Dynamical Mean-Field Theory for Materials

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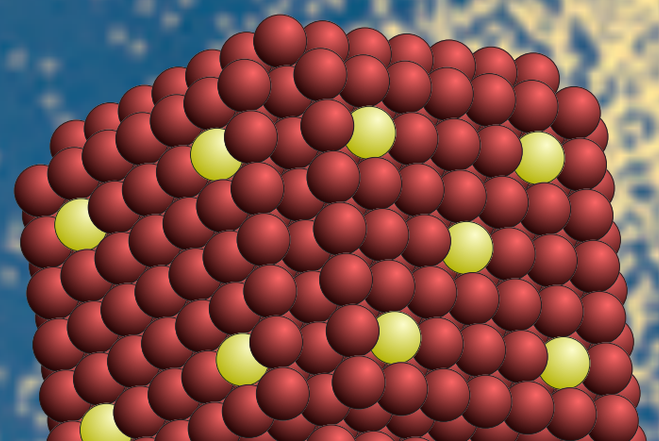


organization of the lecture

- introduction
- from DMFT to LDA+DMFT
  - Hubbard dimer
  - one-band Hubbard model
  - multi-band Hubbard model
- building materials-specific models
  - model construction
  - basis localization and interaction range
  - spin orbit & double counting
- conclusion

introduction

strong correlations: what are they?

all of physics and chemistry is correlation

Born-Oppenheimer approximation, non-relativistic

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

why is it a *problem*?

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

Philip Warren Anderson

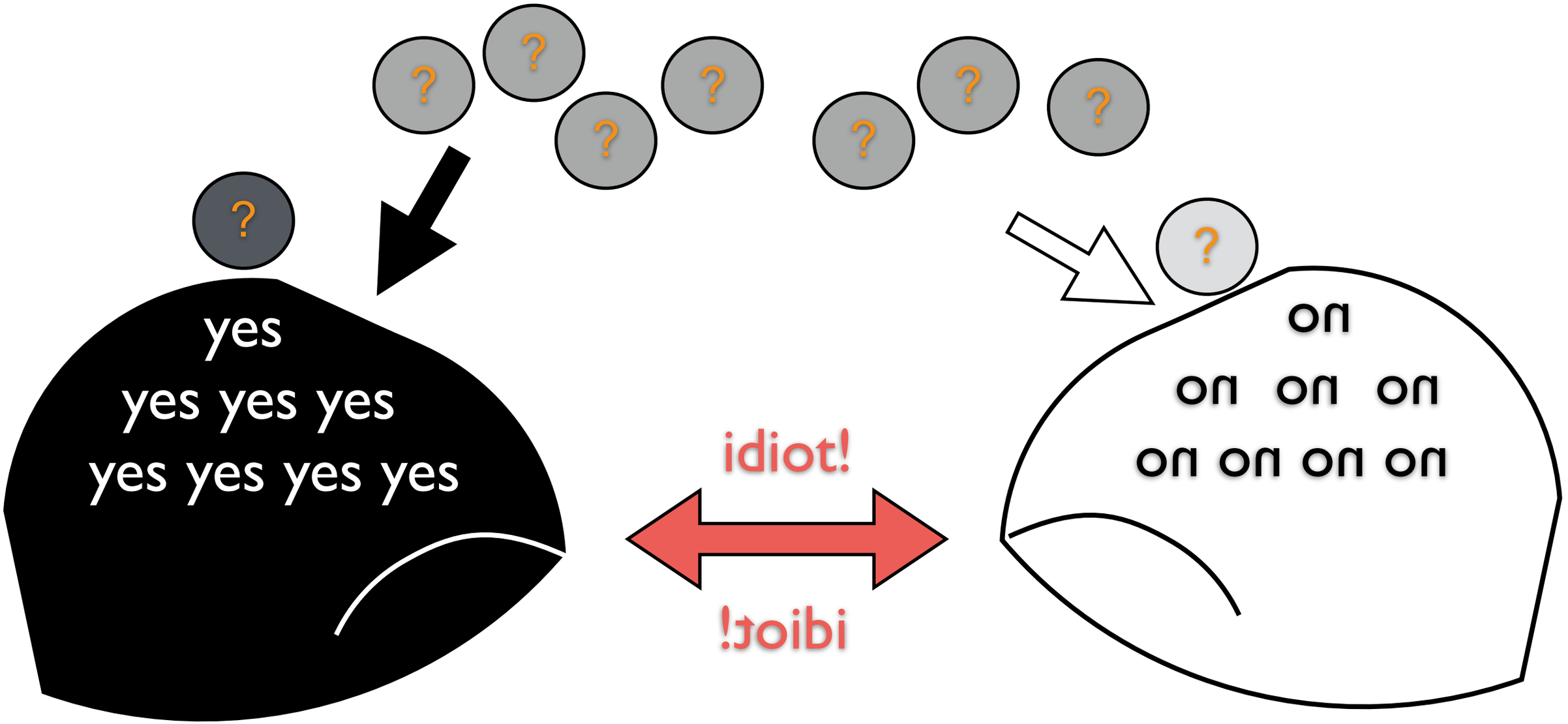
more is different

4 August 1972, Volume 177, Number 4047

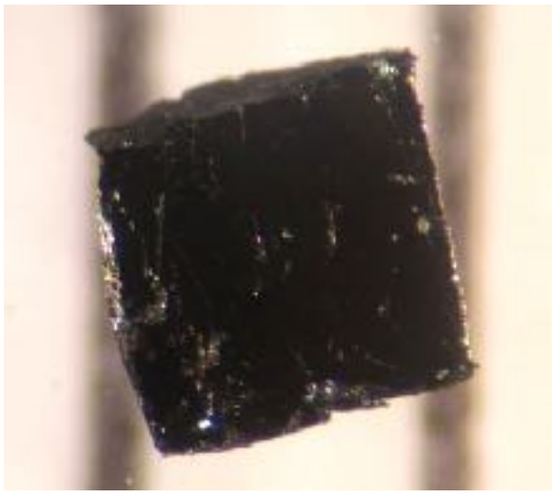
SCIENCE

emergence in social media

formation of polarized opinion-bubbles



emergence in solid-state systems

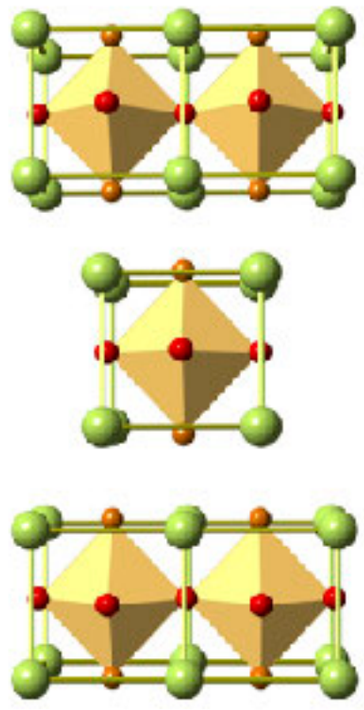


BSCCO-2223, photo from wikipedia

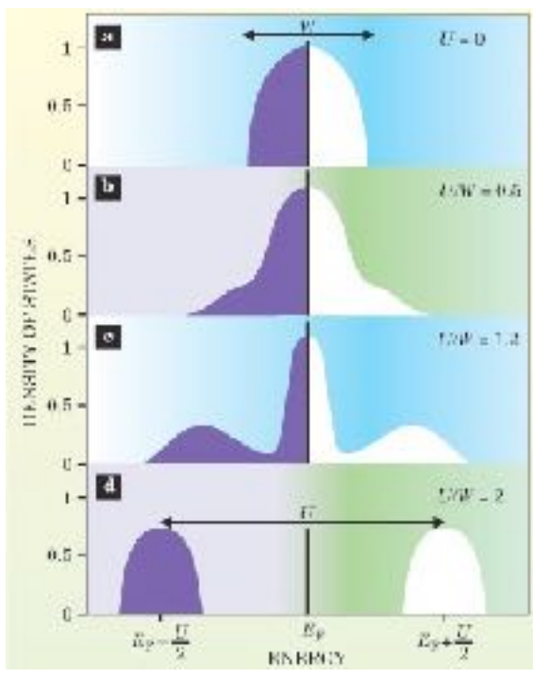
superconductivity

high-Tc superconductivity

non-conventional superconductivity

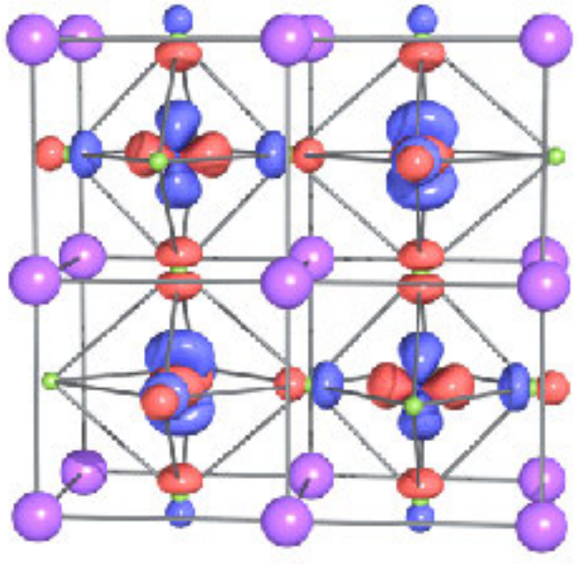


G. Zhang and E. Pavarini,
Rapid Research Letters **12**, 1800211 (2018)



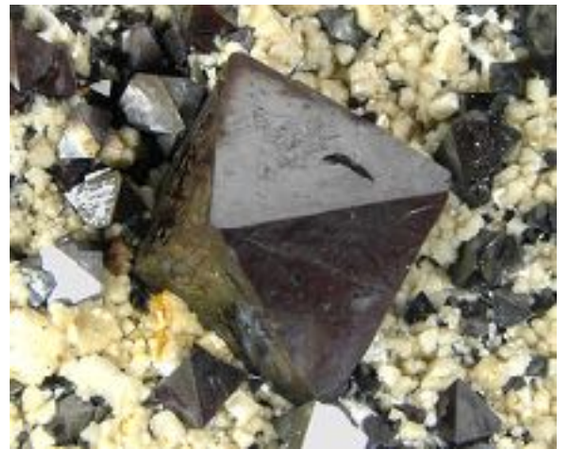
Mott transition

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

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

electron-electron interaction

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

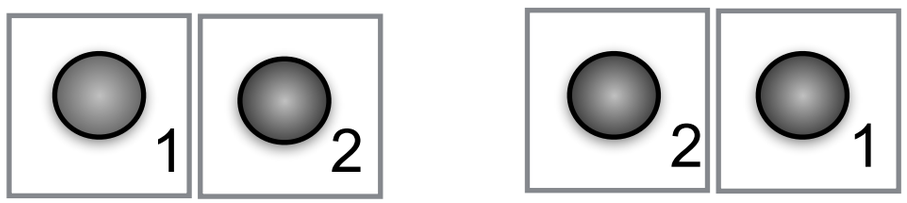
quantum N-body problem

already 1 body is difficult

- uncertainty principle $\Delta x \Delta v \geq \frac{1}{2}\frac{\hbar}{m}$
- described via wavefunction $\Psi(\mathbf{r}) \quad |\Psi(\mathbf{r})|^2$
- eigenvalue problem & discrete energies $\hat{H}_0 \Psi(\mathbf{r}) = \varepsilon \Psi(\mathbf{r})$

2-bodies non interacting

- particles are identical **and** indistinguishable



- fermions $\psi(r_1)\psi(r_2) - \psi(r_2)\psi(r_1)$

Slater determinant

$$\hat{H}_0 = \sum_i \hat{H}_i^0$$

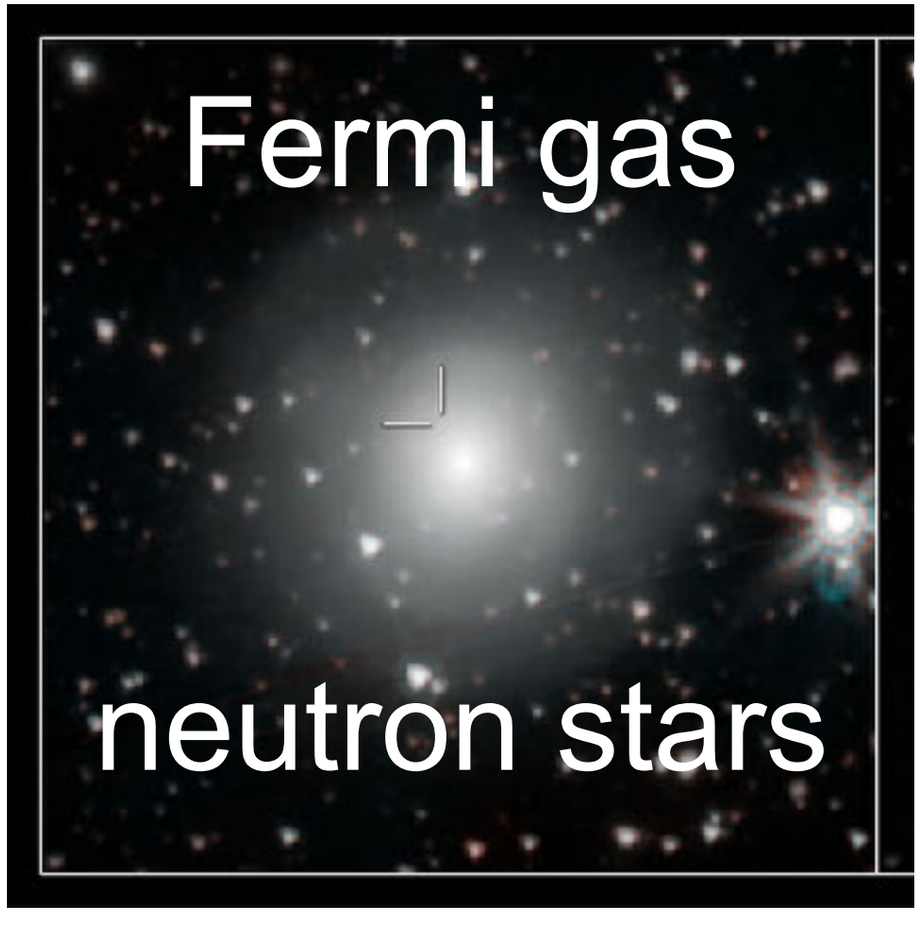
quantum N-body problem, no interaction

$$\hat{H}_0 = \sum_i \hat{H}_i^0 \qquad \hat{H}_i^0 \Psi(r_i) = \varepsilon_i \Psi(r_i) \qquad E = \sum_i \varepsilon_i$$

$$\Psi = \Psi(r_1)\Psi(r_2)...\Psi(r_N)$$

(classical/mean field)

+ antisymmetrization
(Slater determinant)



bad news: the exact solution is not an option

kinetic energy

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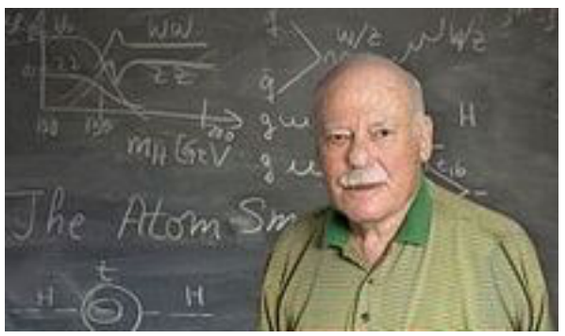
$$\hat{H}_e = \boxed{-\frac{1}{2}\sum_i \nabla_i^2} \boxed{+\frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|}} \boxed{-\sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|}} \boxed{+\frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha -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

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.

E. Pavarini and E. Koch, Autumn School on Correlated Electron 2013, Introduction

what can be done then ?

a way out: density-functional theory

1964

PHYSICAL REVIEW VOLUME 136, NUMBER 3B 9 NOVEMEBR 1964

Inhomogeneous Electron Gas*

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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 interacting electron gas in an external potential $v(\mathbf{r})$. It is proved that there exists a universal functional of the d
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.

