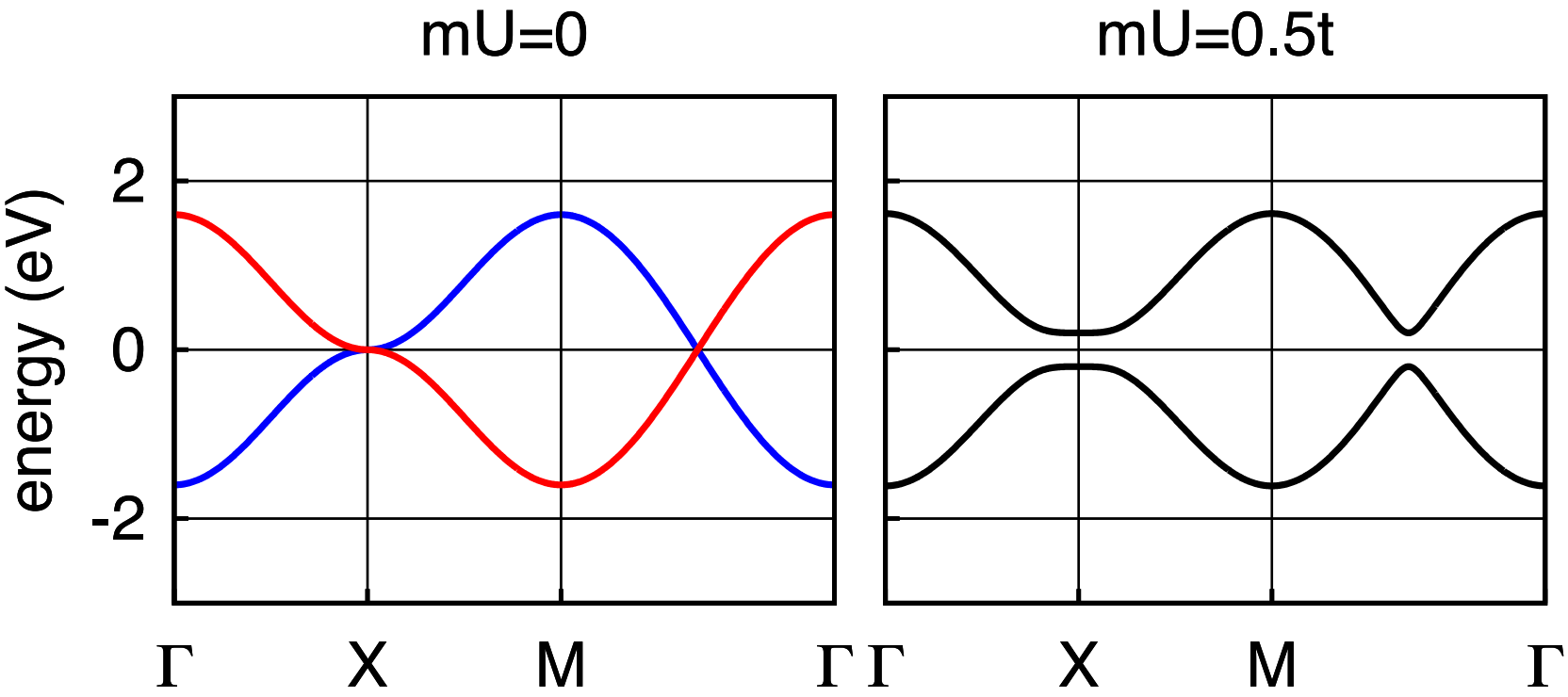


antiferromagnetic case



CuO_2

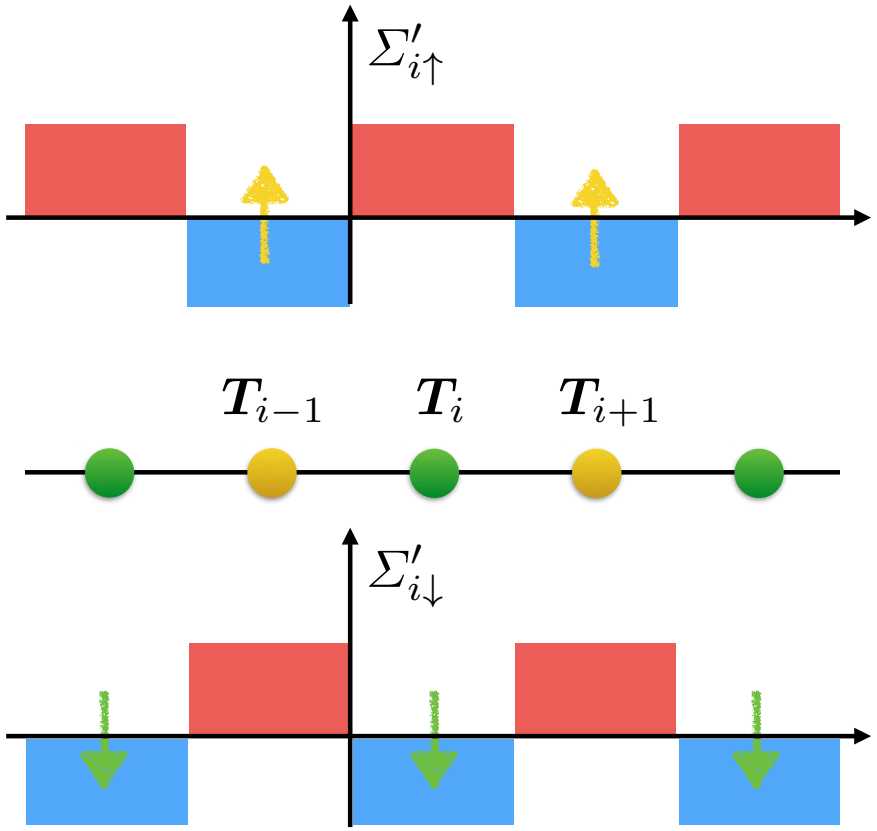




Mott transition: HF vs DMFT

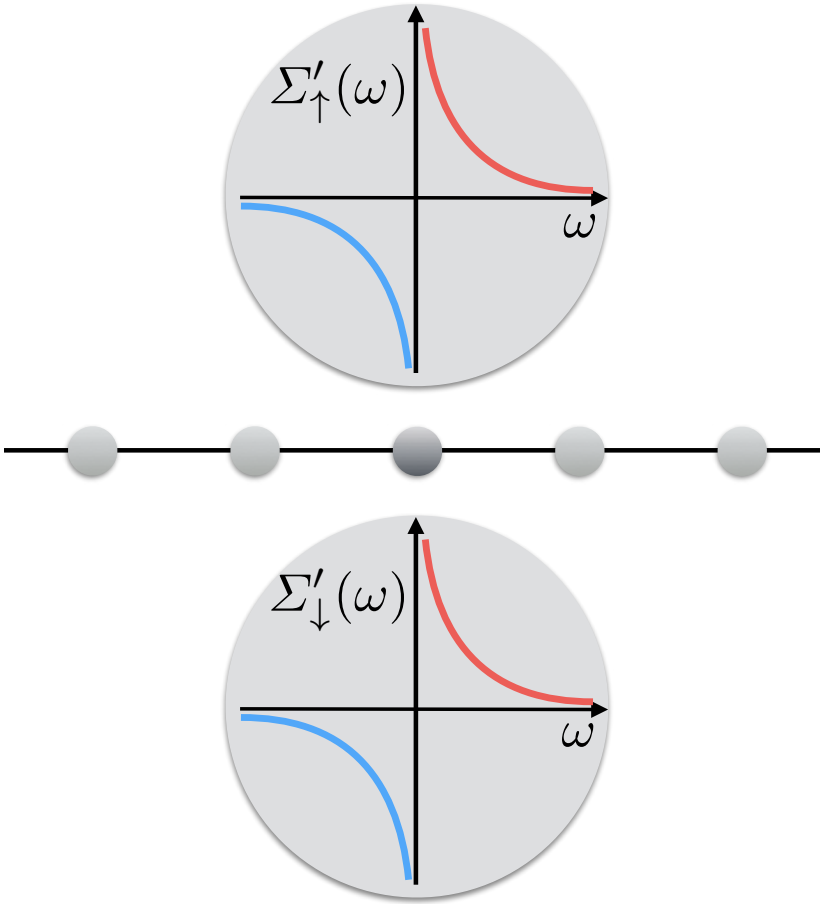
LDA+*U*

Hartree-Fock



LDA+DMFT

DMFT



see also my lecture notes in correl17

dynamical self-energy

two-site Hubbard dimer

$$\Sigma_l^\sigma(i\nu_n) = \frac{1}{2}\left(\Sigma^\sigma(\pi, i\nu_n) + \Sigma^\sigma(0, i\nu_n)\right) = \frac{U}{2} + \frac{U^2}{4}\,\frac{i\nu_n + \mu - \varepsilon_d - \frac{U}{2}}{(i\nu_n + \mu - \varepsilon_d - \frac{U}{2})^2 - (3t)^2}$$

frequency dependence = additional poles

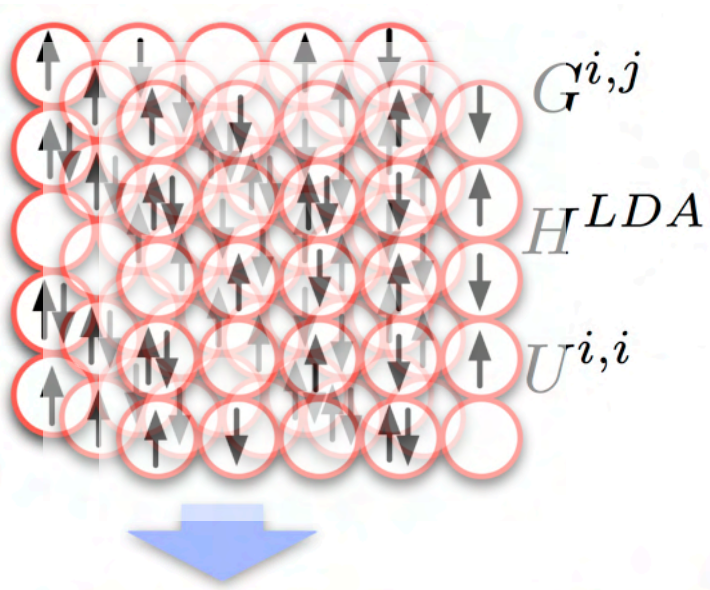
III: DMFT for materials

multi-band Hubbard model

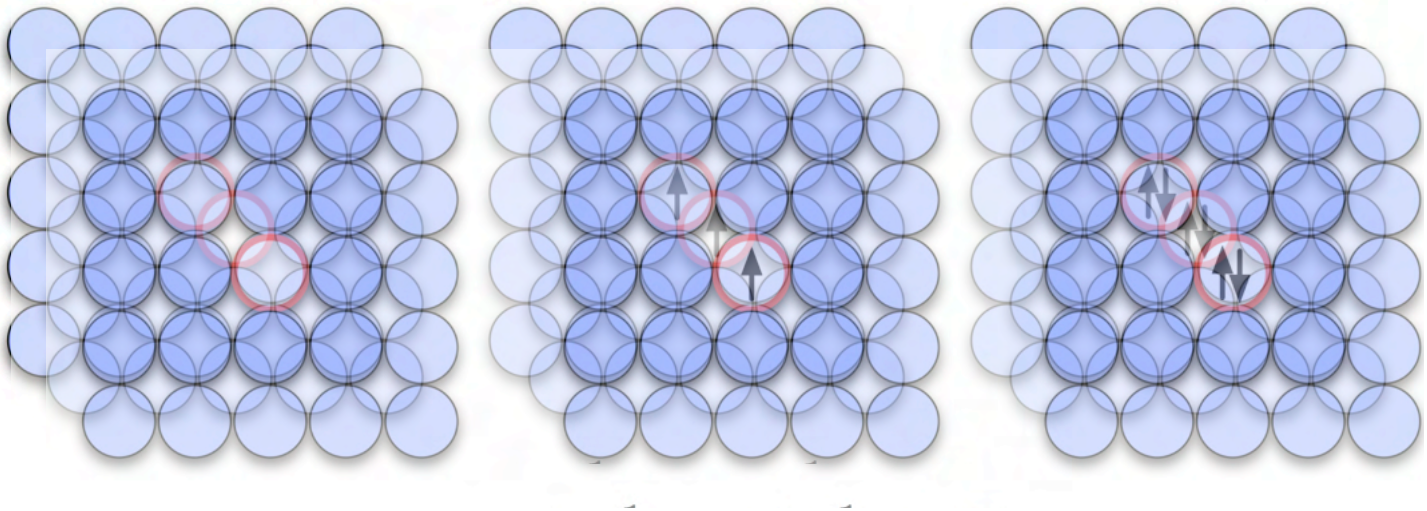
DMFT for real materials

realistic models

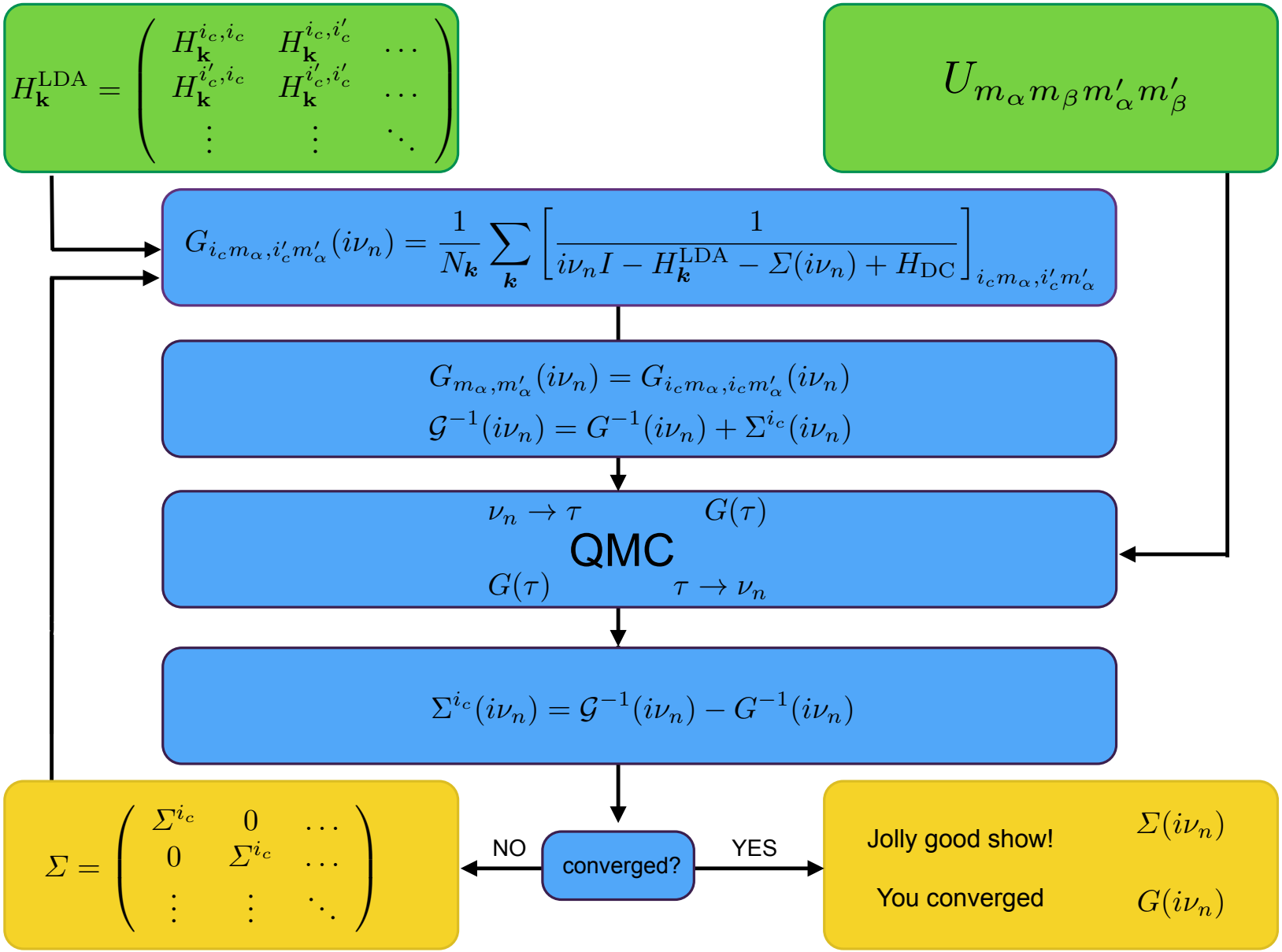
$$\hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}$$



realistic self-consistent quantum-impurity (QI) model



in theory, more indices



in practice, QMC-based solvers

computational time

limited number of orbitals/site

finite temperature

sign problem

some *interactions* are worse than others

some *bases* are worse than others

we need **minimal** material-specific models

materials-specific models from DFT band-structure calculations

let us go back to the basics

$$\hat{H}_e = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$

electronic Hamiltonian in 2nd quantization

$$\hat{H}_e = \underbrace{-\sum_{ab} t_{ab} c_a^\dagger c_b}_{\hat{H}_0} + \underbrace{\frac{1}{2}\sum_{aa'bb'} U_{aa'bb'}\, c_a^\dagger c_{a'}^\dagger c_{b'} c_b}_{\hat{H}_U}$$

complete one-electron basis set!

parameters

$$t_{ab} = -\int d\mathbf{r}\, \overline{\phi_a}(\boldsymbol{r}) \Big(-\frac{1}{2}\nabla^2 \underbrace{- \sum_\alpha \frac{Z_\alpha}{|\boldsymbol{r} - \boldsymbol{R}_\alpha|}}_{v_{\mathrm{en}}(\boldsymbol{r})} \Big) \phi_b(\boldsymbol{r})$$

hopping integrals

$$U_{aa'bb'} = \int d\mathbf{r}_2 \int d\mathbf{r}_2\, \overline{\phi_a}(\boldsymbol{r}_1)\, \overline{\phi_{a'}}(\boldsymbol{r}_2)\, \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}\, \phi_{b'}(\boldsymbol{r}_2)\, \phi_b(\boldsymbol{r}_1)$$

Coulomb integrals

in theory all basis are identical

in practice some bases are better than others

$$\hat{H}_e = \underbrace{-\sum_{ab} t_{ab} c_a^\dagger c_b}_{\hat{H}_0} + \underbrace{\frac{1}{2} \sum_{aa'bb'} U_{aa'bb'}\ c_a^\dagger c_{a'}^\dagger c_{b'} c_b}_{\hat{H}_U}$$

Kohn-Sham Wannier orbitals

$$\hat{H}_e = \underbrace{-\sum_{ab} \tilde{t}_{ab}\, c_a^\dagger c_b}_{\hat{H}_0 = \hat{H}_e^{\mathrm{LDA}}} + \underbrace{\frac{1}{2} \sum_{aba'b'} \tilde{U}_{aa'bb'}\ c_a^\dagger c_{a'}^\dagger c_{b'} c_b - \hat{H}_{\mathrm{DC}}}_{\Delta \hat{H}_U}$$

what do the parameters contain?