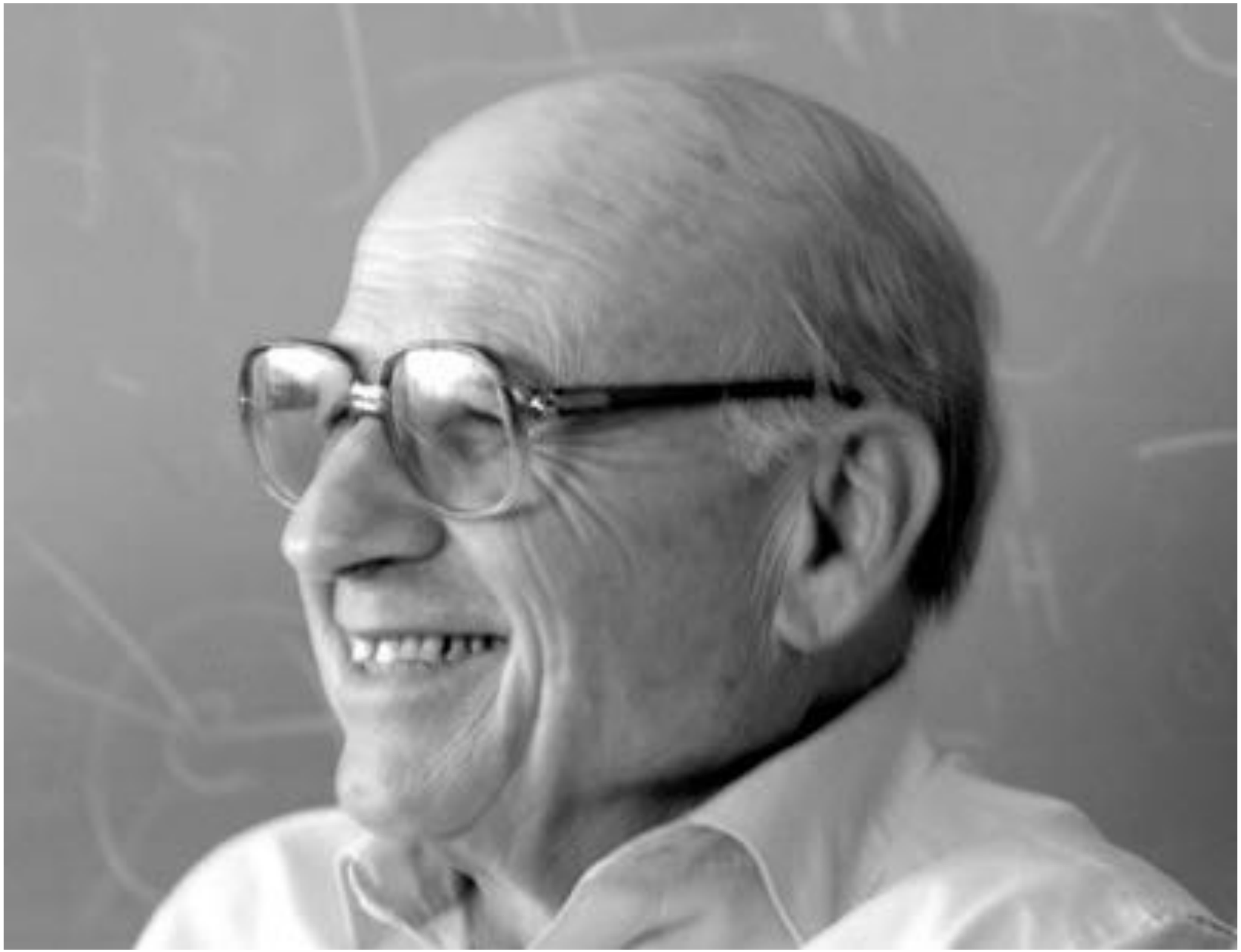
It is then a matter of interest to see how properties of the homogeneous gas can be utilized in theoretical

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



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)

physics is understanding

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)**

(RO Jones, *DFT for emergents*, Autumn School on Correlated Electrons 2013)

a way out: density-functional theory

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

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

Kohn-Sham auxiliary Hamiltonian

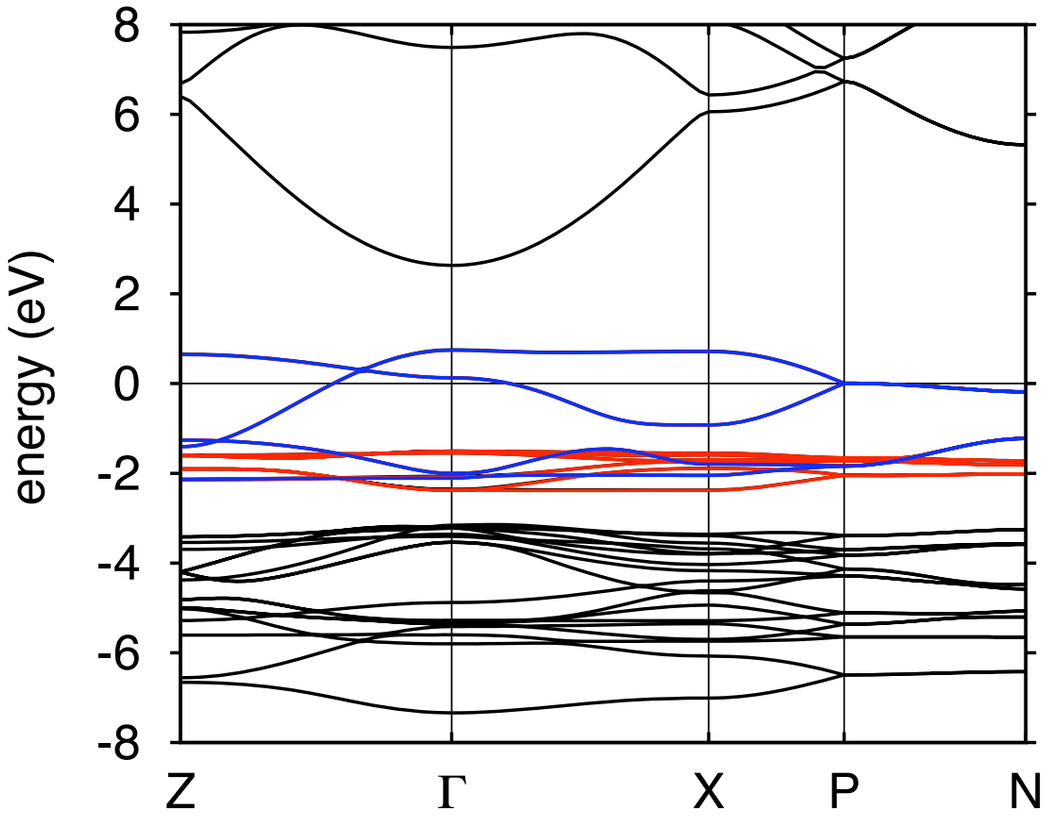
$$\hat{h}_e = \sum_i \left[-\frac{1}{2}\nabla_i^2 + v_R(\boldsymbol{r}_i)\right] = \sum_i \hat{h}_e(\boldsymbol{r}_i)$$

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

(in practice: LDA,GGA,…)

unexpected successes of DFT

Kohn-Sham eigenvalues as elementary excitations!



band structures, material trends, prediction

unexpected successes of DFT

Philip Warren Anderson

"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)***

but "very deep problems" remain (1998)

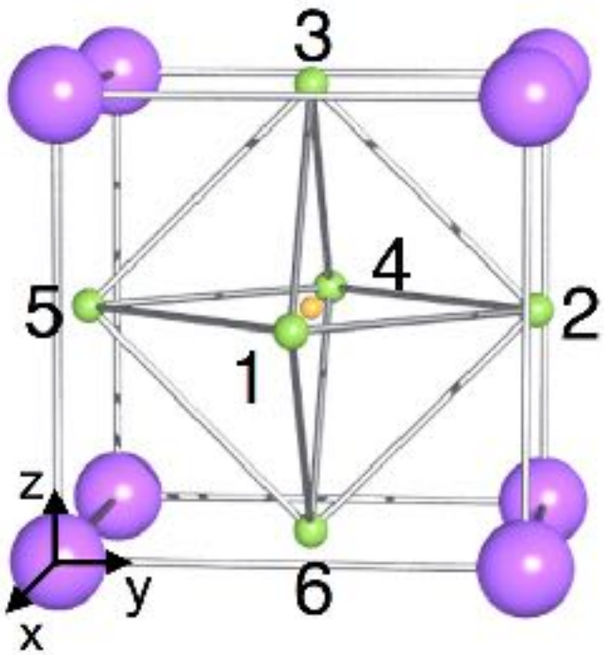
origin of failures: one-electron picture

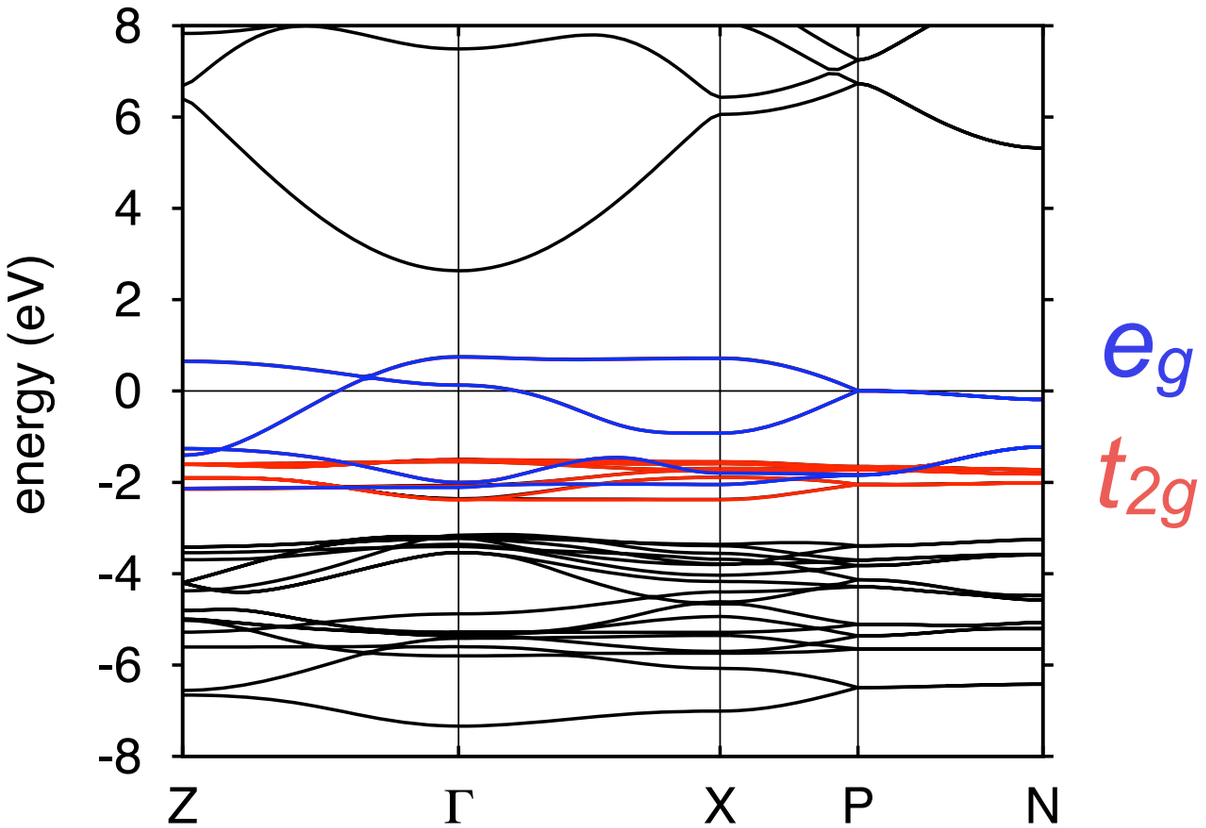
(R.O. Jones, *DFT for emergents*, Autumn School on Correlated Electrons 2013)

big disappointments

$KCuF_3$

DFT (LDA): it is a metal!

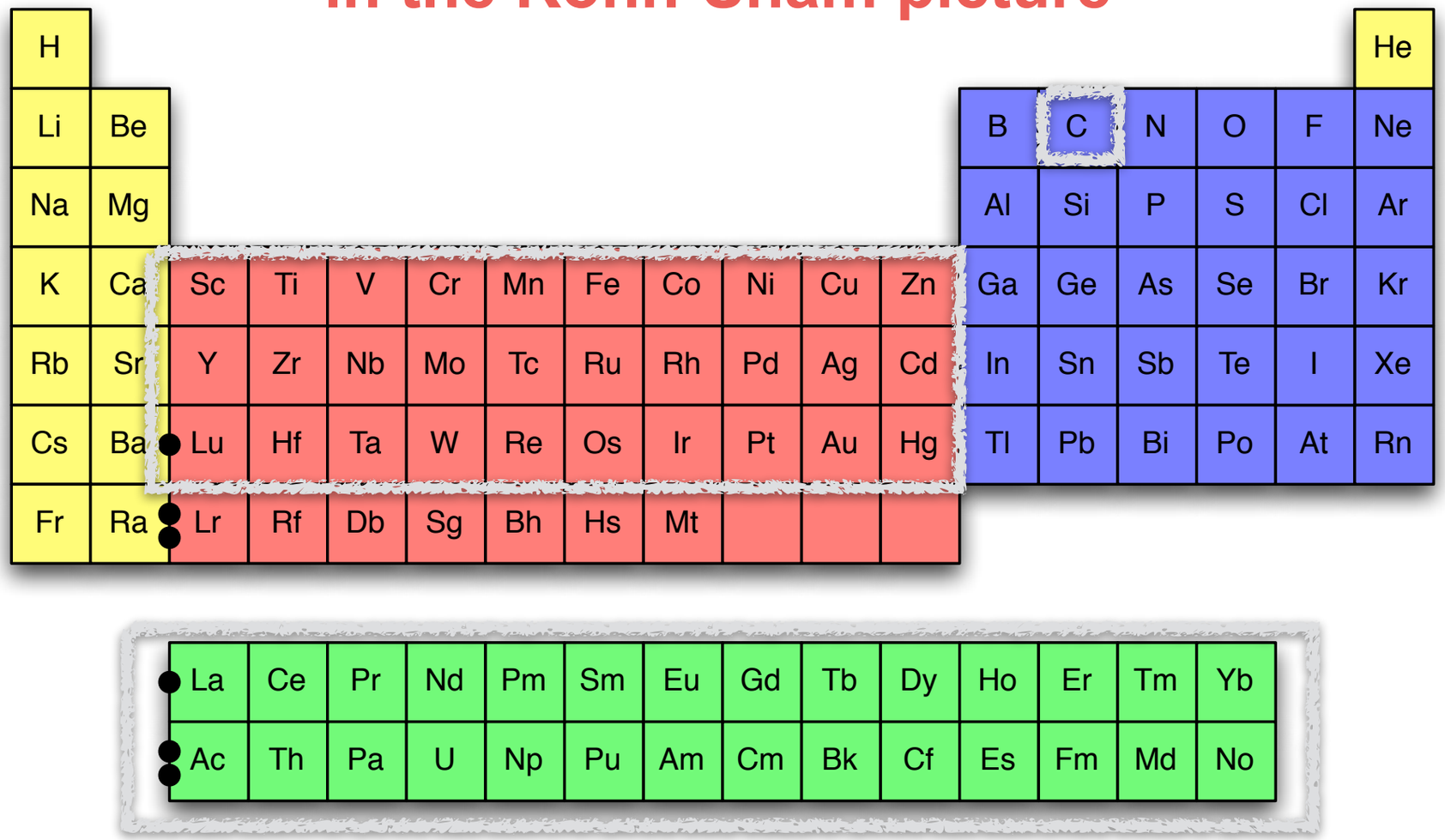




Experiments: it is an insulator! and above 40 K a **paramagnetic** insulator

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

ab-initio methods fail…

but it can be explained with simple models!

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.