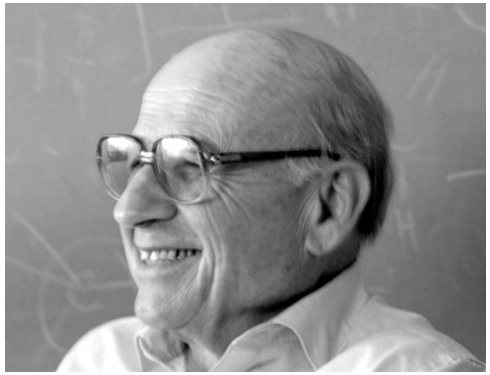
$$\tilde{t}_{ab} = -\int d\mathbf{r}\, \overline{\phi_a^{\mathrm{KS}}}(\boldsymbol{r})\left(-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r})\right)\phi_b^{\mathrm{KS}}(\boldsymbol{r})$$

Hartree

$$v_R(\boldsymbol{r}) = -\sum_\alpha \frac{Z_\alpha}{|\boldsymbol{r}-\boldsymbol{R}_\alpha|} + \int d\boldsymbol{r}'\frac{n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + \frac{\delta E_{\mathrm{xc}}[n]}{\delta n} = v_{en}(\boldsymbol{r}) + v_H(\boldsymbol{r}) + v_{xc}(\boldsymbol{r})$$

potential

exchange-correlation



Walter Kohn

Nobel Prize in Chemistry (1998)

Kohn-Sham equations

understand and predict properties of solids, molecules, biological systems, geological systems...

in theory all basis are identical

in practice some bases are better than others

$$\hat{H}_e = \underbrace{-\sum_{ab} t_{ab} c_a^\dagger c_b}_{\hat{H}_0} + \underbrace{\frac{1}{2}\sum_{aa'bb'} U_{aa'bb'}\; c_a^\dagger c_{a'}^\dagger c_{b'} c_b}_{\hat{H}_U}$$

Kohn-Sham Wannier orbitals

$$\hat{H}_e = \underbrace{-\sum_{ab} \tilde{t}_{ab}\, c_a^\dagger c_b}_{\hat{H}_0 = \hat{H}_e^{\mathrm{LDA}}} + \underbrace{\frac{1}{2}\sum_{aba'b'} \tilde{U}_{aa'bb'}\; c_a^\dagger c_{a'}^\dagger c_{b'} c_b - \hat{H}_{\mathrm{DC}}}_{\Delta\hat{H}_U}$$

remember

this is not foreseen in DFT

we are using the KS basis
no matter how it was produced

weakly-correlated systems

one-electron approximation

$$\hat{H}_e = \underbrace{-\sum_{ab} \tilde{t}_{ab}\, c_a^\dagger c_b}_{\hat{H}_0 = \hat{H}_e^{\mathrm{LDA}}} + \underbrace{\frac{1}{2}\sum_{aba'b'} \tilde{U}_{aa'bb'}\, c_a^\dagger c_{a'}^\dagger c_{b'} c_b}_{\Delta \hat{H}_U} - \hat{H}_{\mathrm{DC}}$$

$$\hat{H}_{\mathrm{eff}} \sim \hat{S}^{-1} \hat{H}_e \hat{S} \sim \hat{H}_e^{\mathrm{LDA}}$$

strongly-correlated systems

Hubbard-like approximation

$$\hat{H}_e = \underbrace{-\sum_{ab} \tilde{t}_{ab}\, c_a^\dagger c_b}_{\hat{H}_0 = \hat{H}_e^{\mathrm{LDA}}} + \underbrace{\frac{1}{2} \sum_{aba'b'} \tilde{U}_{aa'bb'}\; c_a^\dagger c_{a'}^\dagger c_{b'} c_b - \hat{H}_{\mathrm{DC}}}_{\Delta \hat{H}_U}$$

$$\hat{H}_{\mathrm{eff}} \sim \hat{S}^{-1} \hat{H}_e\, \hat{S} \sim \hat{H}_{\mathrm{Hubbard-like}}$$

LDA, GGA & so on: minor differences in this context

why Wannier functions?

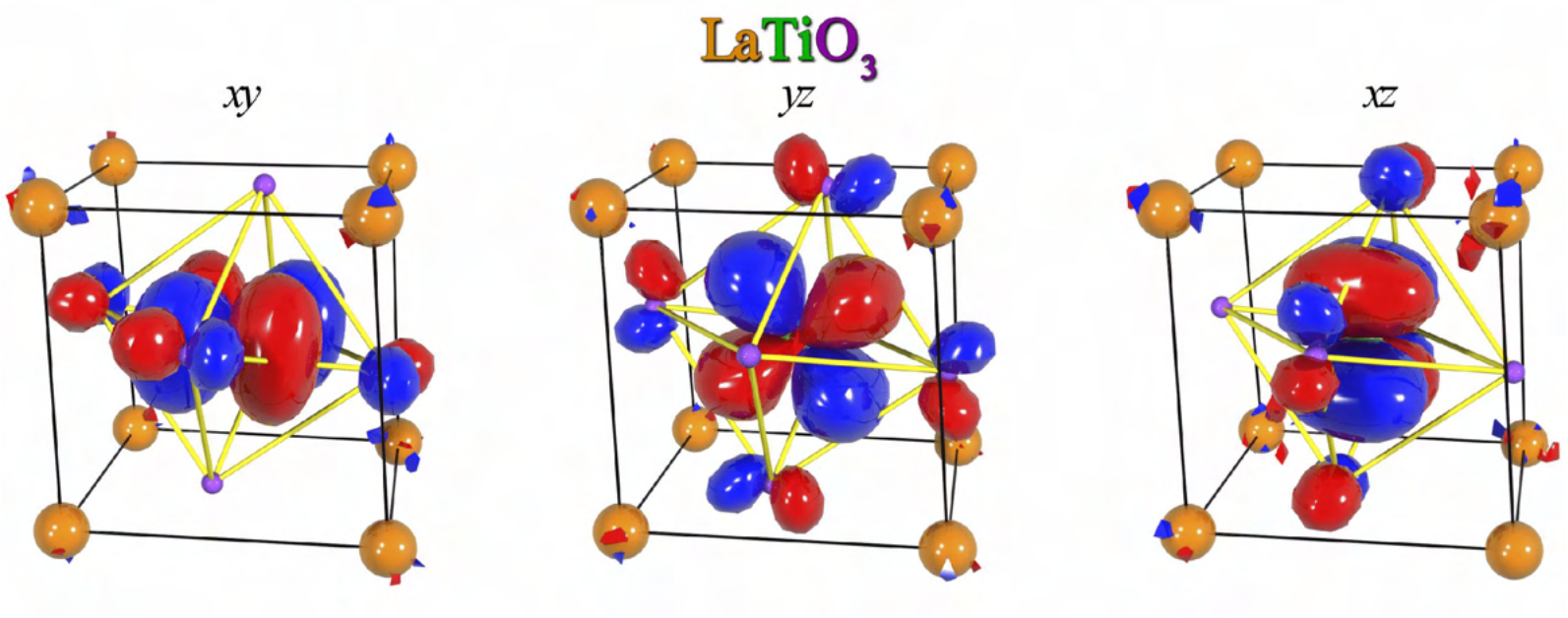
span exactly the one-electron Hamiltonian

can be constructed site-centered & orthogonal & localized

natural basis for **local** Coulomb terms

very good for weakly correlated systems

information on lattice and chemistry



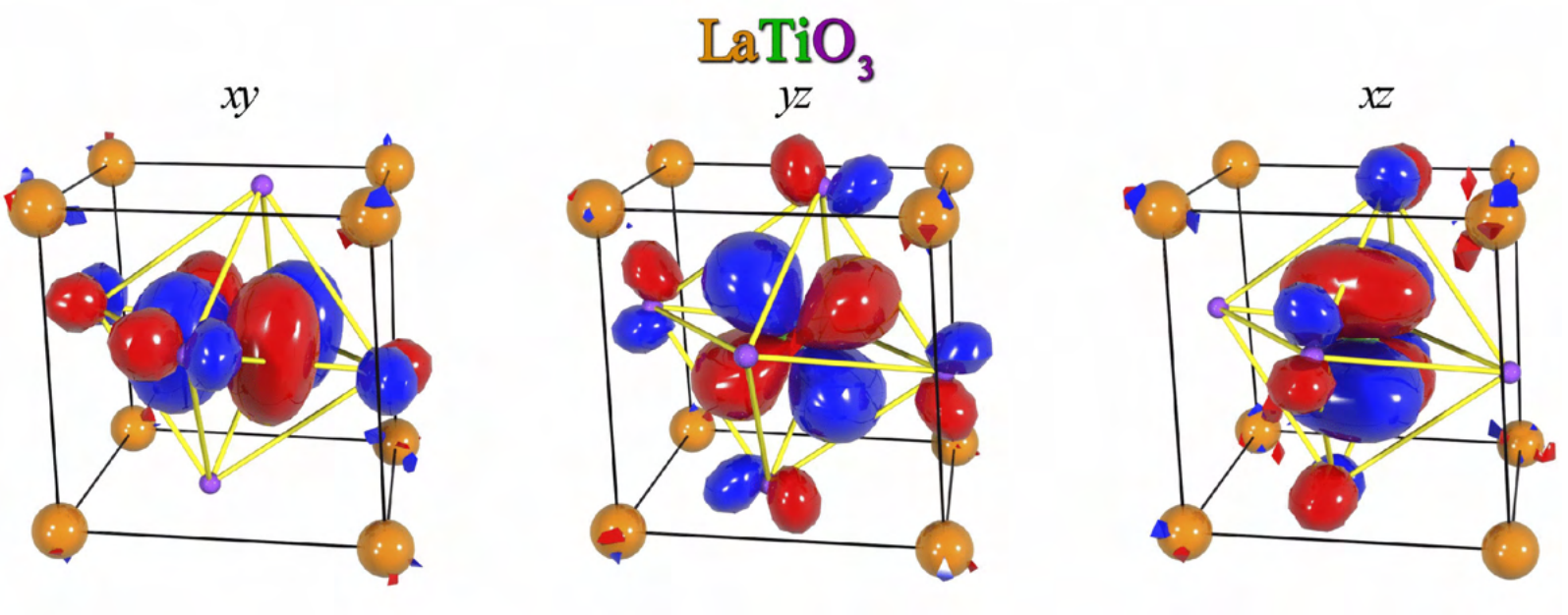
E. Pavarini, A. Yamasaki, J. Nuss, O.K. Andersen, New. J. Phys **7**, *188 (2005)*

why Wannier functions?