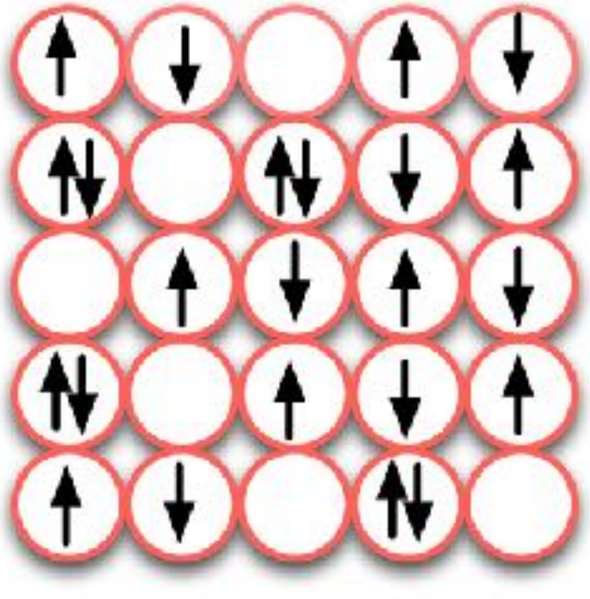
Capturing the essence of a phenomenon while being simple: the ingredients of a top model in physics. Since the early days of quantum mechanics, many models, Hamiltonians and theories aiming to provide a deeper understanding of various properties of condensed matter have been put forward — with varying 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

Hubbard model at half-filling

atomic hoppings atomic

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



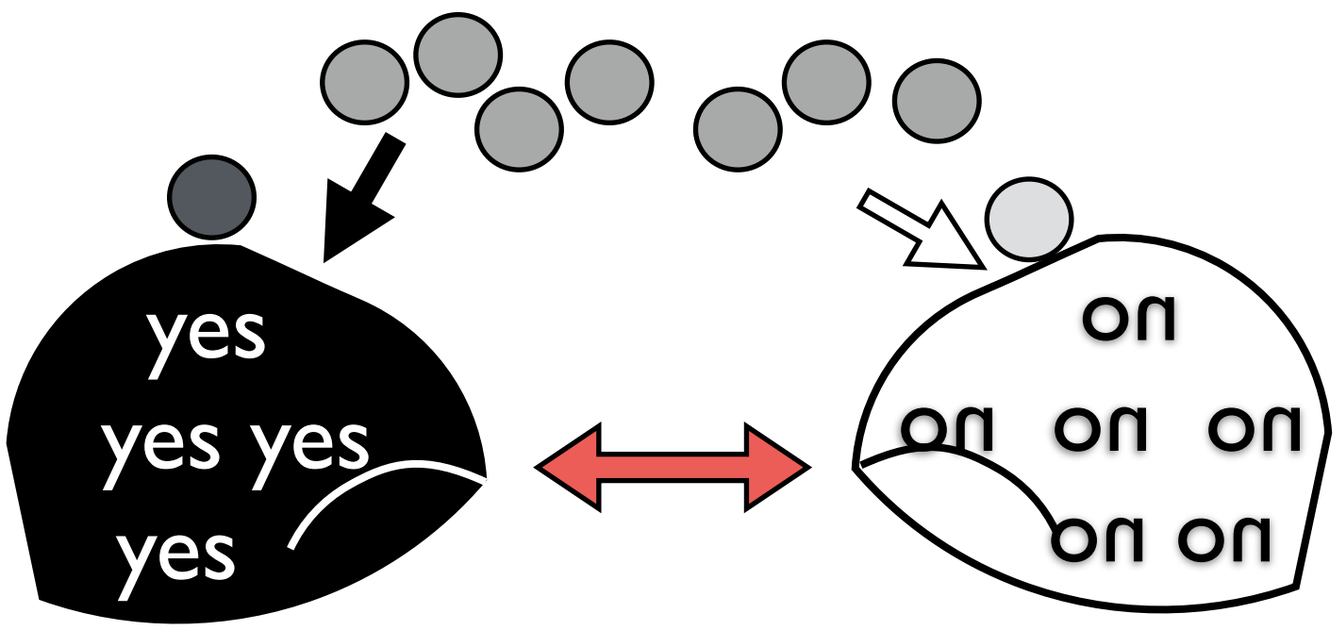
1. *t=0*: collection of atoms, **insulator**
2. *U=0*: half-filled band, **metal**

canonical model for Mott transition

Mott systems: two irreconcilable philosophies?

- improve exchange-correlation functional
  - materials-specific aspects are key

- give up DFT and use canonical models
  - generic mechanism-specific aspects are key)



both right and wrong

how do we connect canonical models and DFT ?

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 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?

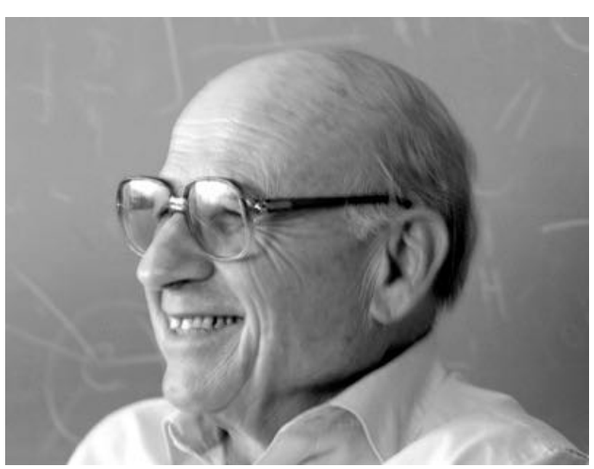
$$\tilde{t}_{ab} = -\int d\mathbf{r}\, \overline{\phi_a^{\mathrm{KS}}}(\boldsymbol{r})\left(-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r})\right)\phi_b^{\mathrm{KS}}(\boldsymbol{r})$$

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...

weakly-correlated systems

one-electron approximation

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

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

very good approach for weakly correlated systems

why not also for Mott systems ?

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

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

one-electron approximation

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 $T_{c\,\max}$

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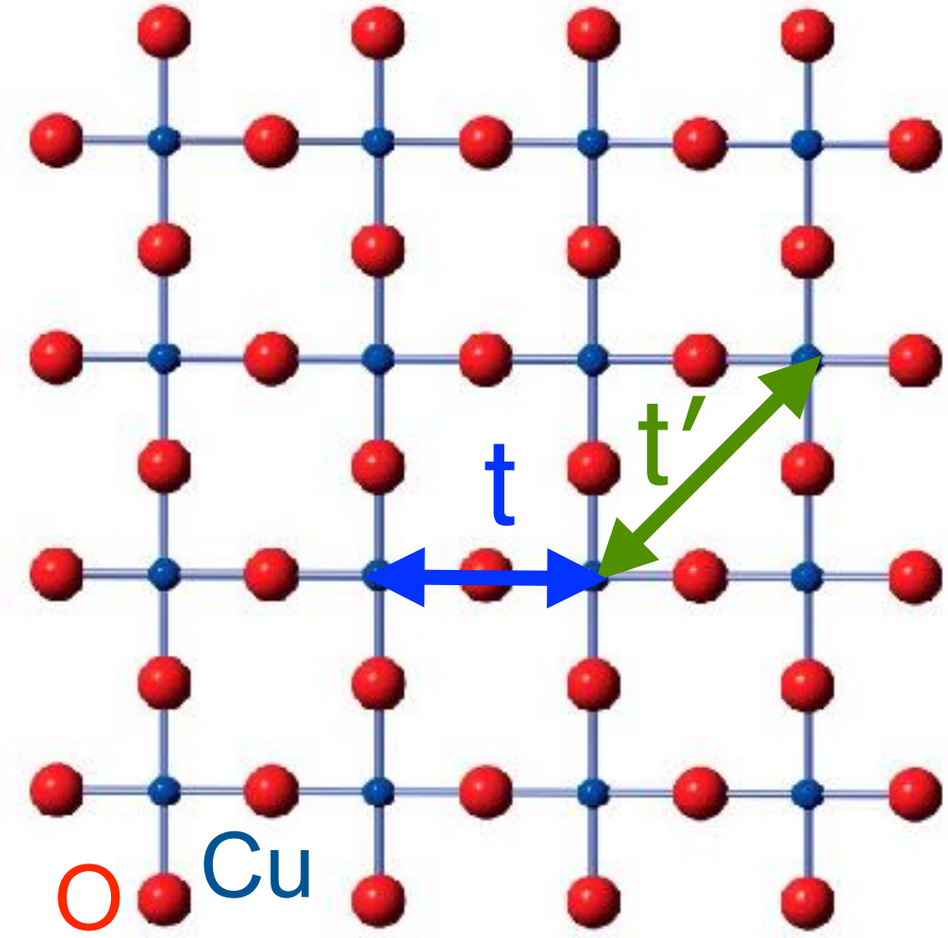
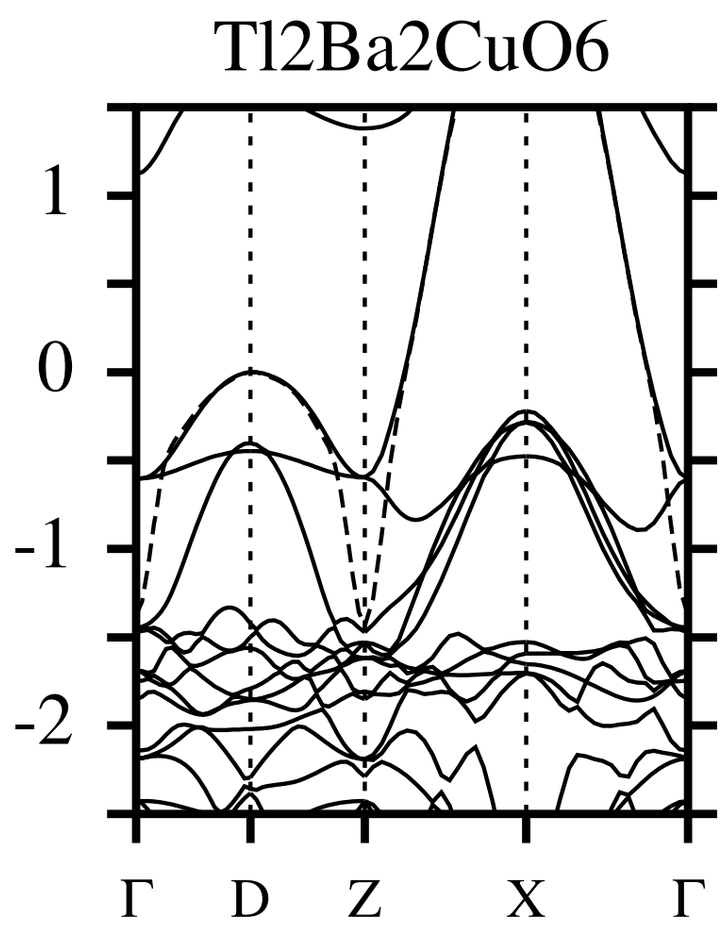
(Received 4 December 2000; published 10 July 2001)

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.