$$\hat{H}_e = \hat{H}_0 + \hat{H}_U \longrightarrow \hat{H}^{\mathrm{LDA}} + \boxed{\hat{H}_U - \hat{H}_{dc}}$$

ΔU

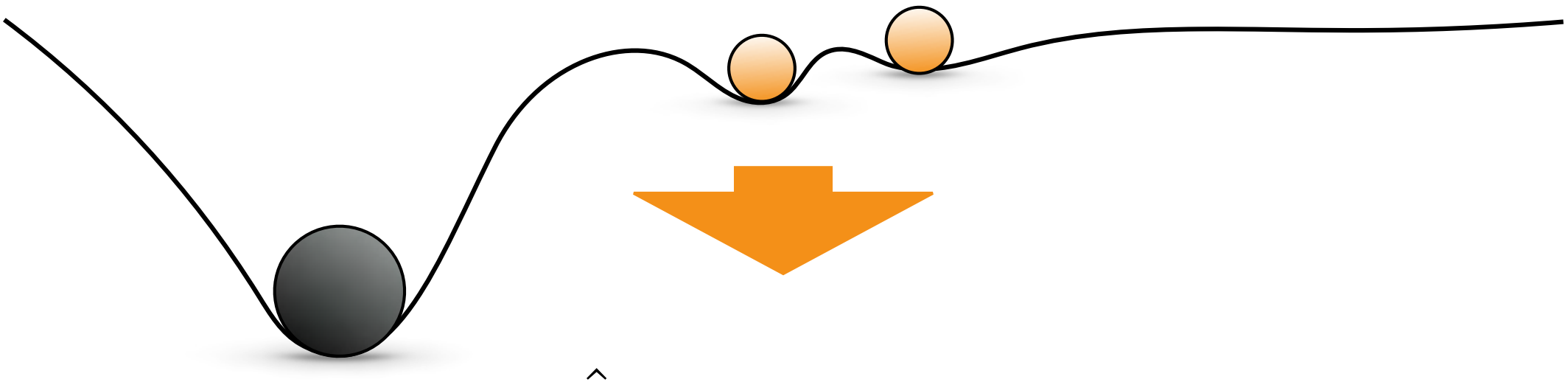
if long range Hartree and mean-field exchange-correlation already are well described by LDA (GGA,..), ΔU is local



E. Pavarini, A. Yamasaki, J. Nuss, O.K. Andersen, New. J. Phys **7**, *188 (2005)*

light electrons

$$\hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}$$

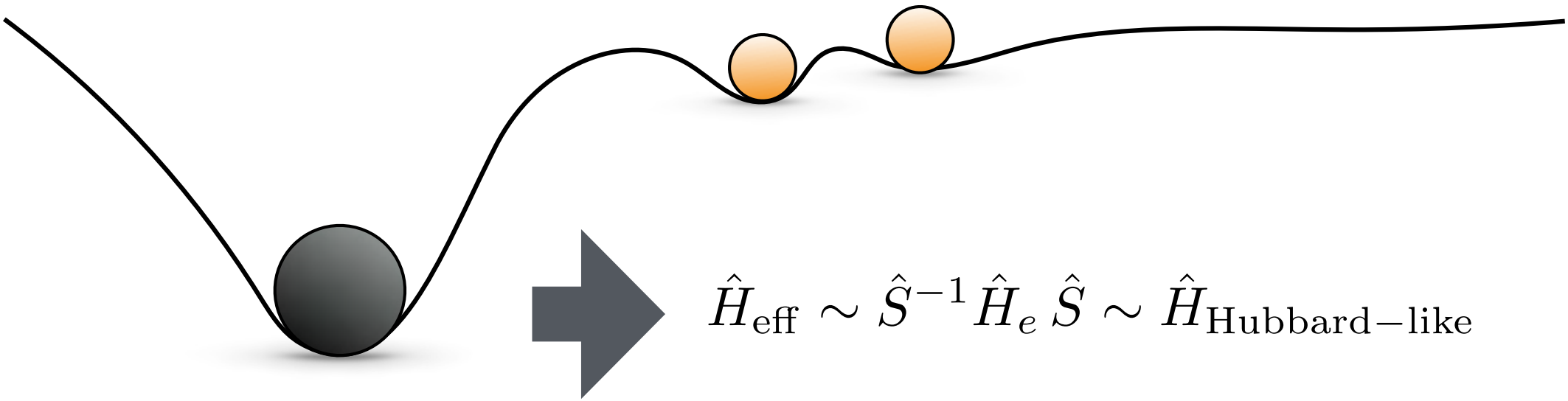


$$\hat{\tilde{H}}_e = \sum_{ab} \tilde{t}_{ab} c_a^\dagger c_b$$

independent-electron approximation

heavy electrons

$$\hat{H}_e = \underbrace{-\sum_{ab} \tilde{t}_{ab}\, c_a^\dagger c_b}_{\hat{H}_0 = \hat{H}_e^{\mathrm{LDA}}} + \underbrace{\frac{1}{2} \sum_{aba'b'} \tilde{U}_{aa'bb'}\; c_a^\dagger c_{a'}^\dagger c_{b'} c_b - \hat{H}_{\mathrm{DC}}}_{\Delta \hat{H}_U}$$

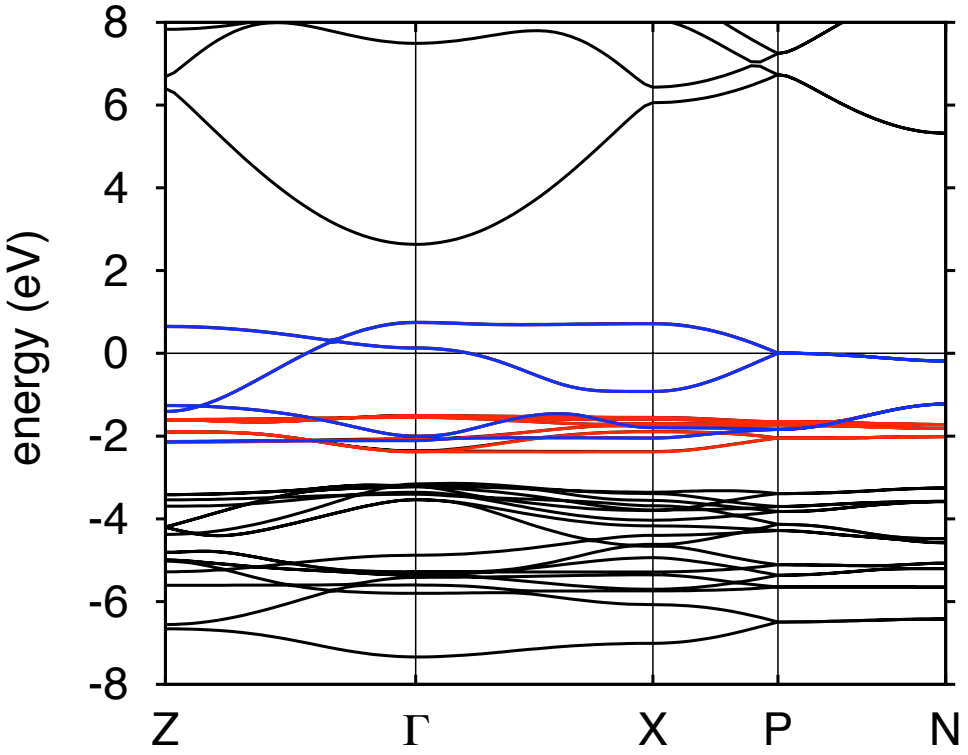


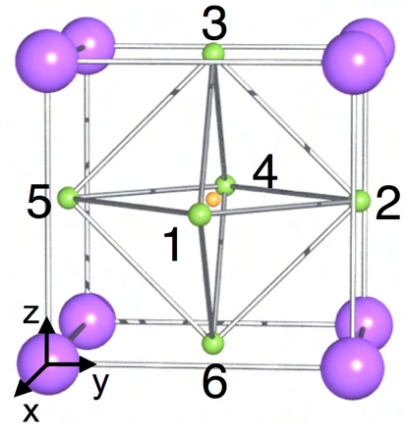
$$\hat{H}_{\mathrm{eff}} \sim \hat{S}^{-1} \hat{H}_e \hat{S} \sim \hat{H}_{\mathrm{Hubbard-like}}$$

minimal model for a given class of phenomena
as system-specific as possible

how many degrees of freedom?

$KCuF_3$

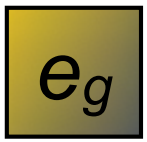




e_g

t_{2g}

integrate out light electrons

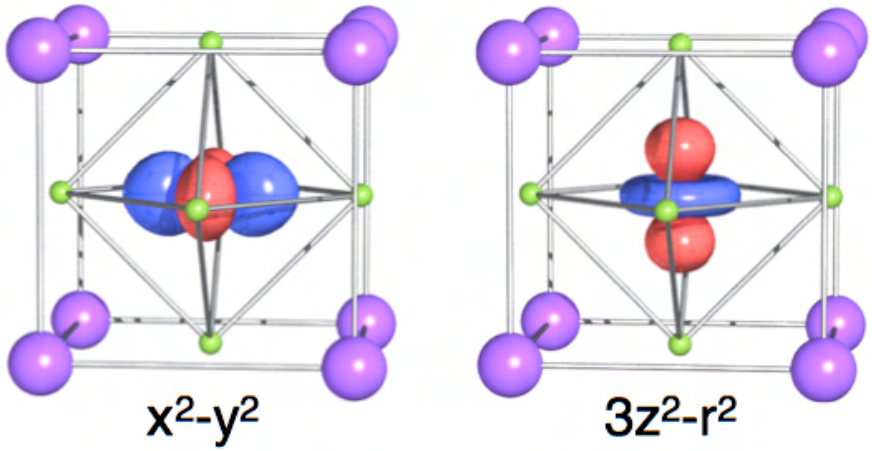


how many degrees of freedom?

no downfolding

more parameters & H_{DC}

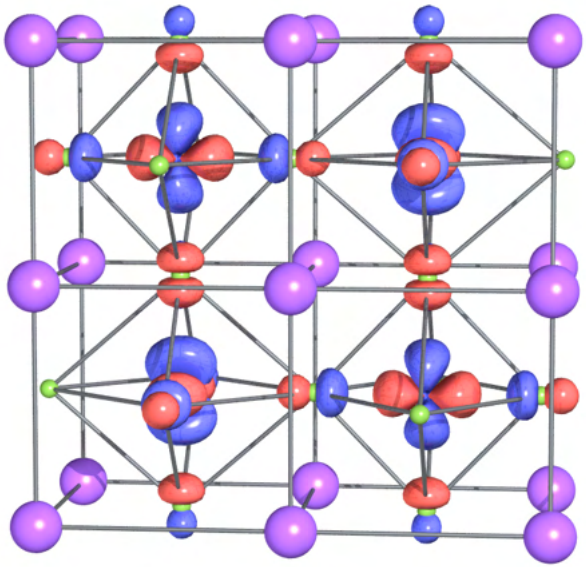
WF more localized



massive downfolding

fewer parameters & no H_{DC}

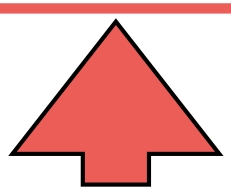
WF less localized



E. Pavarini, E. Koch, A.I. Lichtenstein, Phys. Rev. Lett. ***101****, 266405 (2008)*

how important is localization?

$$\hat{H}_e = \hat{H}_0 + \hat{H}_U \longrightarrow \hat{H}^{\mathrm{LDA}} + \boxed{\hat{H}_U - \hat{H}_{dc}}$$



local or almost local

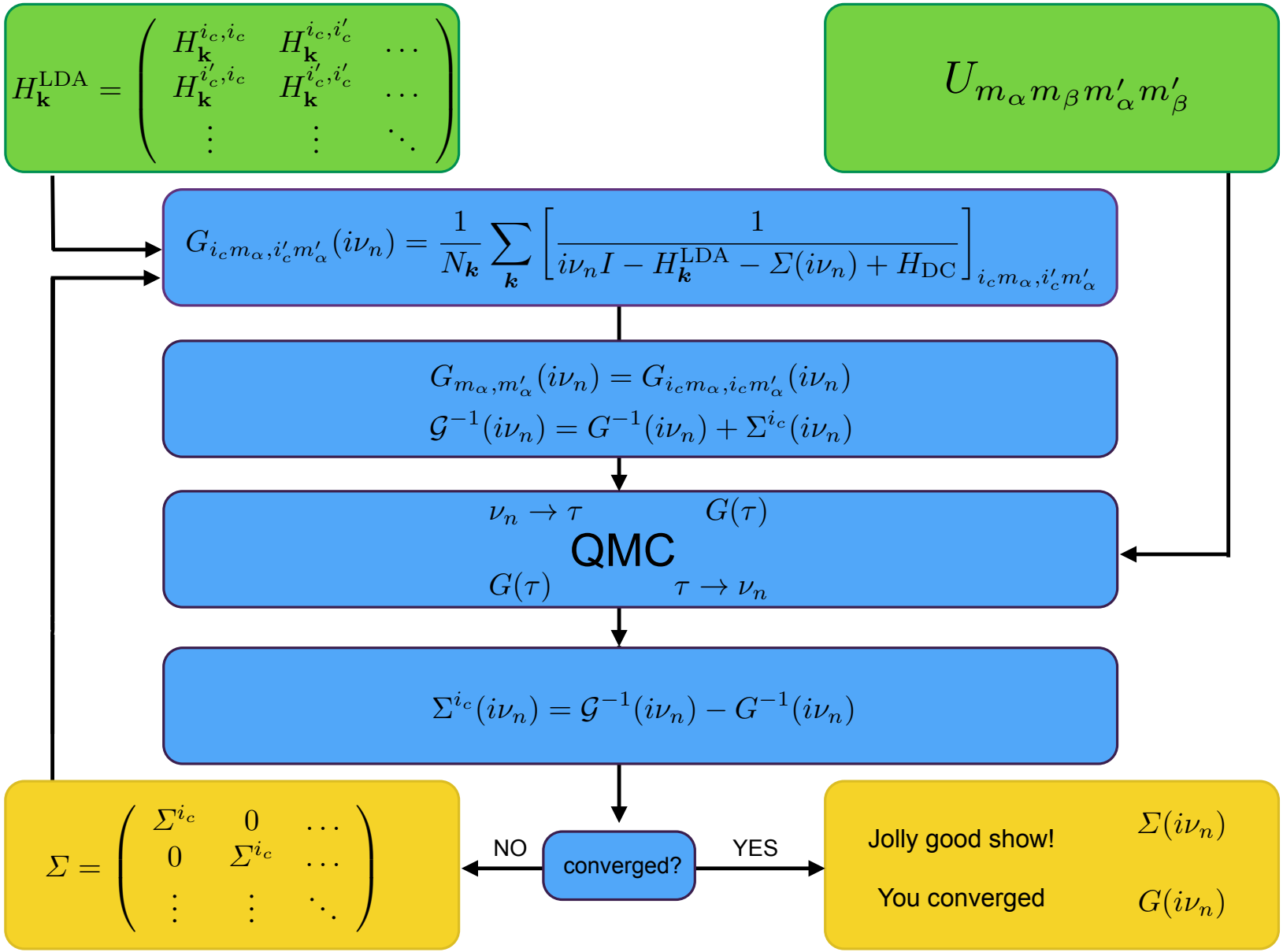
strong correlations arise from strong local Coulomb

$$U^{iji'j'}_{np\ n'p'} = \int d\mathbf{r}_1 \int d\mathbf{r}_2\ \overline{\psi_{in\sigma}}(\mathbf{r}_1)\overline{\psi_{jp\sigma'}}(\mathbf{r}_2)\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\psi_{j'p'\sigma'}(\mathbf{r}_2)\psi_{i'n'\sigma}(\mathbf{r}_1).$$

$$\psi_{im\sigma}(\boldsymbol{r})\overline{\psi_{i'm'\sigma'}}(\boldsymbol{r}) \sim \delta_{i,i'}\delta(\boldsymbol{r} - \boldsymbol{T}_i)$$

$$U^{iji'j'}_{mp\ m'p'} \propto \frac{\delta_{i,i'}\delta_{j,j'}}{|\boldsymbol{T}_i - \boldsymbol{T}_j|},$$