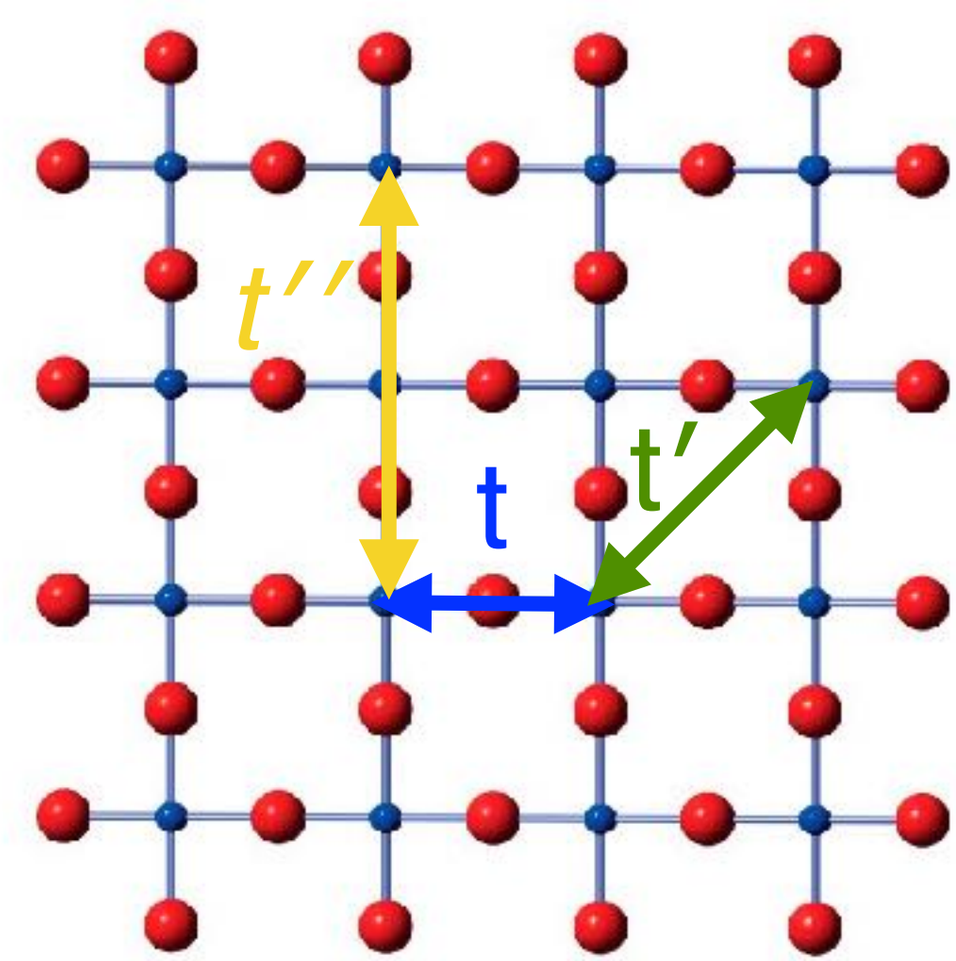
CuO_2



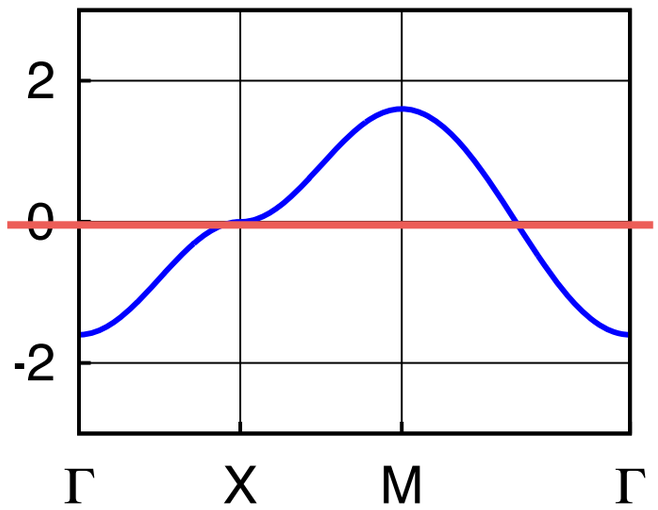


electron counting argument

one electron per site

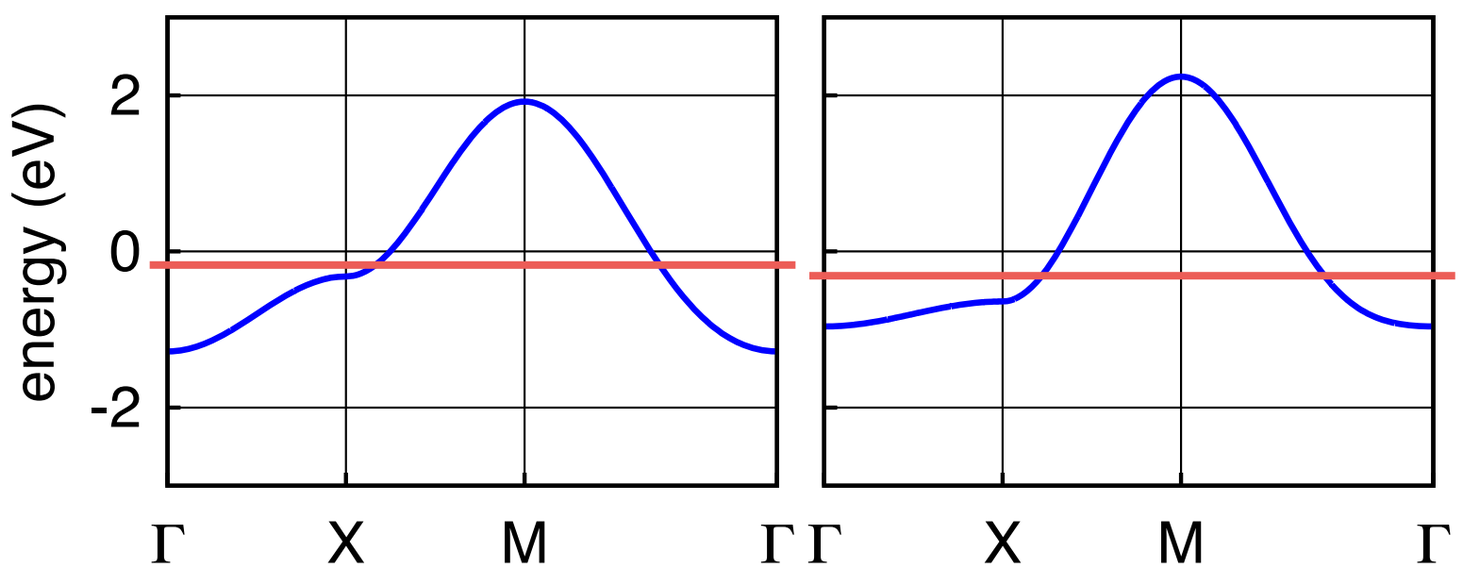


$$\varepsilon_{\boldsymbol{k}} = -2t[\cos k_x + \cos k_y]$$

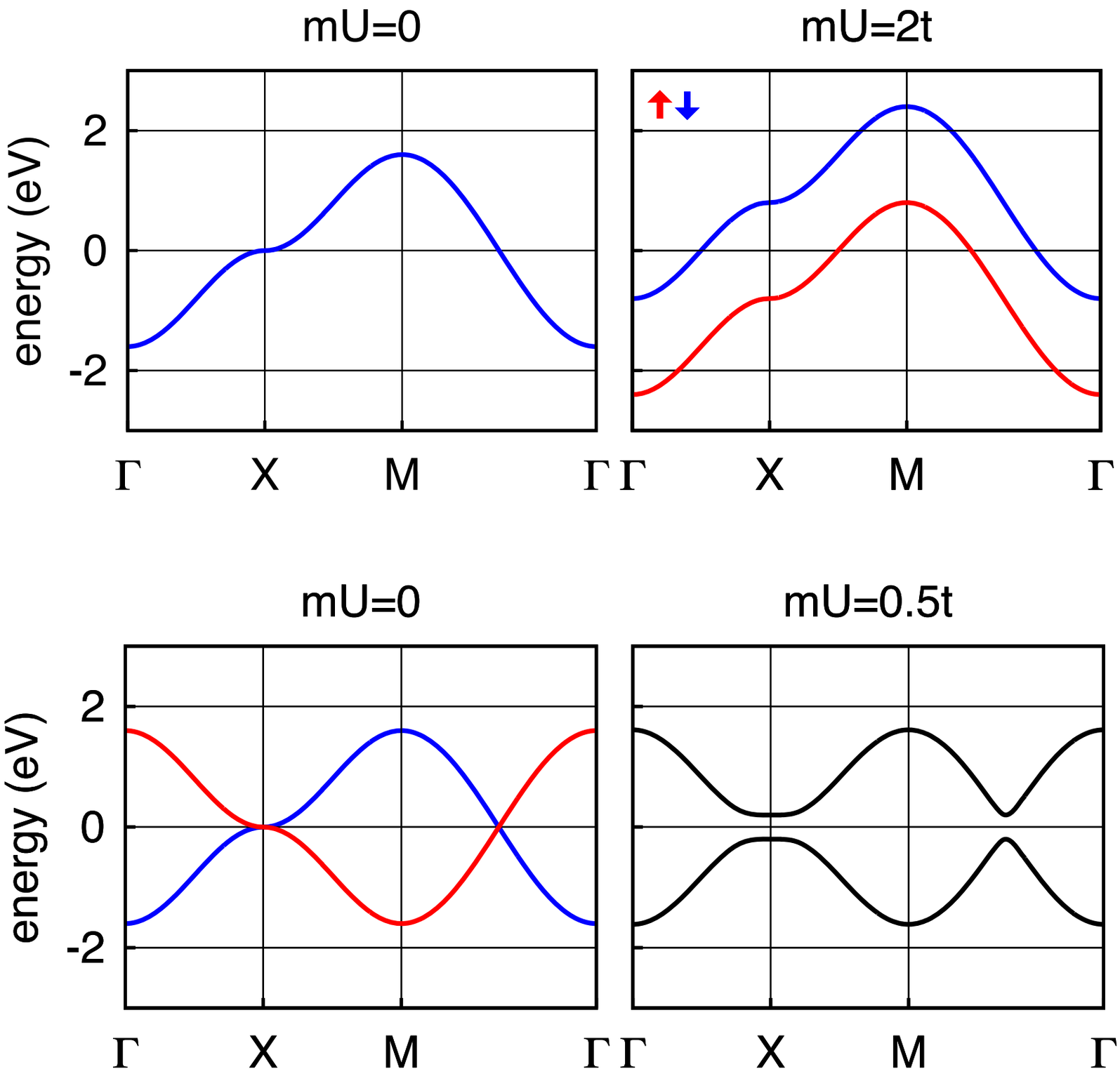


t′/t= =0.2

t′/t= =0.4



to open a gap we must lower the symmetry



methods to lower the symmetry

magnetic/orbital/charge order

spin-glass

....

Slater insulator

Mott insulators have different properties than Slater insulators

the ***gap*** is only one of them

it is not only about the gap

strongly-correlated systems

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

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

it is the **local** Coulomb interaction that matters

minimal model for a given class of phenomena

as system-specific as possible

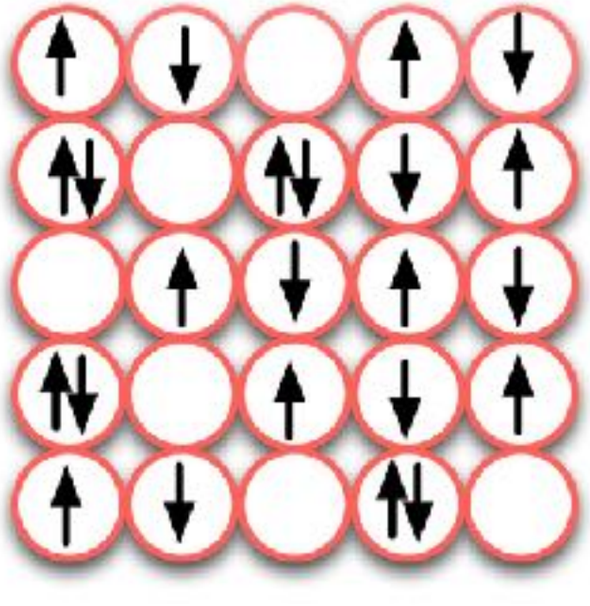
we have to **build** & **solve** materials-specific Hubbard-like models

let us discuss first how to **solve** them

Hubbard model

atomic hoppings atomic

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



at half filling:

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

how do we solve it?

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)

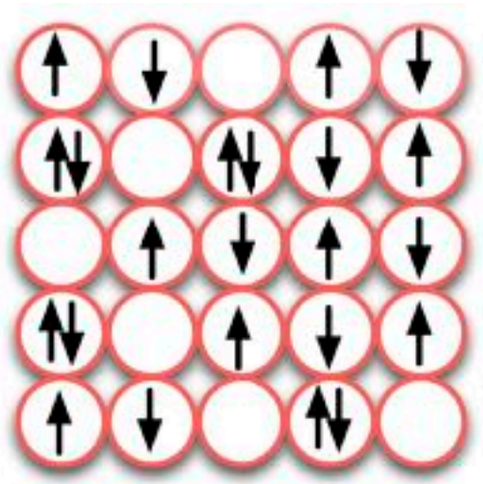
- A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992)

- M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992)

1989-1992: dynamical mean-field theory

Hubbard model

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

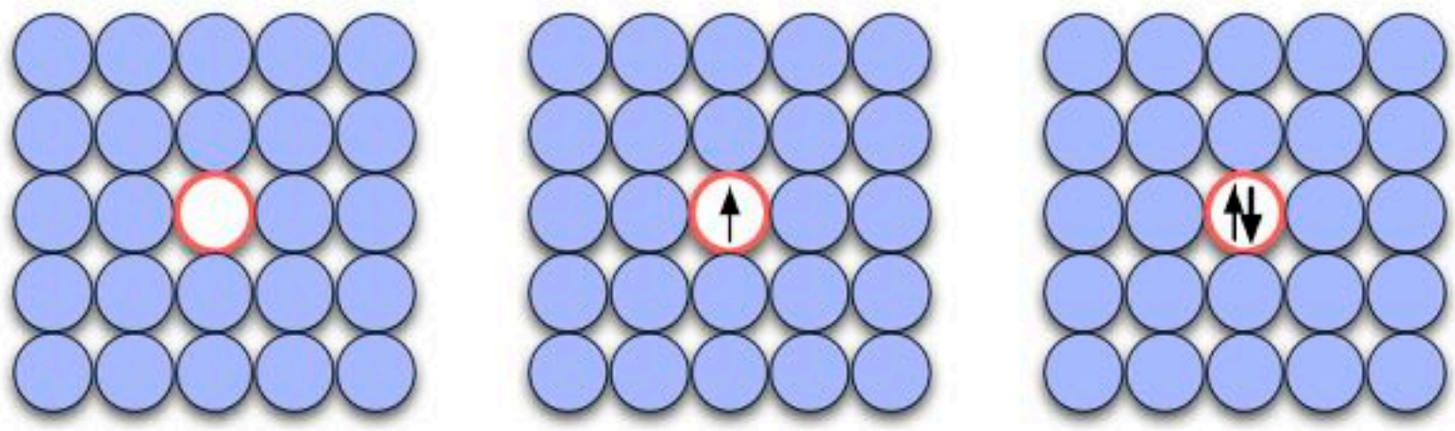


$G^{i,j}$

H^{LDA}

$U^{i,i}$

self-consistent
quantum-impurity model



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

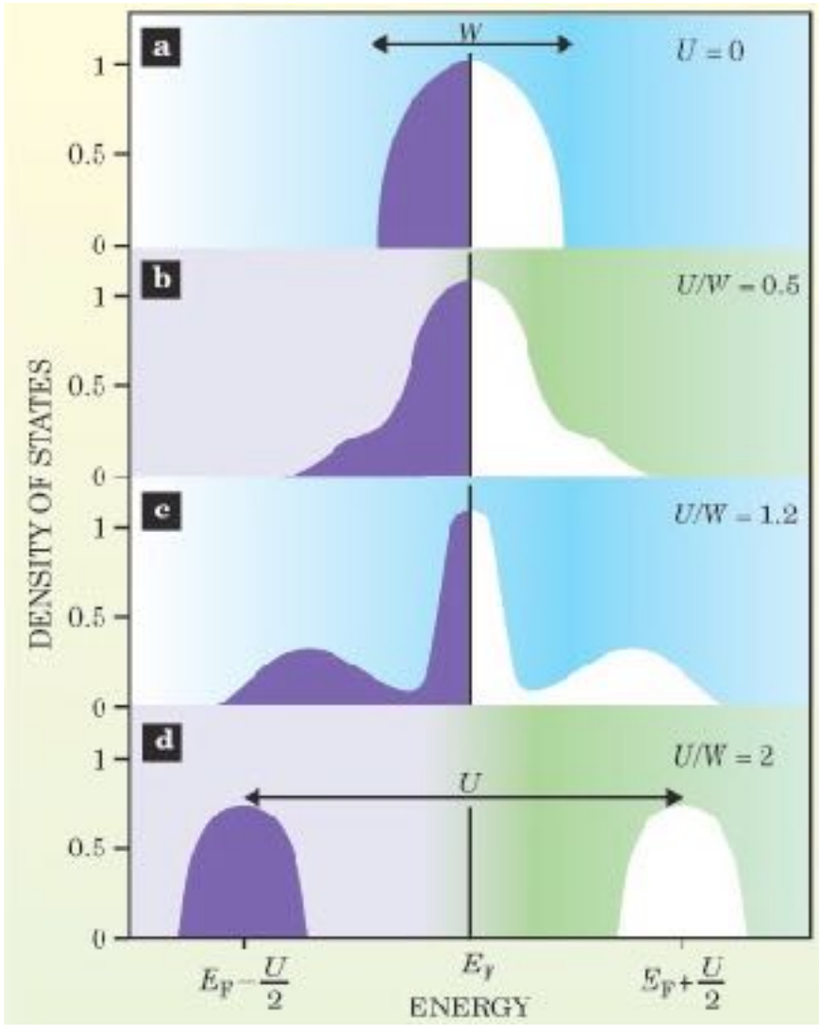
k-independent self-energy

main difficulty: solve self-consistent quantum impurity problem

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

dynamical mean-field theory

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



Bethe Lattice

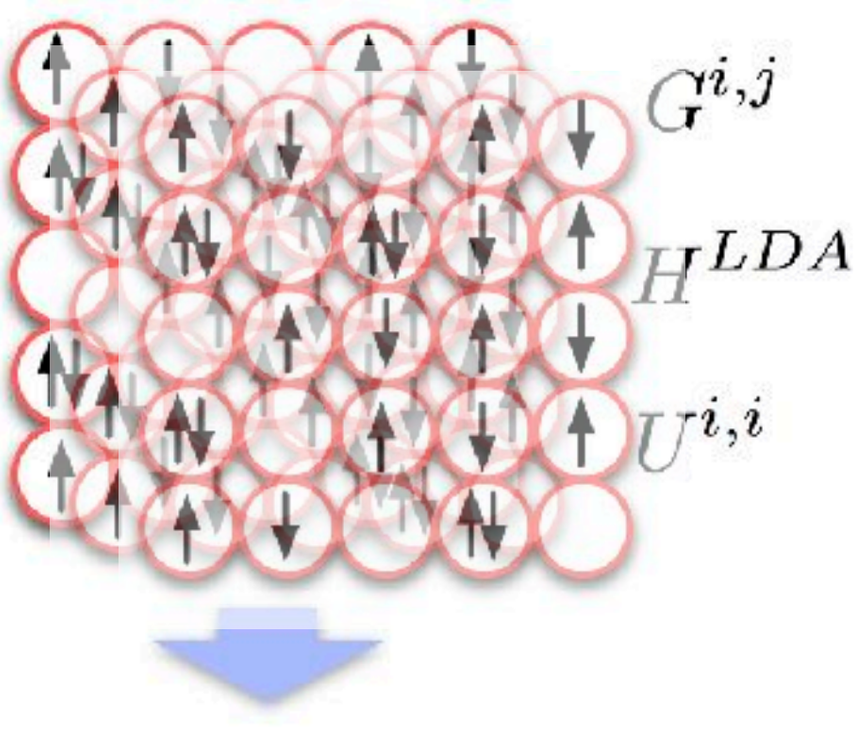
W: band width

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

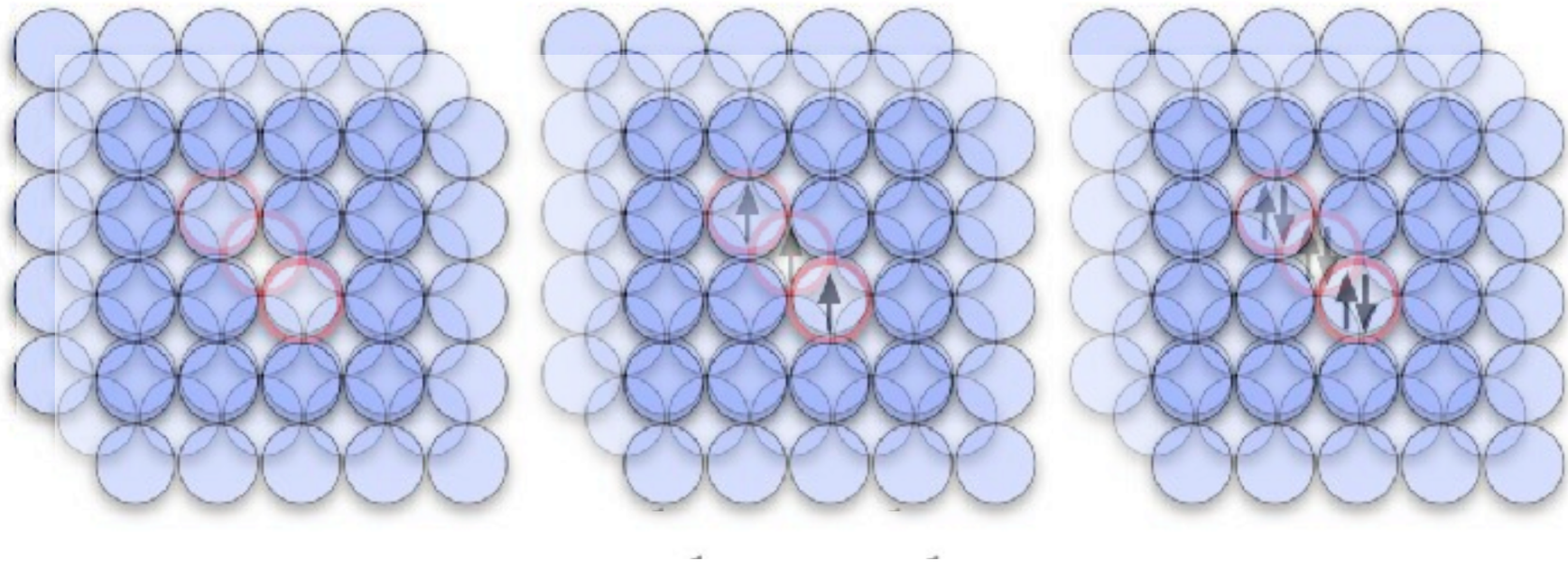
DMFT for real materials

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



how does it work?