LDA+DMFT

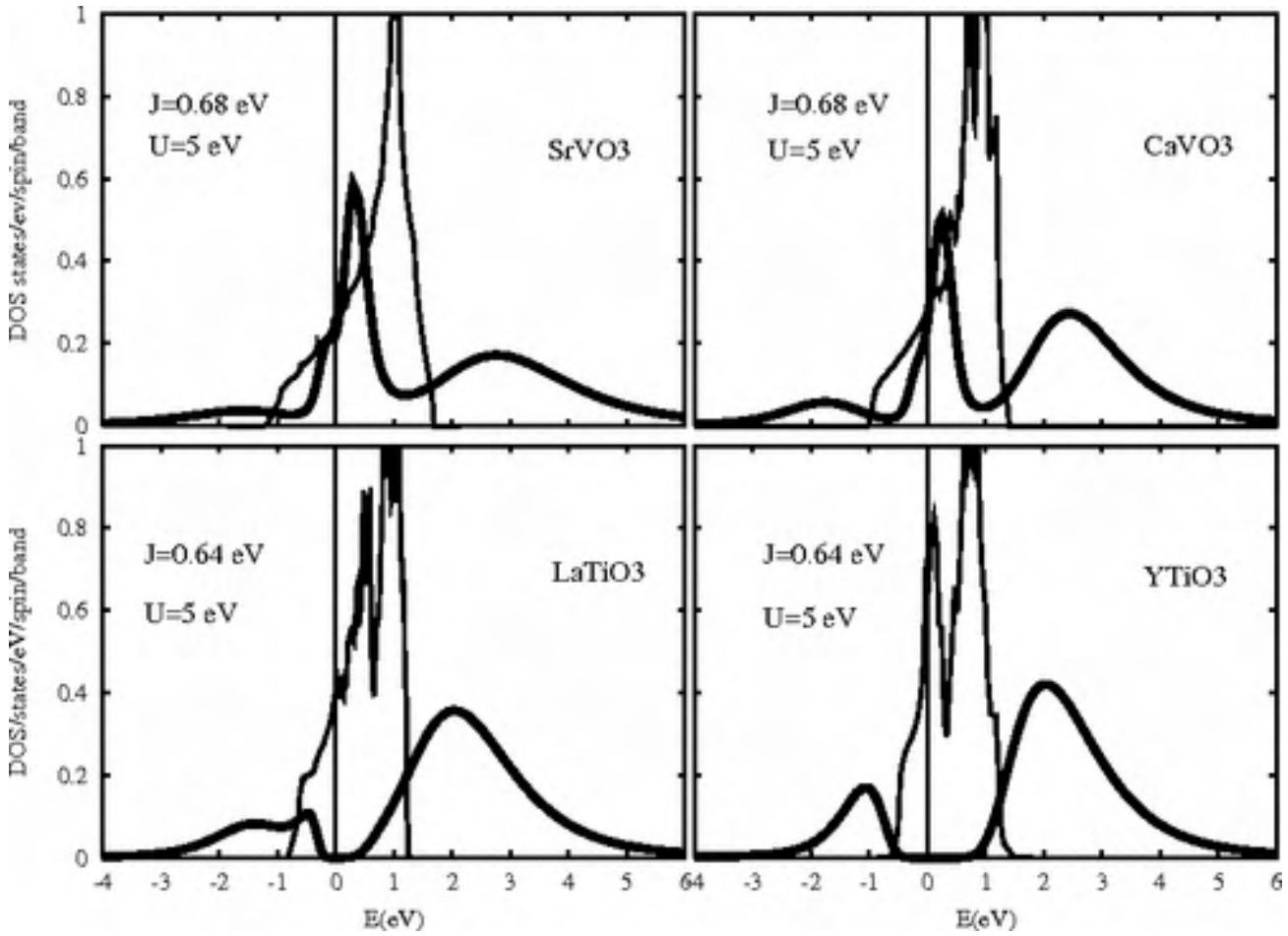

$H_{\mathbf{k}}^{\mathrm{LDA}} = \begin{pmatrix} H_{\mathbf{k}}^{i_c,i_c} & H_{\mathbf{k}}^{i_c,i'_c} & \dots \\ H_{\mathbf{k}}^{i'_c,i_c} & H_{\mathbf{k}}^{i'_c,i'_c} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$
$U_{m_\alpha m_\beta m'_\alpha m'_\beta}$
$G_{i_c m_\alpha, i'_c m'_\alpha}(i\nu_n) = \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \left[\frac{1}{i\nu_n I - H_{\boldsymbol{k}}^{\mathrm{LDA}} - \Sigma(i\nu_n) + H_{\mathrm{DC}}} \right]_{i_c m_\alpha, i'_c m'_\alpha}$
$G_{m_\alpha, m'_\alpha}(i\nu_n) = G_{i_c m_\alpha, i_c m'_\alpha}(i\nu_n)$
$\mathcal{G}^{-1}(i\nu_n) = G^{-1}(i\nu_n) + \Sigma^{i_c}(i\nu_n)$
$\nu_n \to \tau$
$G(\tau)$
QMC
$G(\tau)$
$\tau \to \nu_n$
$\Sigma^{i_c}(i\nu_n) = \mathcal{G}^{-1}(i\nu_n) - G^{-1}(i\nu_n)$
$\Sigma = \begin{pmatrix} \Sigma^{i_c} & 0 & \dots \\ 0 & \Sigma^{i_c} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$
NO
converged?
YES
Jolly good show!
$\Sigma(i\nu_n)$
You converged
$G(i\nu_n)$

details matter!

VOLUME 92, NUMBER 17 PHYSICAL REVIEW LETTERS week ending 30 APRIL 2004

Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites

E. Pavarini,[1] S. Biermann,[2] A. Poteryaev,[3] A. I. Lichtenstein,[3] A. Georges,[2] and O. K. Andersen[4]



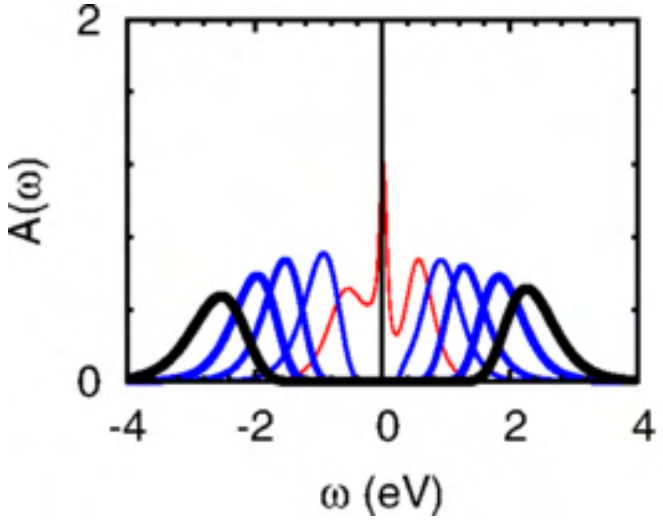
t_{2g}^1

Δ=200-300 meV

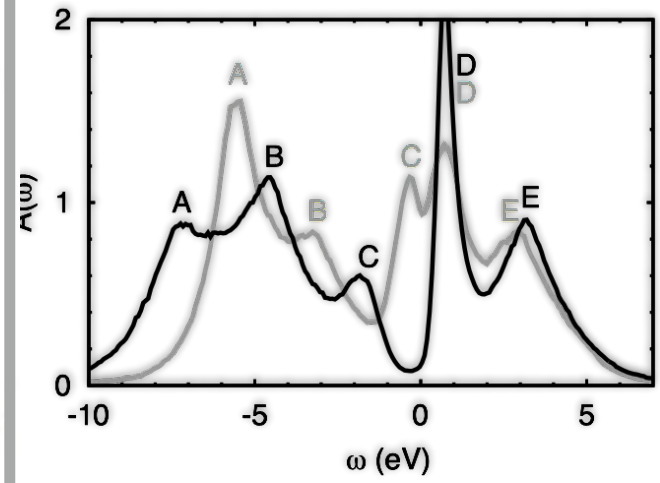
small crystal-field+hoppings play key role

what can we do so far?

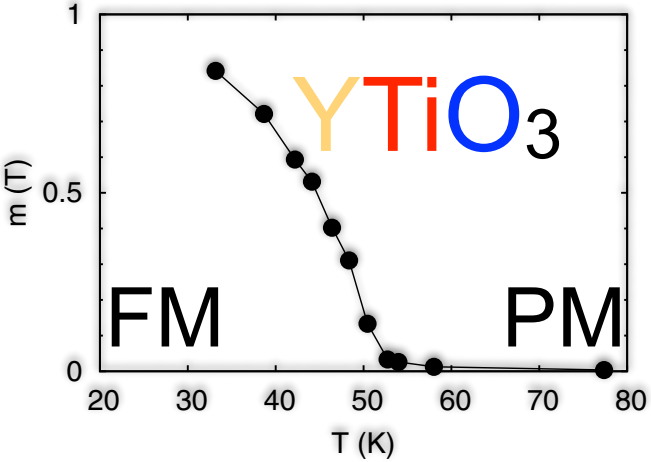
spectral functions



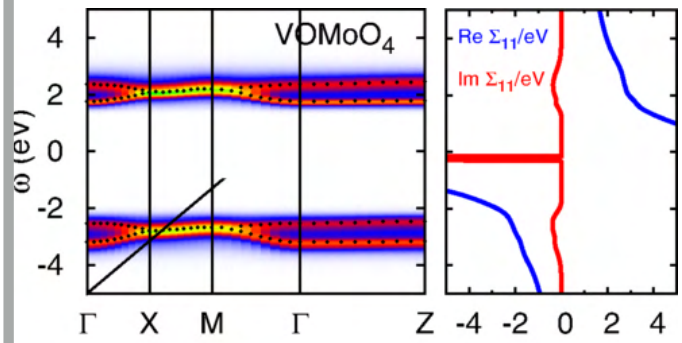
many orbitals



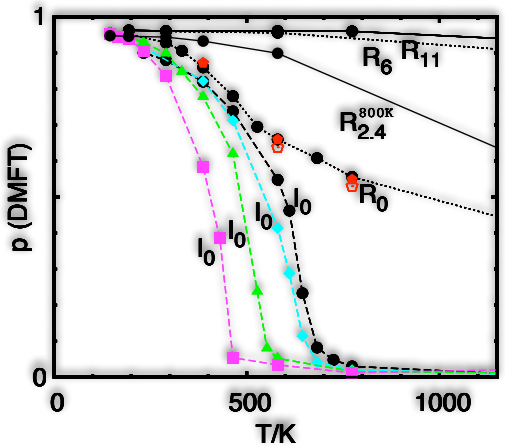
low T



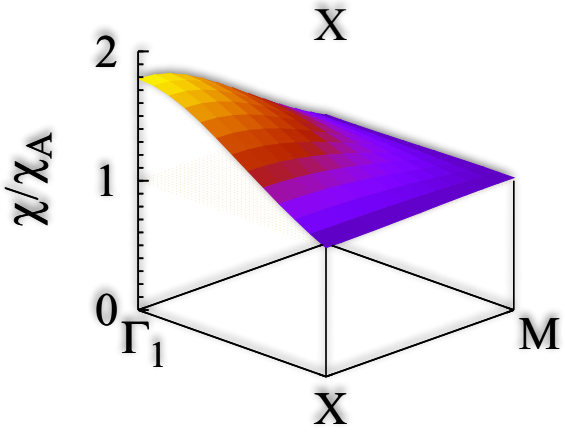
correlated bands



phase transitions

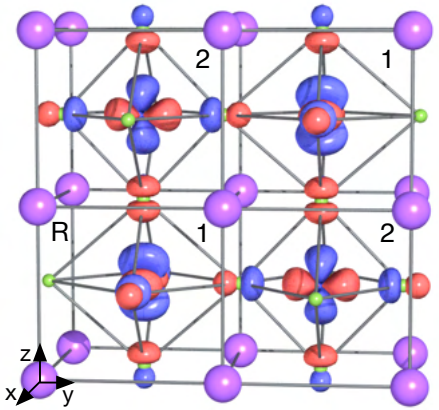


susceptibilities

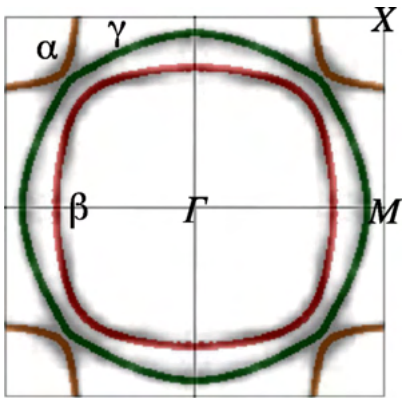


what can we do so far?