DMFT for the Hubbard dimer

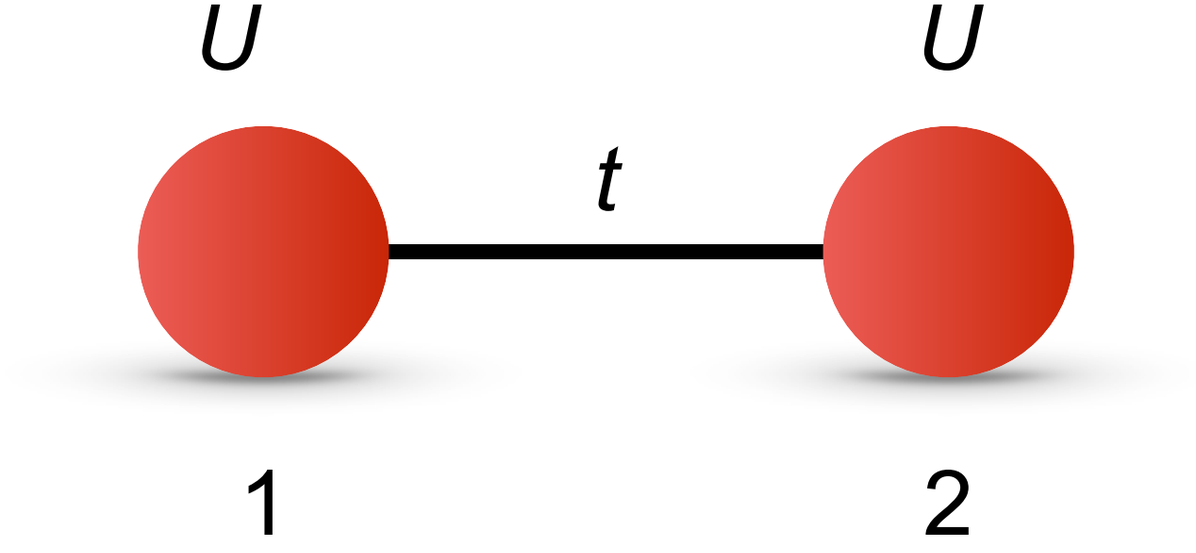
this is a **toy** model: coordination number is one

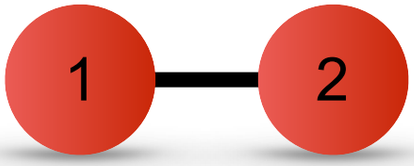
DMFT is exact for $t=0$, $U=0$ and in the **infinite dimension** limit

the Hubbard dimer

the Hubbard dimer

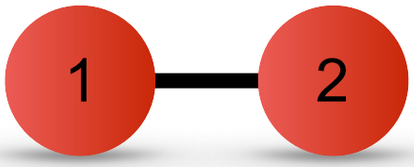
$$\hat{H} = \varepsilon_d \sum_{i\sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left(c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$





t=0: exact diagonalization

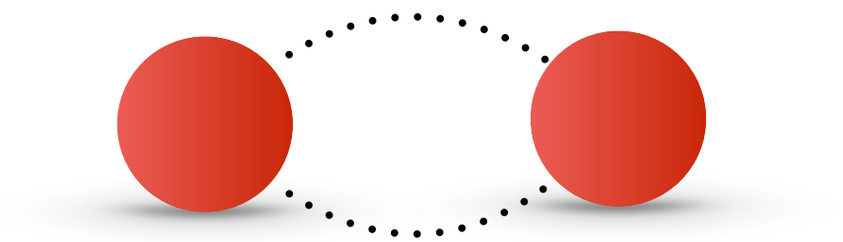
$\lvert N,S,S_z\rangle$			N	S	$E(N,S)$
$\lvert 0,0,0\rangle$	$=$	$\lvert 0\rangle$	0	0	0
$\lvert 1,1/2,\sigma\rangle_1$	$=$	$c^\dagger_{1\sigma}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 1,1/2,\sigma\rangle_2$	$=$	$c^\dagger_{2\sigma}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 2,1,1\rangle$	$=$	$c^\dagger_{2\uparrow}c^\dagger_{1\uparrow}\lvert 0\rangle$	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	$4\varepsilon_d+2U$

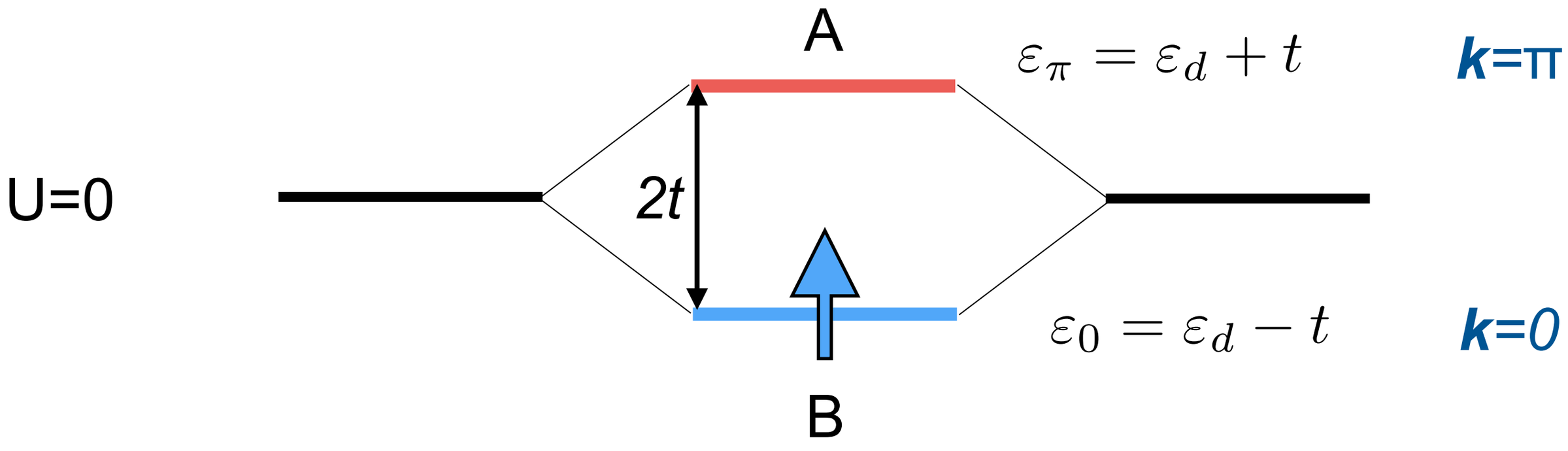


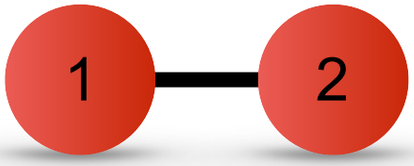
finite *t*: exact diagonalization

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





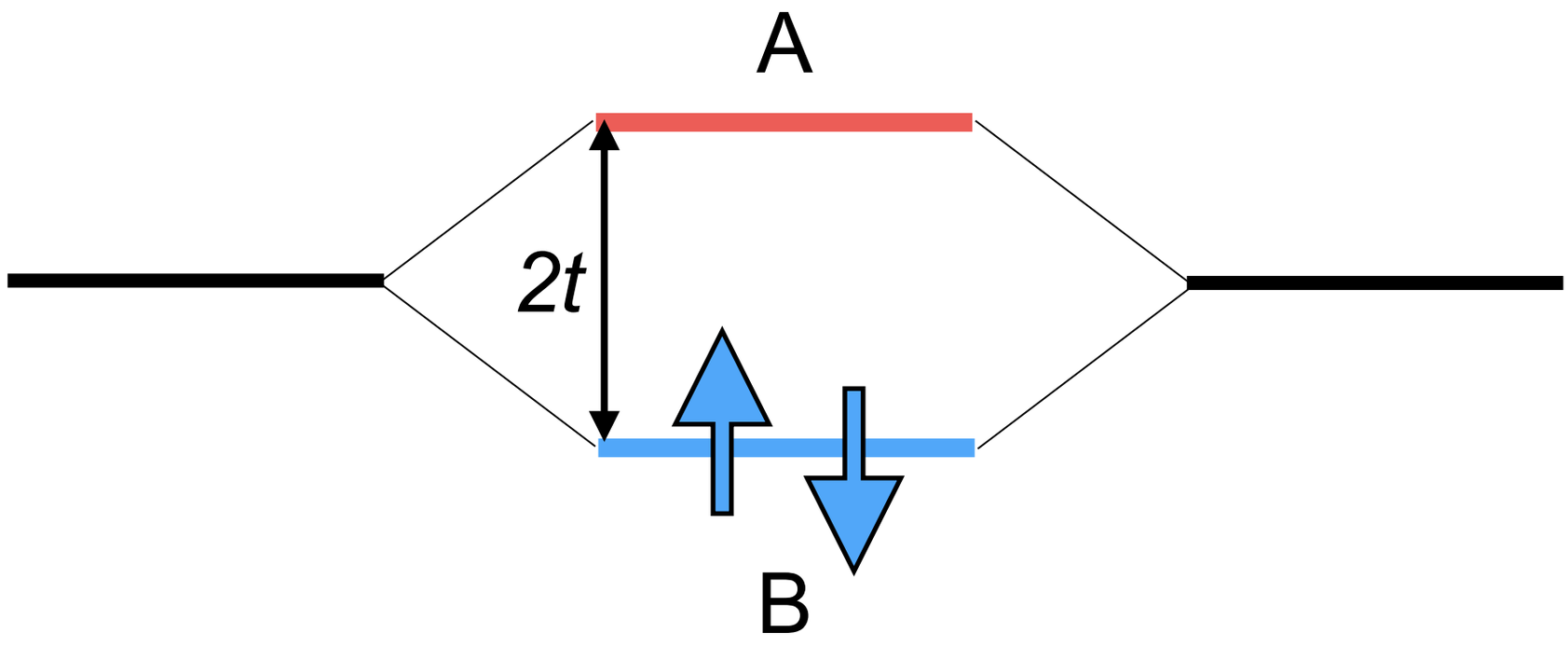


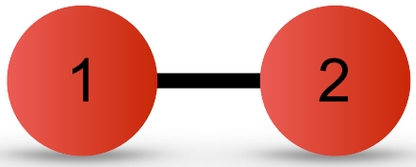
finite *t*: exact diagonalization

half filling (N=2)

$\lvert 2,S,S_z\rangle_\alpha$	$E_\alpha(2,S)$	$d_\alpha(2,S)$
$\lvert 2,0,0\rangle_+ = b_1\lvert 2,0,0\rangle_0 - \frac{b_2}{\sqrt{2}}\big(\lvert 2,0,0\rangle_1 + \lvert 2,0,0\rangle_2\big)$	$2\varepsilon_d + \frac{U}{2} + \frac{1}{4}\big(U + 2\Delta(t,\frac{U}{2})\big)$	1
$\lvert 2,0,0\rangle_o = \frac{1}{\sqrt{2}}\big(\lvert 2,0,0\rangle_1 - \lvert 2,0,0\rangle_2\big)$	$2\varepsilon_d + U$	1
$\lvert 2,1,m\rangle_o = \lvert 2,1,m\rangle$	$2\varepsilon_d + \frac{U}{2}$	3
$\lvert 2,0,0\rangle_- = b_2\lvert 2,0,0\rangle_0 + \frac{b_1}{\sqrt{2}}\big(\lvert 2,0,0\rangle_1 + \lvert 2,0,0\rangle_2\big)$	$2\varepsilon_d + \frac{U}{2} + \frac{1}{4}\big(U - 2\Delta(t,\frac{U}{2})\big)$	1

U=0

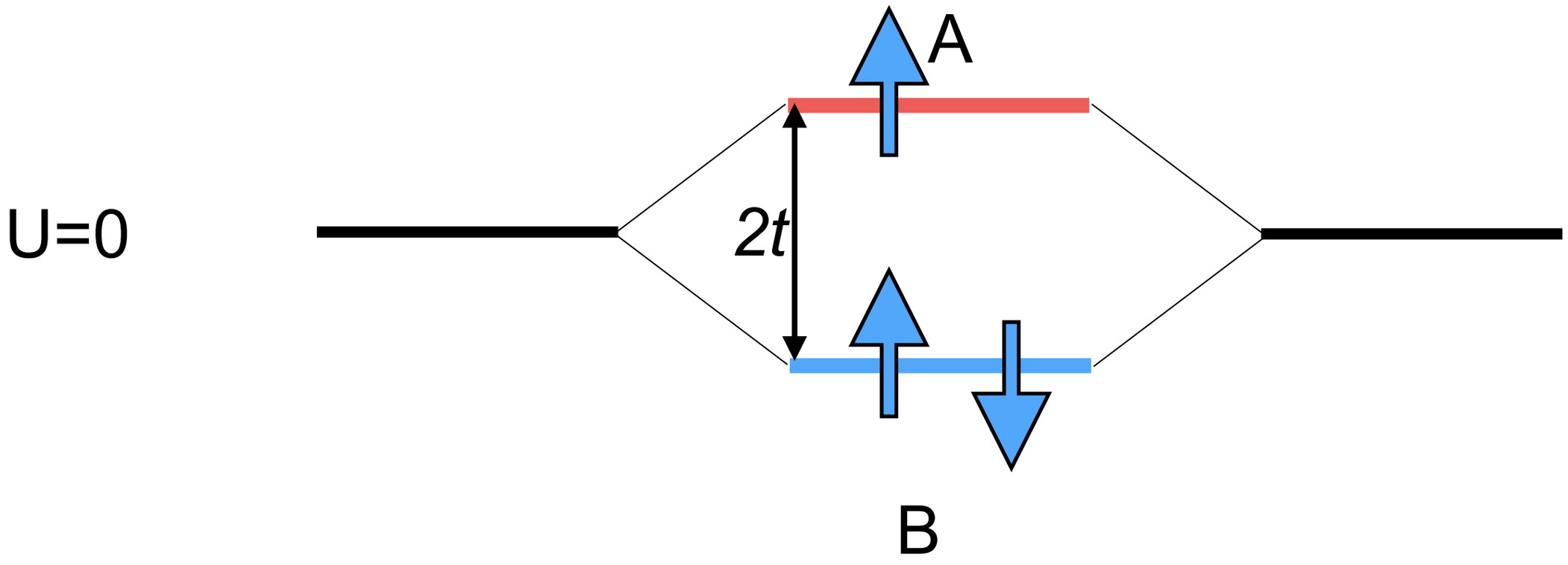


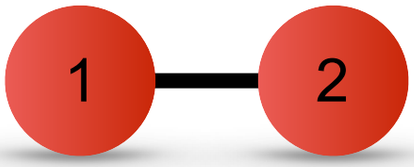


finite *t*: exact diagonalization

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





the local Green function

Lehmann representation

$d^1 \rightarrow d^0$

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

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

E(2)-E(1)

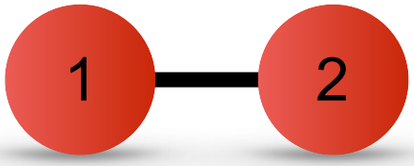
$$|\langle 3|c^\dagger_\sigma|2\rangle|^2$$

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

E(3)-E(2)

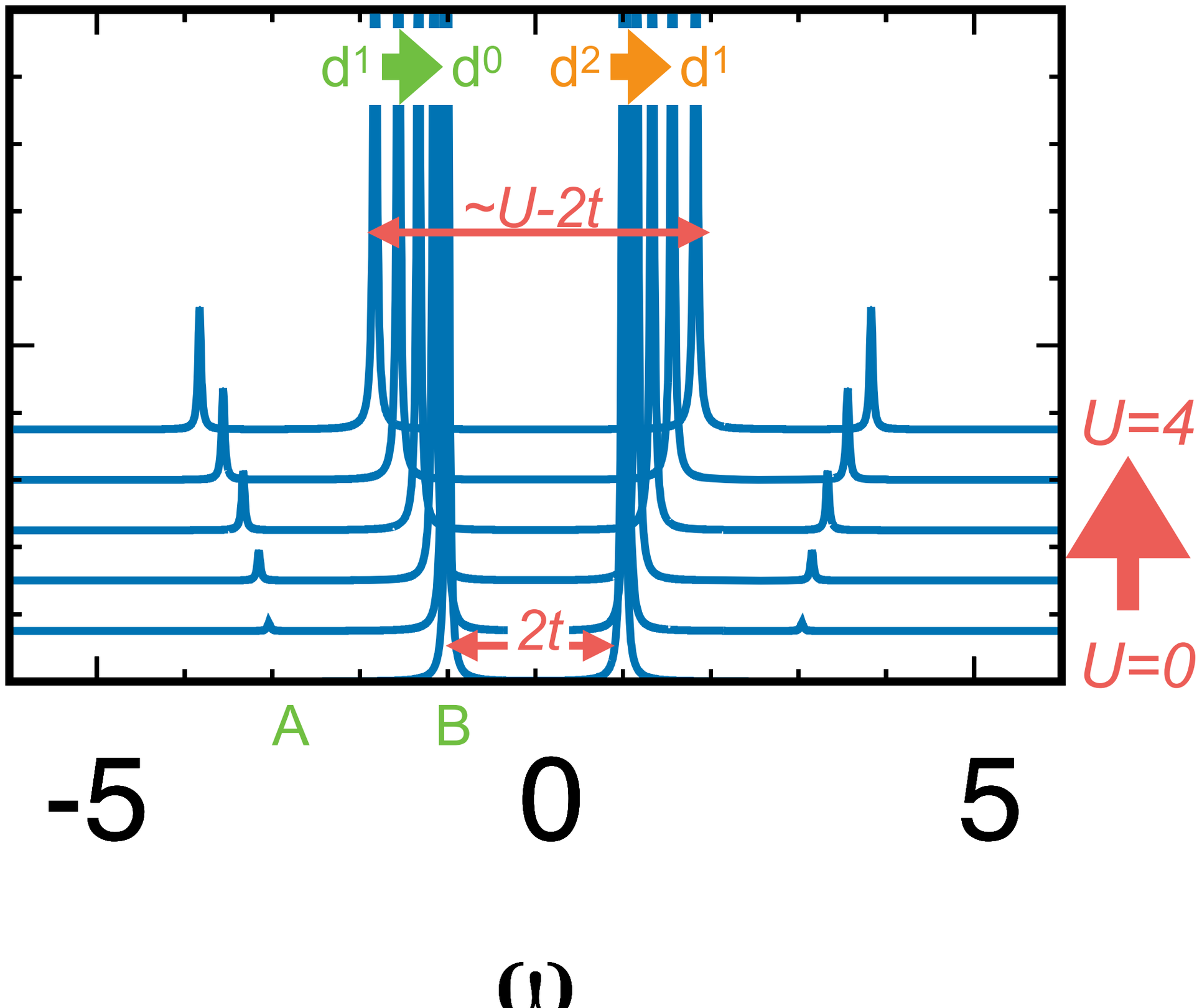
$d^2 \rightarrow d^1$

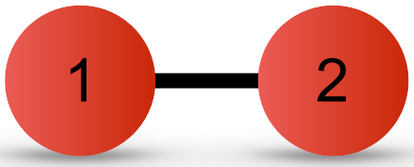
the local spectral function



W=2t

t=1





the local Green function

Lehmann representation

$d^1 \rightarrow d^0$

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

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

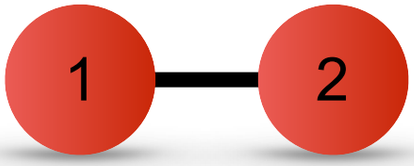
E(2)-E(1)

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

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

E(3)-E(2)

$d^2 \rightarrow d^1$



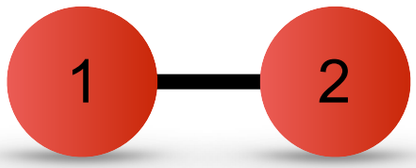
the local Green function

change basis

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

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

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



local Green function

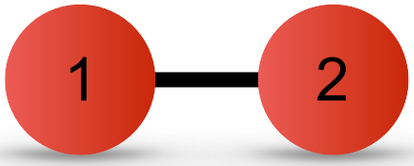
U=0 vs finite *U*

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

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

hybridization function

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



the local Green function

local self-energy

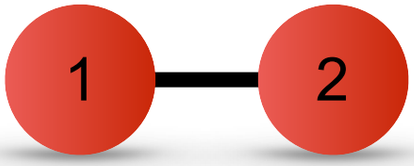
$$\Sigma_l^\sigma(i\nu_n) = \frac{1}{2}\Big(\Sigma^\sigma(\pi, i\nu_n) + \Sigma^\sigma(0, i\nu_n)\Big) = \frac{U}{2} + \frac{U^2}{4}\,\frac{i\nu_n + \mu - \varepsilon_d - \frac{U}{2}}{(i\nu_n + \mu - \varepsilon_d - \frac{U}{2})^2 - (3t)^2}$$

non-local self-energy

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

modified **hybridization function**

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



the local Green function

hybridization function

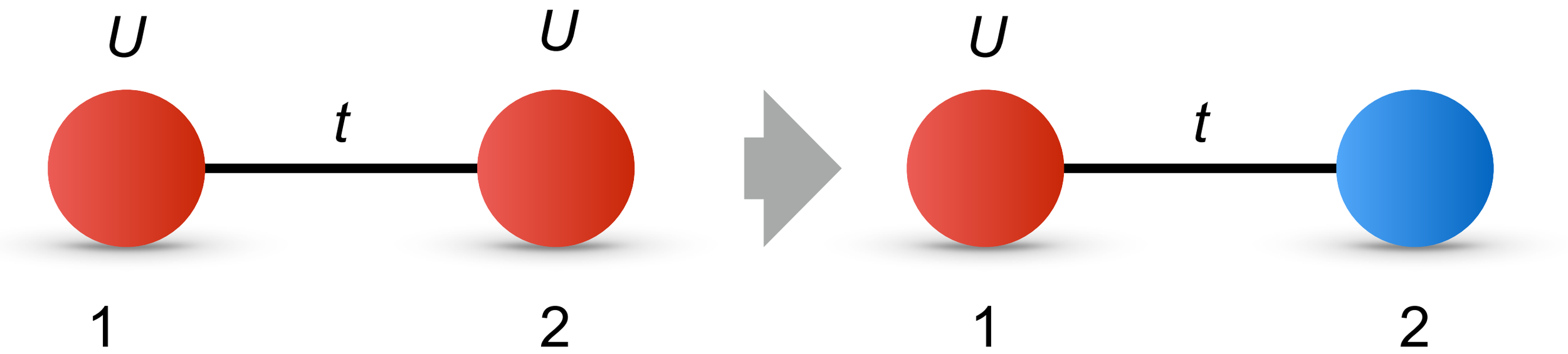
$$F^0(i\nu_n) = \frac{t^2}{i\nu_n - (\varepsilon_d - \mu)},$$

modified **hybridization function**

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

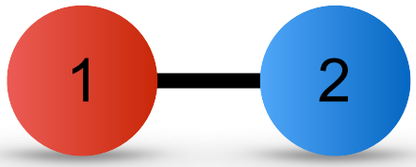
map to a quantum impurity model ?

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 Green function ?



self-consistency

half filling: N=2

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

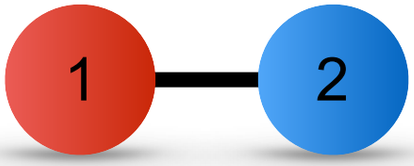
Hubbard

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

Anderson

same occupations of Hubbard dimer

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



solution: Hubbard vs Anderson

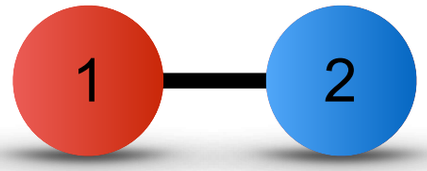
Anderson molecule

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

Hubbard dimer

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

let us neglect the **non-local** self-energy



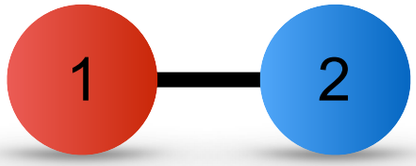
solution: Hubbard vs Anderson

hybridization function

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

modified **hybridization function**

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

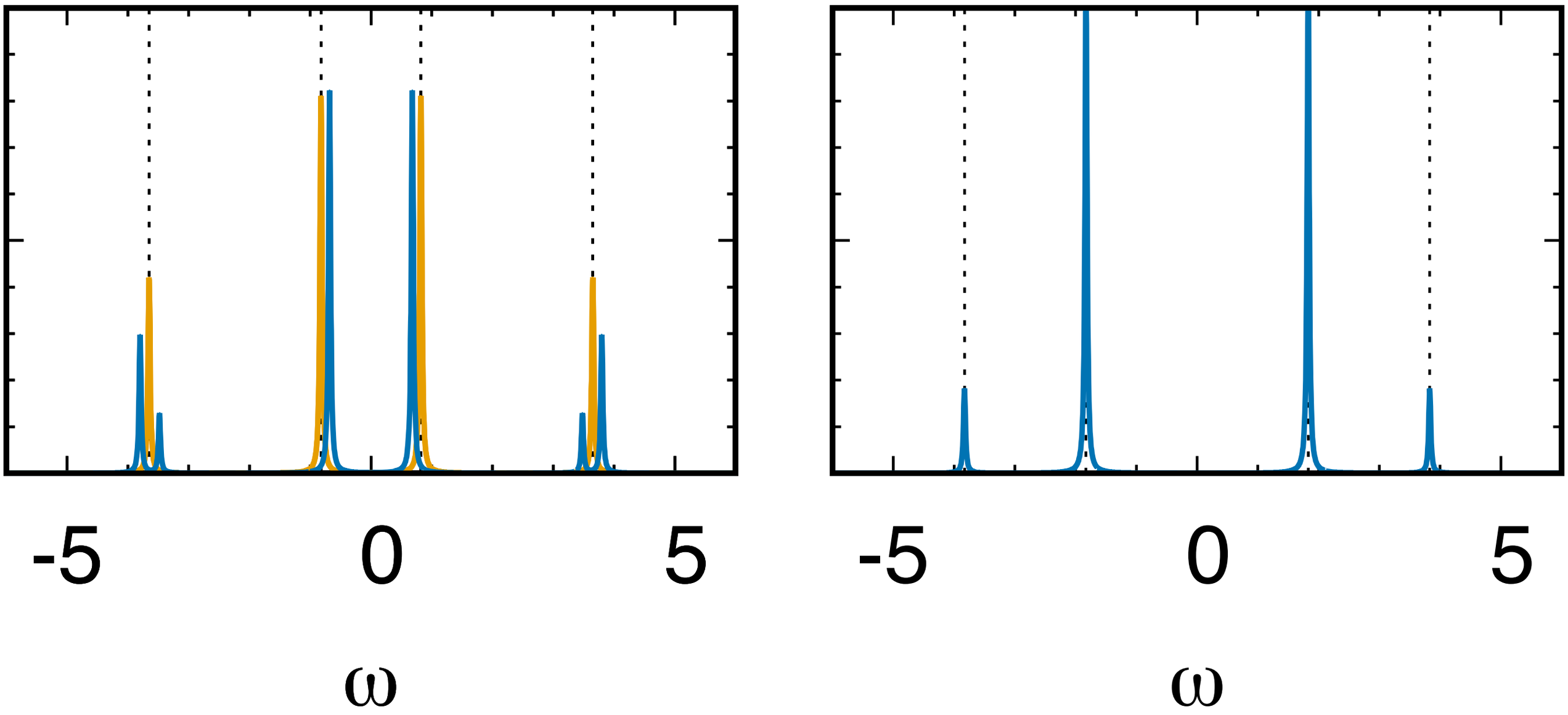


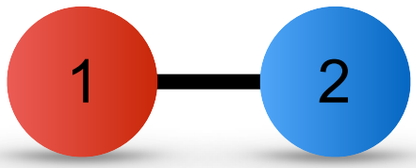
Green function *U=4t*

Anderson vs **Hubbard**

only **local** self-energy

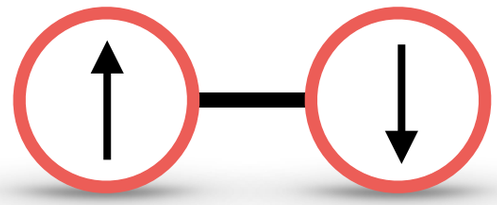
exact





DMFT for the dimer

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

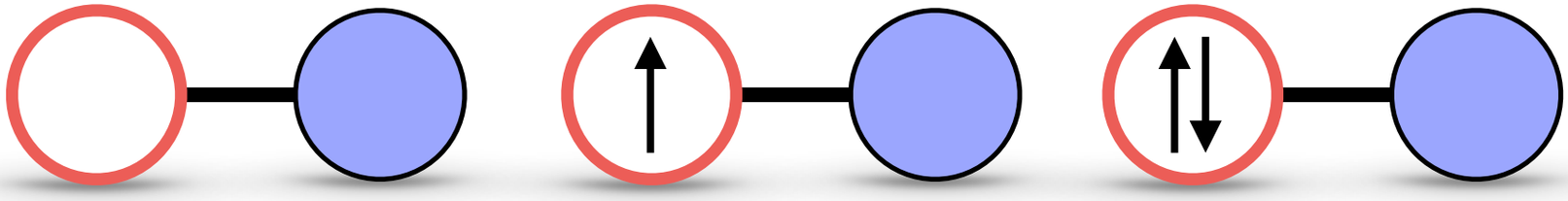


map to quantum impurity model (QIM) in local self-energy approximation

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

QIM solver

self-consistency loop

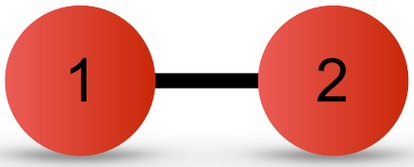


$$\Sigma(\mathbf{k},\omega) \longrightarrow \Sigma_d(\omega)$$

non-local self-energy terms

vs non-local interaction

$$U_{ijij}$$

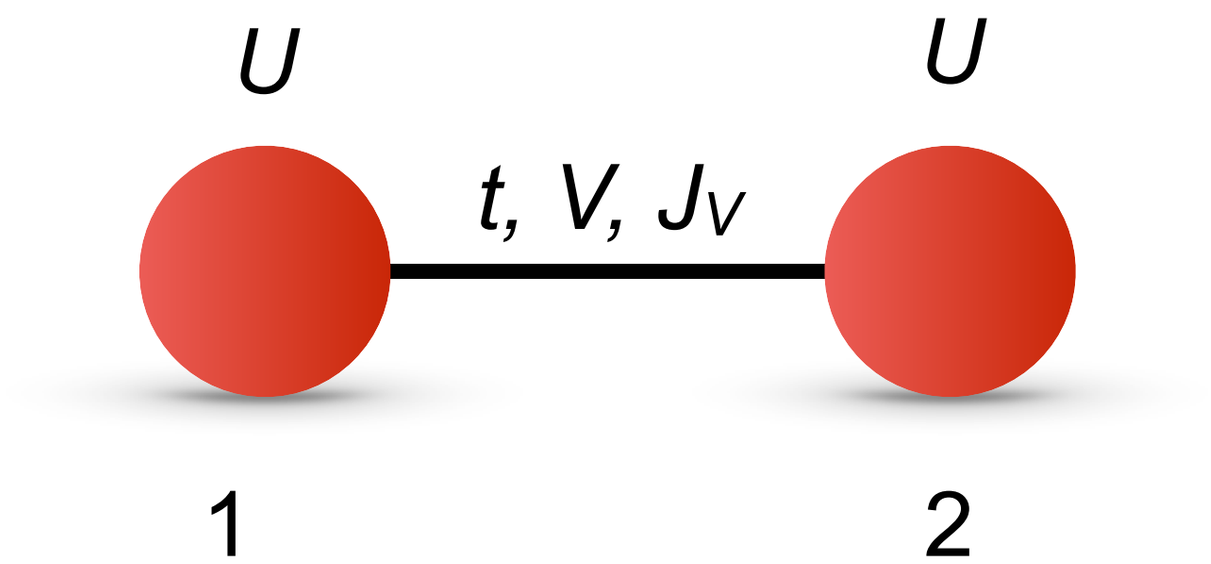


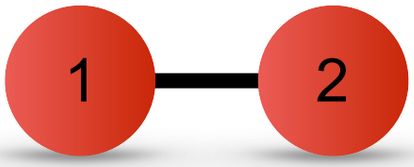
non-local Coulomb terms

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

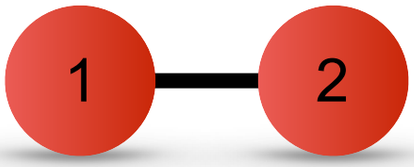
Hubbard

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

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 $U' = U - V$.