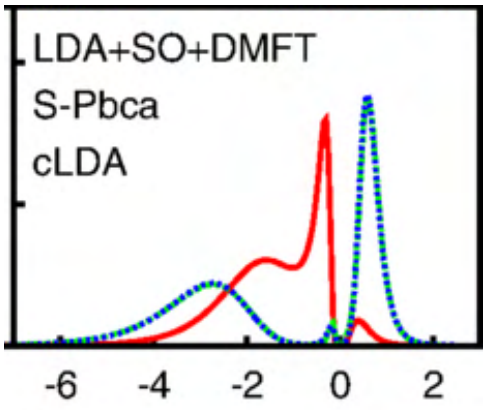
orbital order



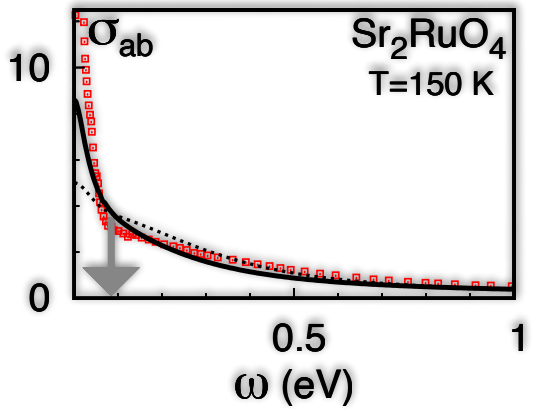
Fermi surface



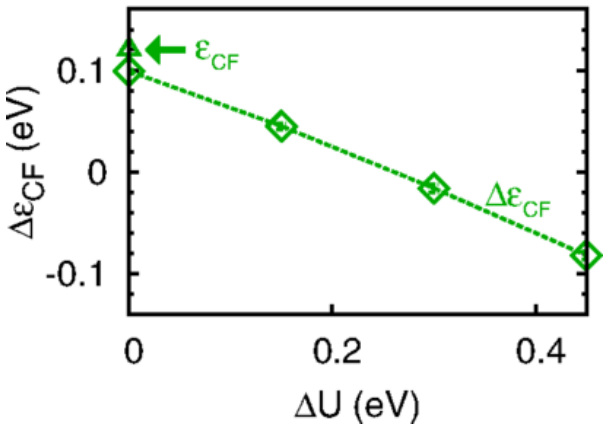
spin-orbit



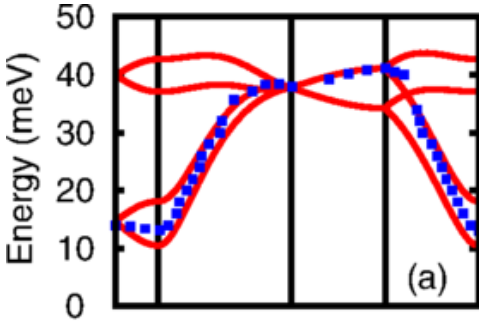
conductivity



realistic Coulomb



spin waves



the LDA+DMFT Fermi surface

LDA

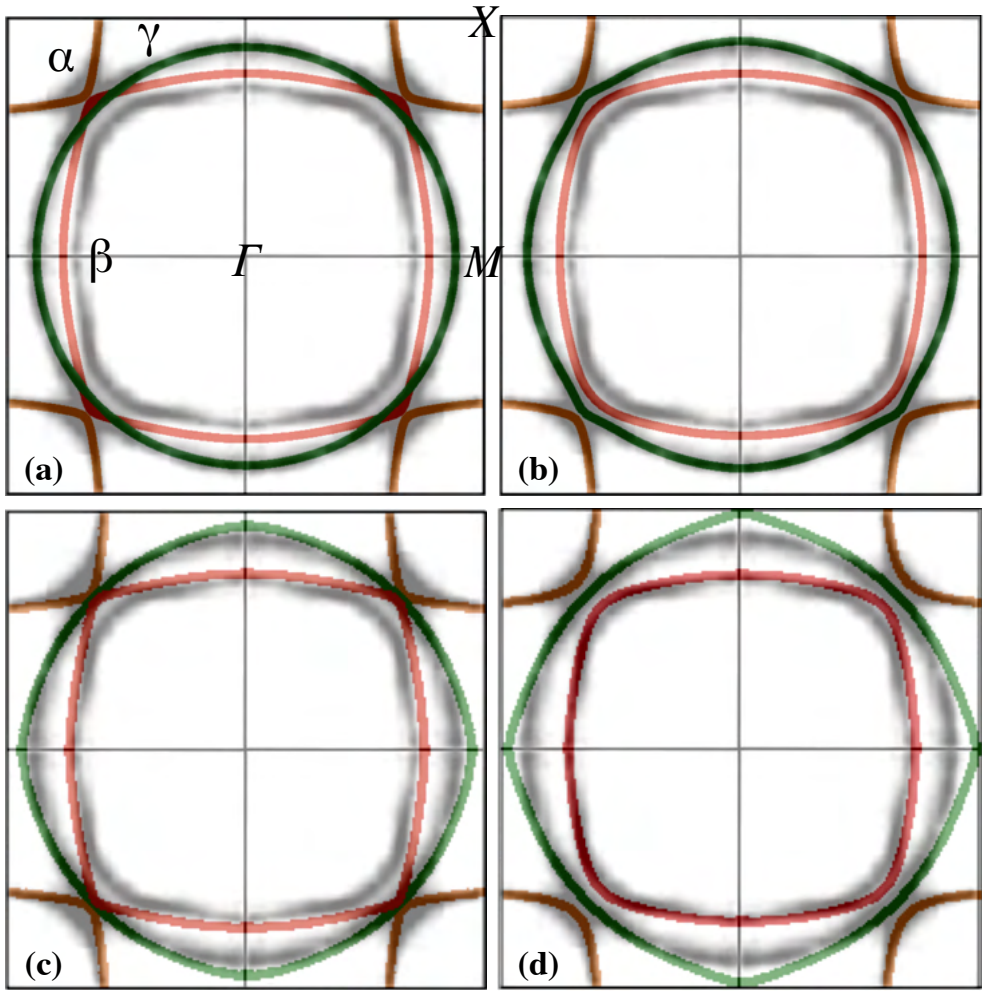
ε_{CF}

LDA+DMFT

ε_{CF}

$\varepsilon_{CF} + \Delta\varepsilon_{CF}$

$\sim 2\varepsilon_{CF}$



LDA+SO

λ

LDA+SO+DMFT

λ

$\lambda + \Delta\lambda \sim 2\lambda$

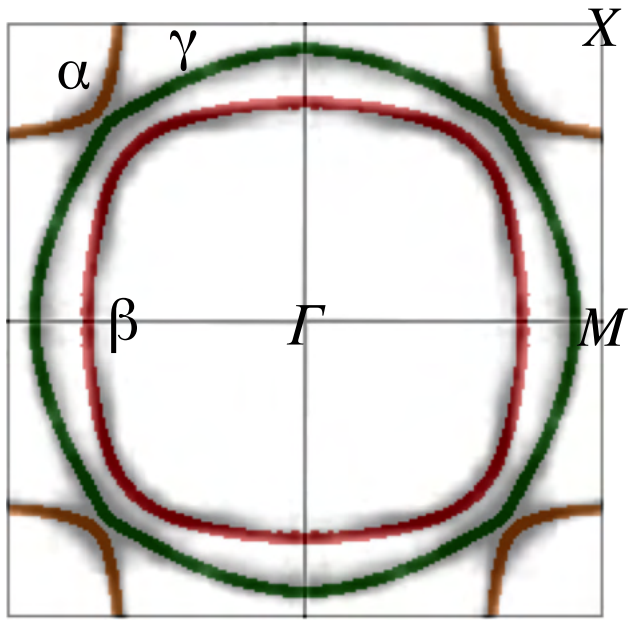
G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)

? a crucial mechanism is still missing ?