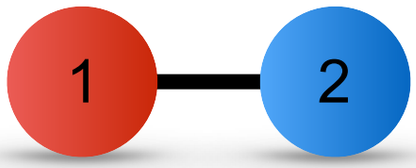
non-local Coulomb terms

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

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

If Coulomb interaction independent on site distance map to effective weakly correlated model

quantum-impurity solvers



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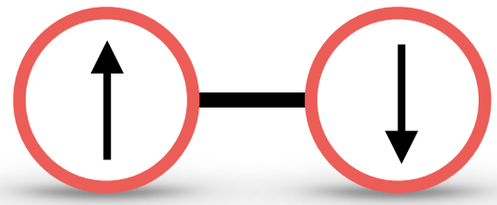

map to quantum impurity model (QIM) in local self-energy approximation

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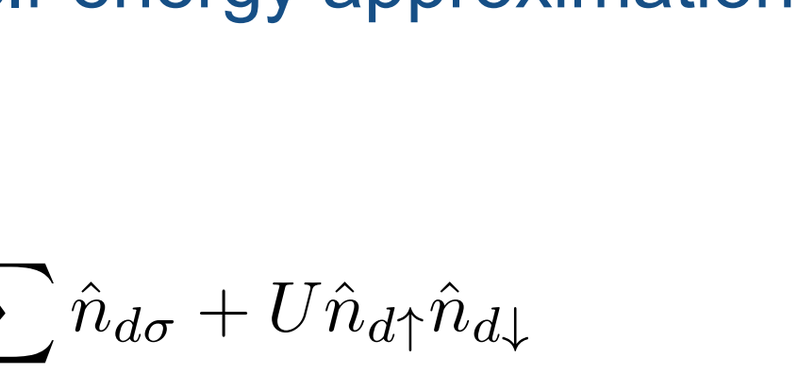
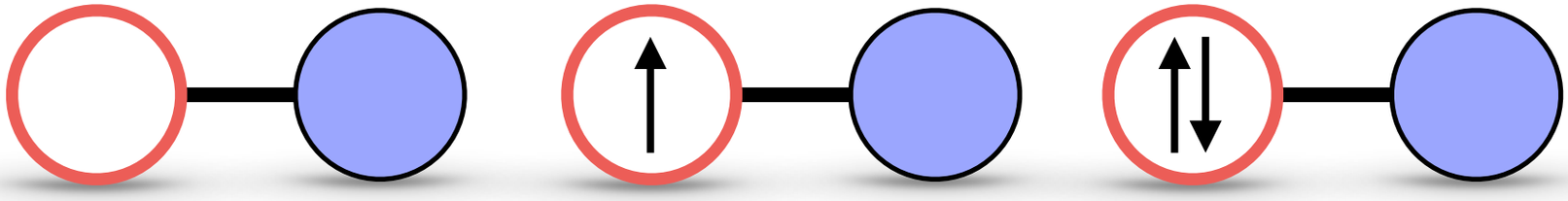
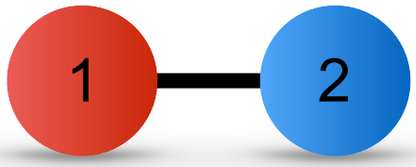
QIM solver

self-consistency loop



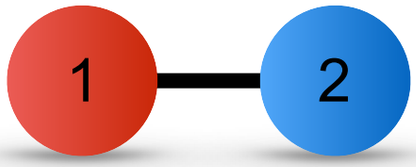




quantum-impurity solver

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

hybridization-expansion CT-QMC



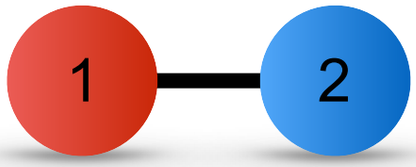
quantum-impurity solver

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)



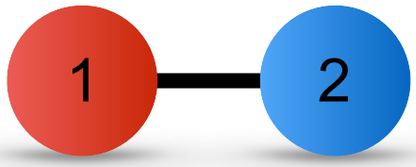
quantum-impurity solver

bath-impurity decoupling

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

$$d^k_{\bar{\boldsymbol{\sigma}},\boldsymbol{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}}) = (t)^{2k}\ {\rm Tr}_{\rm bath}\left(e^{-\beta(\hat{H}_{\rm bath}-\mu\hat{N}_s)}\mathcal{T}\Pi^1_{i=k} c^\dagger_{s\sigma_i}(\tau_i) c_{s\bar{\sigma}_i}(\bar{\tau}_i)\right)/Z_{\rm bath}$$

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



quantum-impurity solver

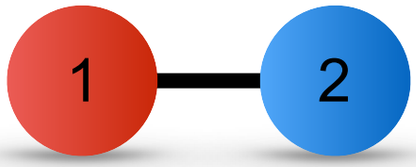
bath-impurity decoupling

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

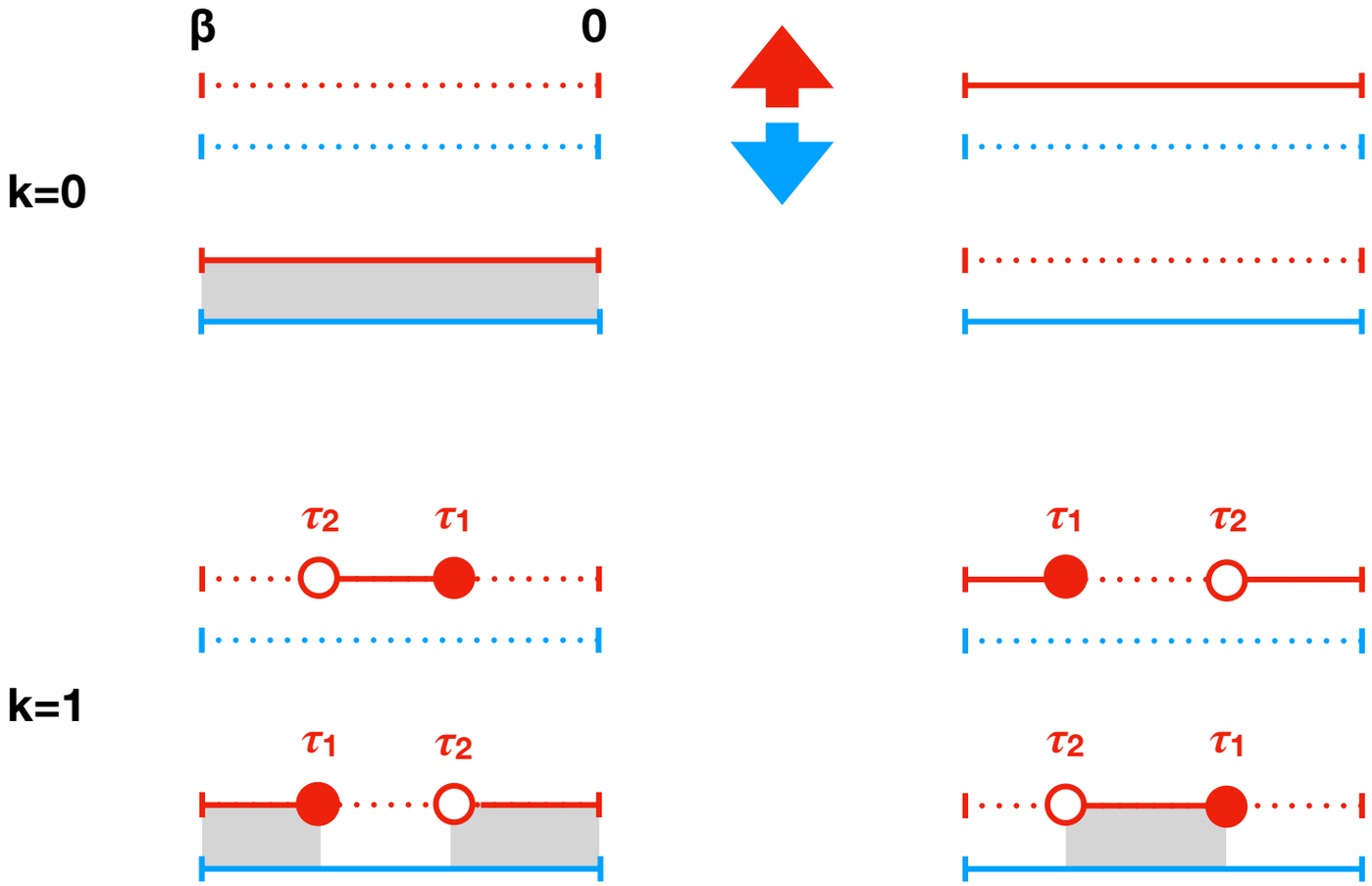
bath $\quad d^k_{\bar{\boldsymbol{\sigma}},\boldsymbol{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}}) = \det\left(F^k_{\bar{\boldsymbol{\sigma}},\boldsymbol{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})\right)$

non-interacting hybridization function

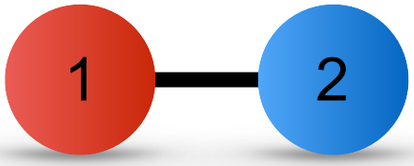
the difficult part: the local trace $\quad t^k_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})$



define configurations



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



quantum-impurity solver

hybridization-expansion CT-QMC

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

configuration *c*: expansion order & segments

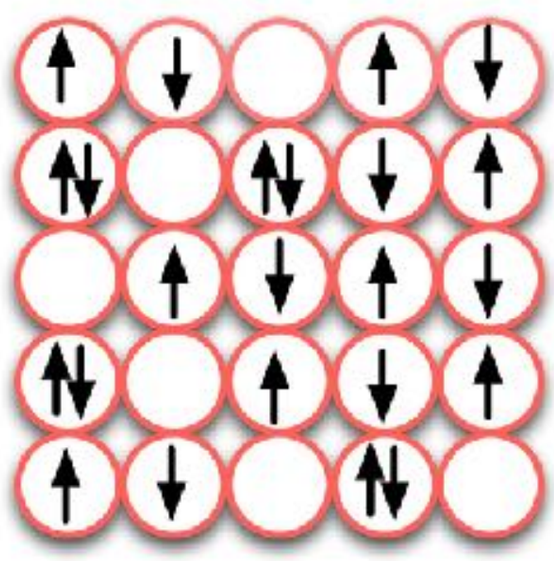
$$w_c = d\boldsymbol{\tau}_c \ d_c \ t_c$$

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

DMFT for the one-band Hubbard model

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

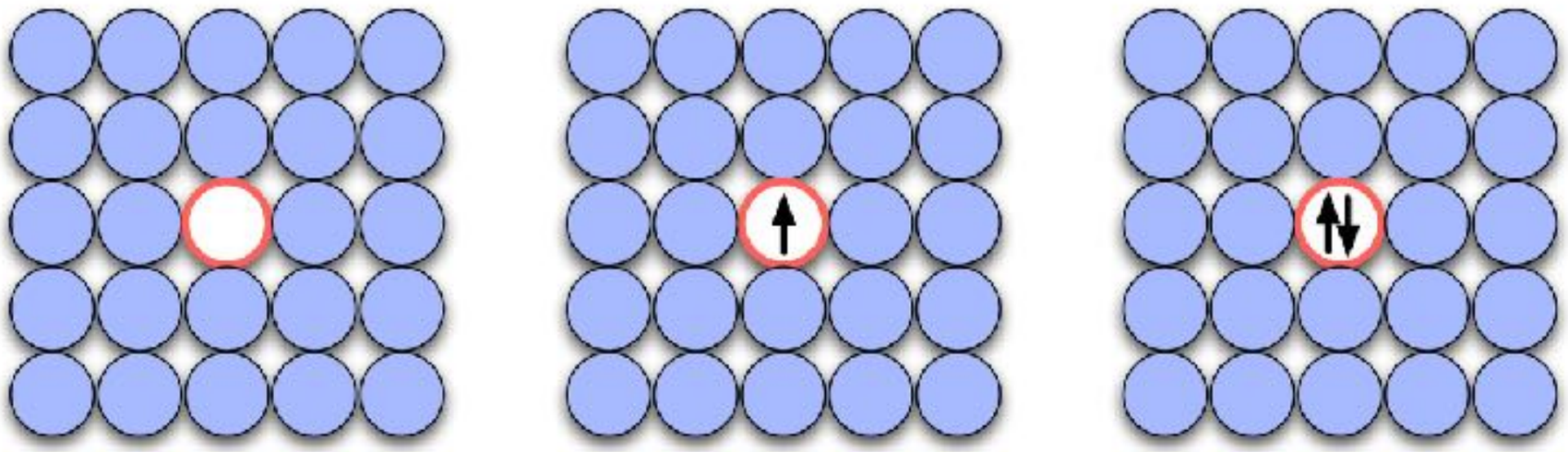
dynamical mean-field theory



$G^{i,j}$

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

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

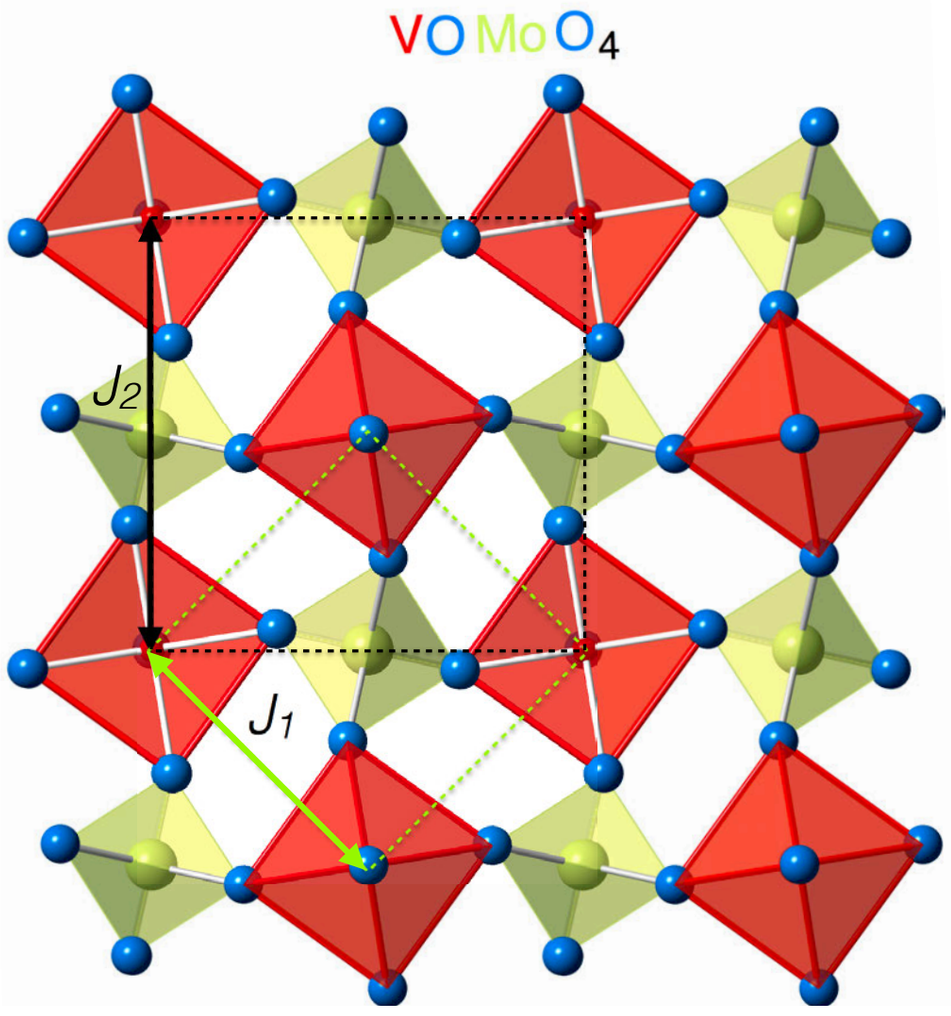
quantum impurity model (QIM)

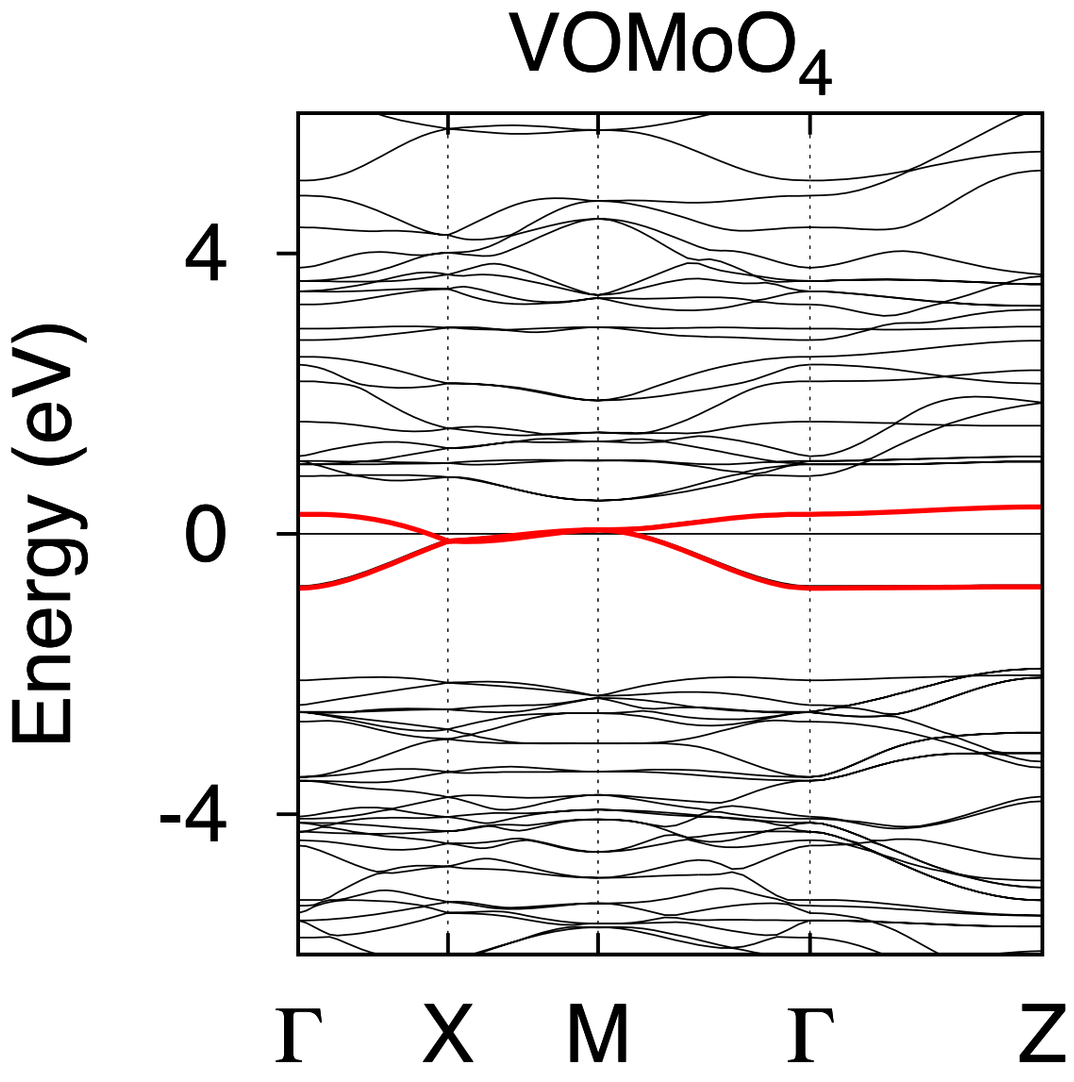
$$\hat{H}^A = \underbrace{\sum_{\boldsymbol{k}\sigma} \varepsilon^s_{\boldsymbol{k}} \hat{n}_{\boldsymbol{k}\sigma}}_{\hat{H}_{\text{bath}}} + \underbrace{\sum_{\boldsymbol{k}\sigma} \left(V^s_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{d\sigma} + \text{h.c.} \right)}_{\hat{H}_{\text{hyb}}}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