Is the Coulomb interaction spherical?

the bare Coulomb interaction is spherical
but the screened interaction has the symmetry of the site

$\varepsilon_{CF} + \Delta' \varepsilon_{CF} \sim \varepsilon_{CF}$

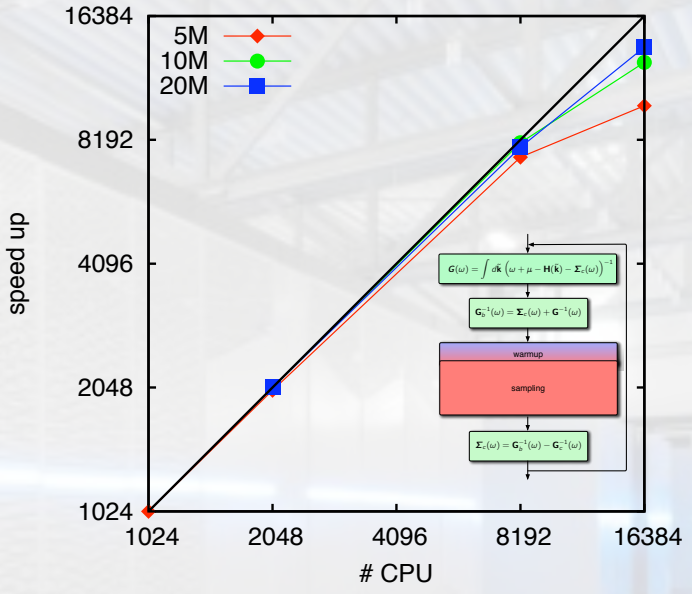


G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)

flexible and efficient solvers

$$H = -\sum_{ii'}\sum_{mm'}\sum_{\sigma} t^{ii'}_{mm'} c^{\dagger}_{im\sigma} c_{i'm'\sigma} + U\sum_{im} n_{im\uparrow} n_{im\downarrow} + \frac{1}{2}\sum_{im\neq m'\sigma\sigma'} (U - 2J - J\delta_{\sigma\sigma'}) n_{im\sigma} n_{im'\sigma'} - J\sum_{m\neq m'} (c^{\dagger}_{m\uparrow} c^{\dagger}_{m'\downarrow} c_{m'\uparrow} c_{m\downarrow} + c^{\dagger}_{m\uparrow} c^{\dagger}_{m\downarrow} c_{m'\uparrow} c_{m'\downarrow})$$

self-energy matrix in spin-orbital space



DMFT and cDMFT

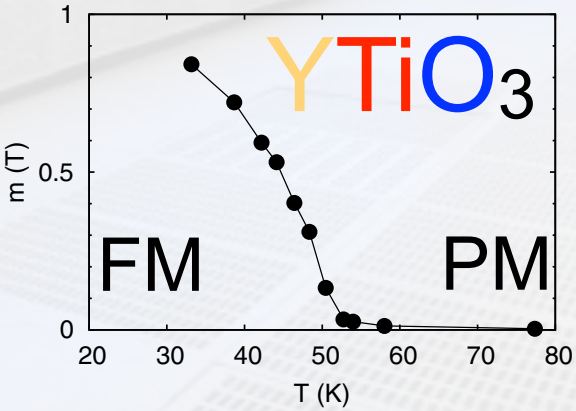
generalized quantum impurity solvers:

general HF QMC

general CT-INT QMC

general CT-HYB QMC

- CT-HYB: A. Flesch, E. Gorelov, E. Koch and E. Pavarini
  Phys. Rev. B **87**, 195141 (2013)
- CT-INT: E. Gorelov et al, PRL 104, 226410 (2010)
- CT-INT+SO: G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini,
  Phys. Rev. Lett. 116, 106402 (2016)

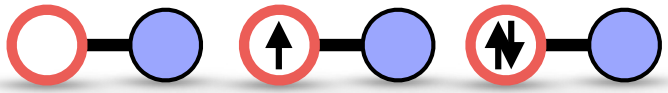


sign problem: smart adapted basis choice

IV: conclusions

DMFT

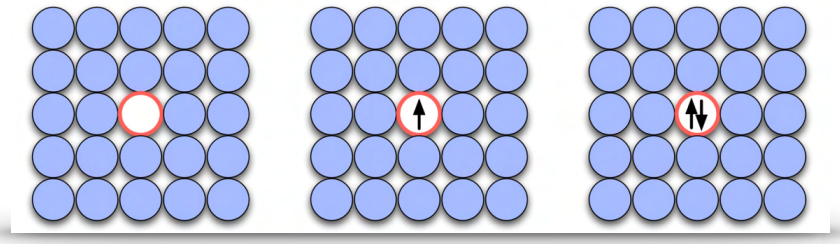
dimer



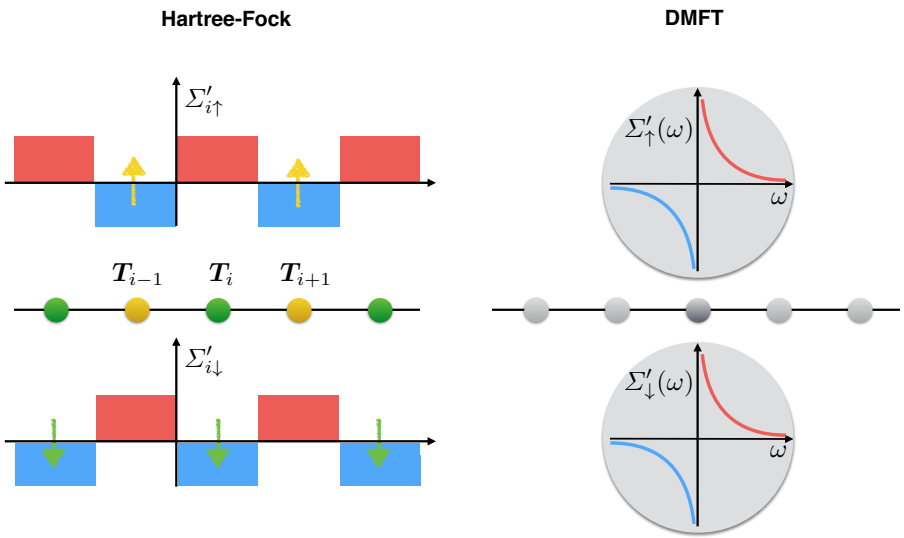
strong-correlations are local

U=V 

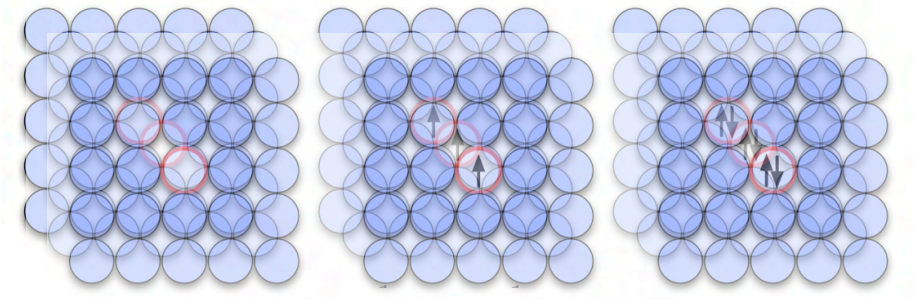
one band



DMFT vs HF

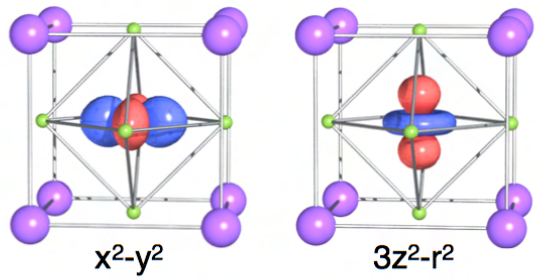


multiband

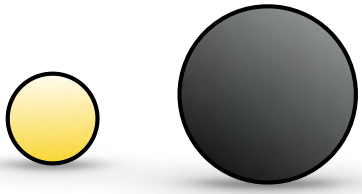


DMFT for materials

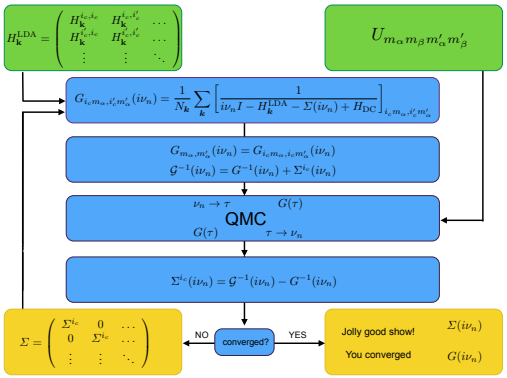
basis choice



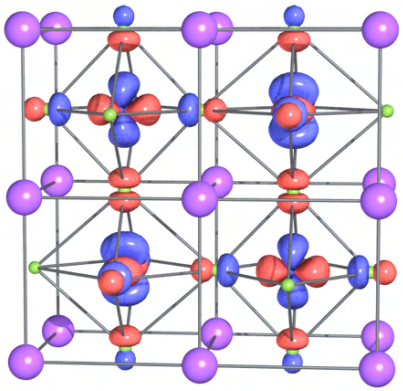
light & heavy electrons



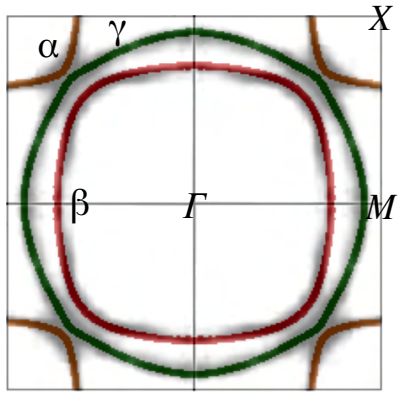
DMFT



downfolding, localization,
double counting & screening



spin-orbit coupling &
non-spherical U



reductionism vs emergence

minimal model for a given class of phenomena

- weakly-correlated systems
  - minimal model: mean-field like

- strongly-correlated Mott systems
  - minimal model: Hubbard like

…but the world is full of surprises :)

unknown unknown

thank you!