QIM solver: **QMC**, ED, NRG, DMRG,…

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

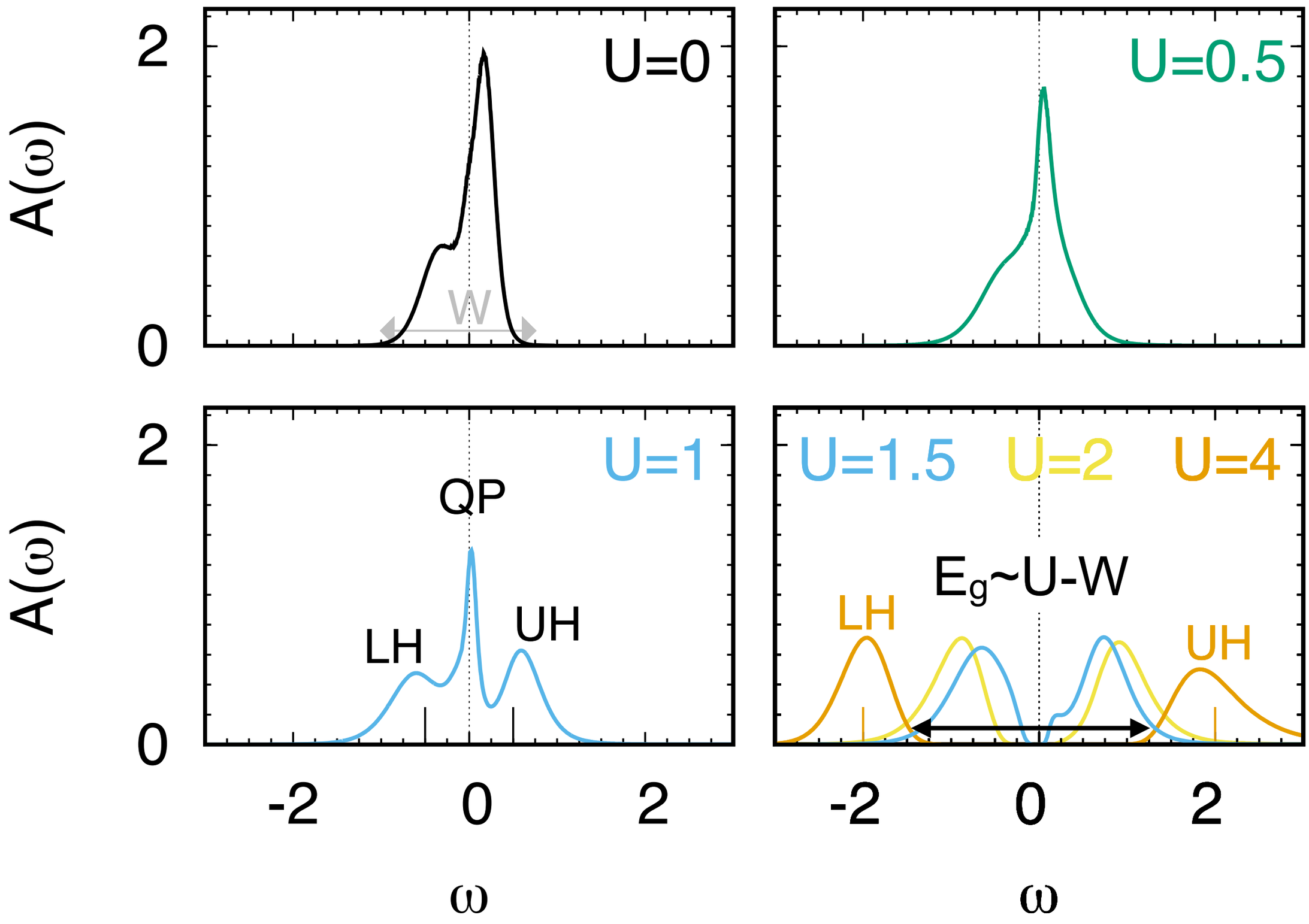
a real-system case: $VOMoO_4$





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

a real-system: $VOMoO_4$



why this cannot be obtained
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

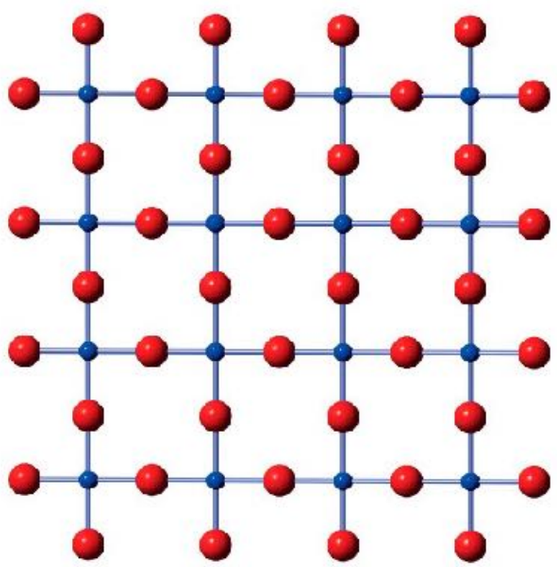
$$\hat{H}_{\mathrm{MF}} = \sum_{\boldsymbol{k}\sigma}\left[\varepsilon_{\boldsymbol{k}} + U\left(\frac{1}{2} - \sigma m\right)\right]\hat{n}_{\boldsymbol{k}\sigma}$$

self-energy

m: magnetization

ferromagnetic Hartree-Fock

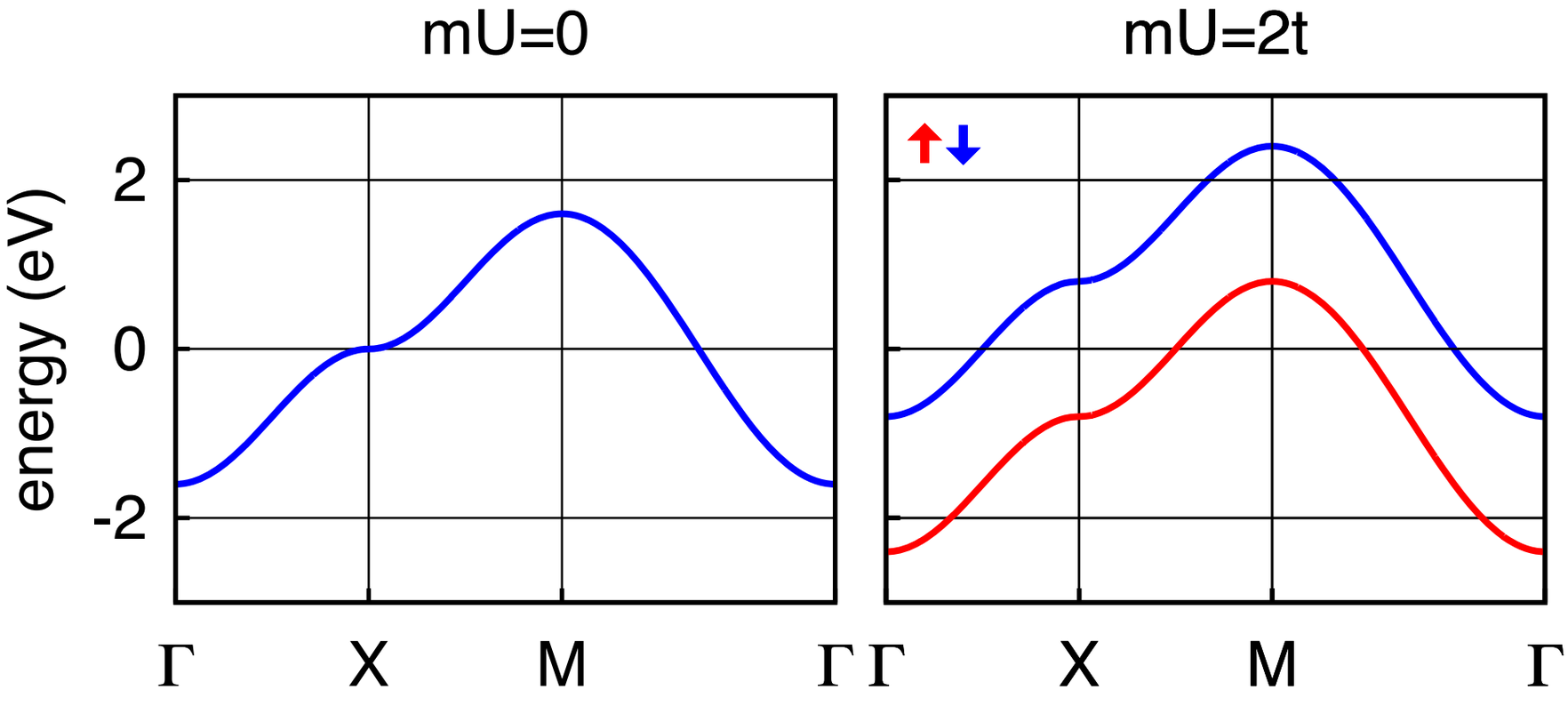
CuO_2



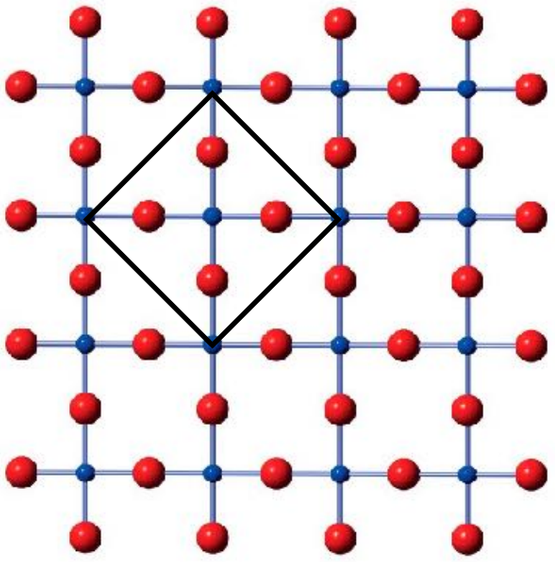
2d-tight binding model

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

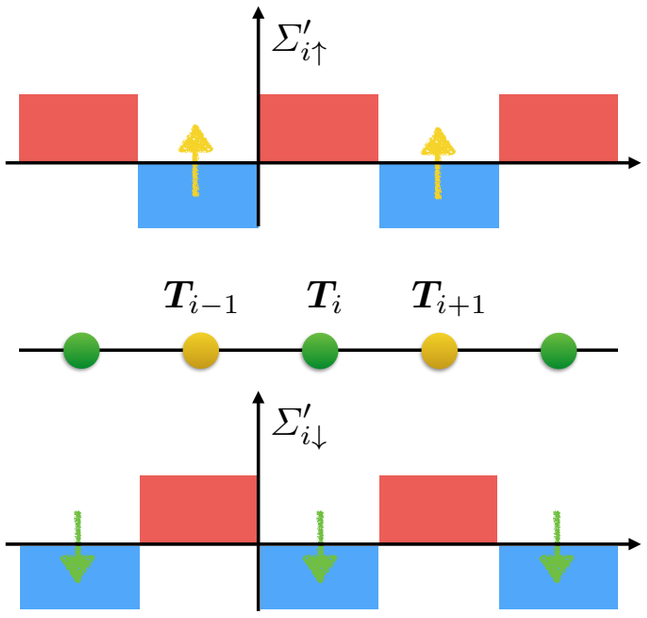
$$\Sigma^{\sigma}(k, i\nu_n) = U\left(\frac{1}{2} - \sigma m\right)$$

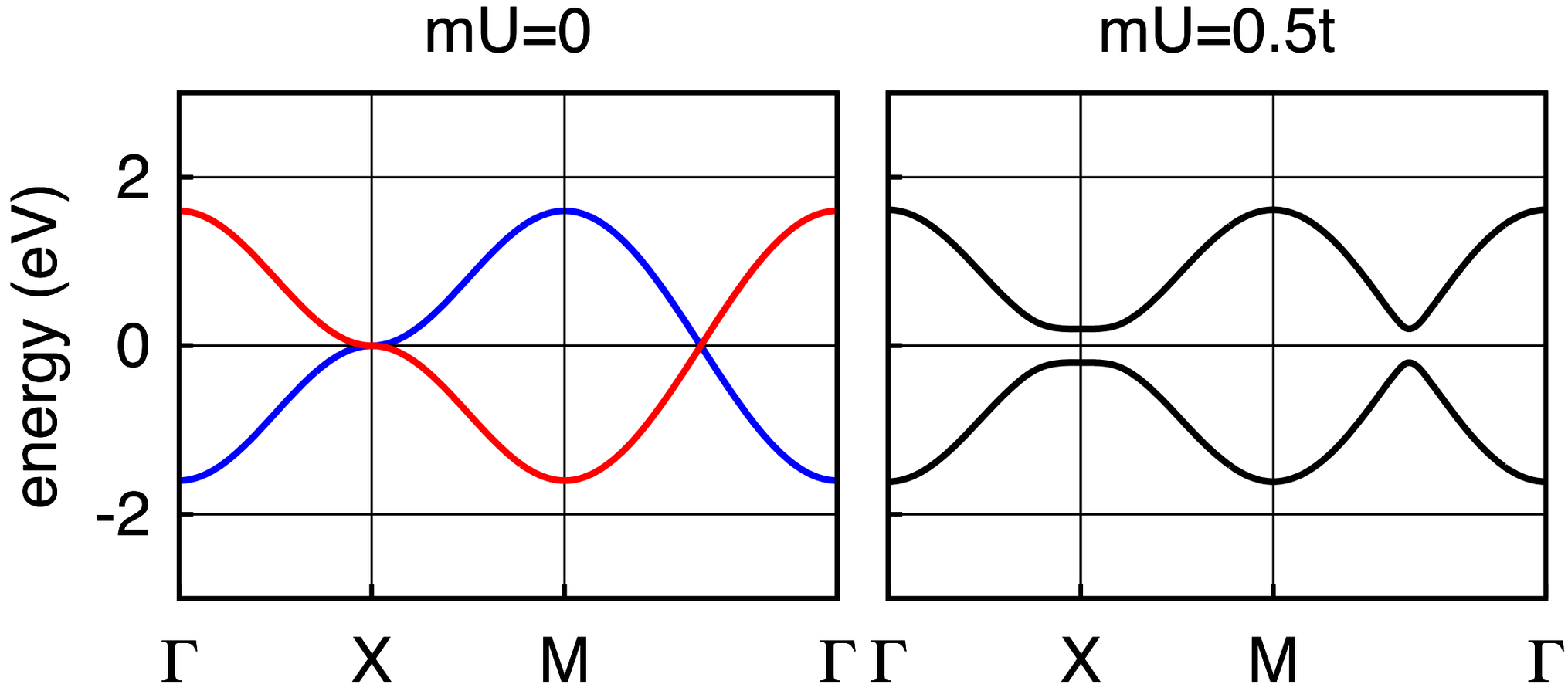


antiferromagnetic case



CuO_2

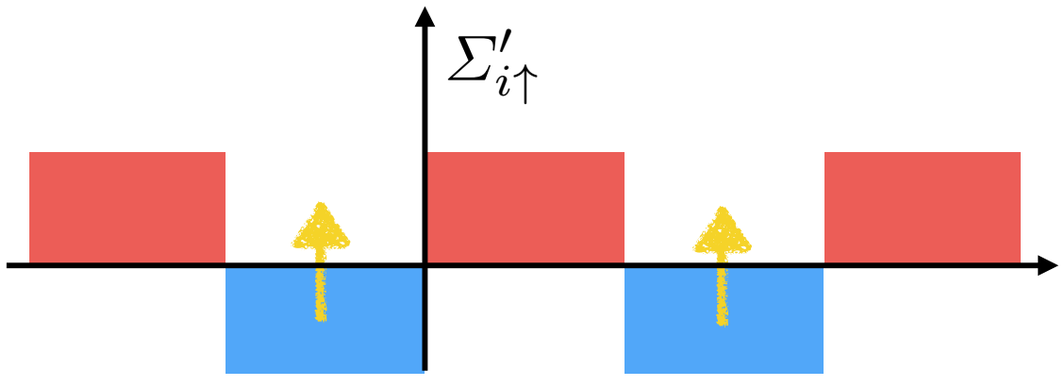


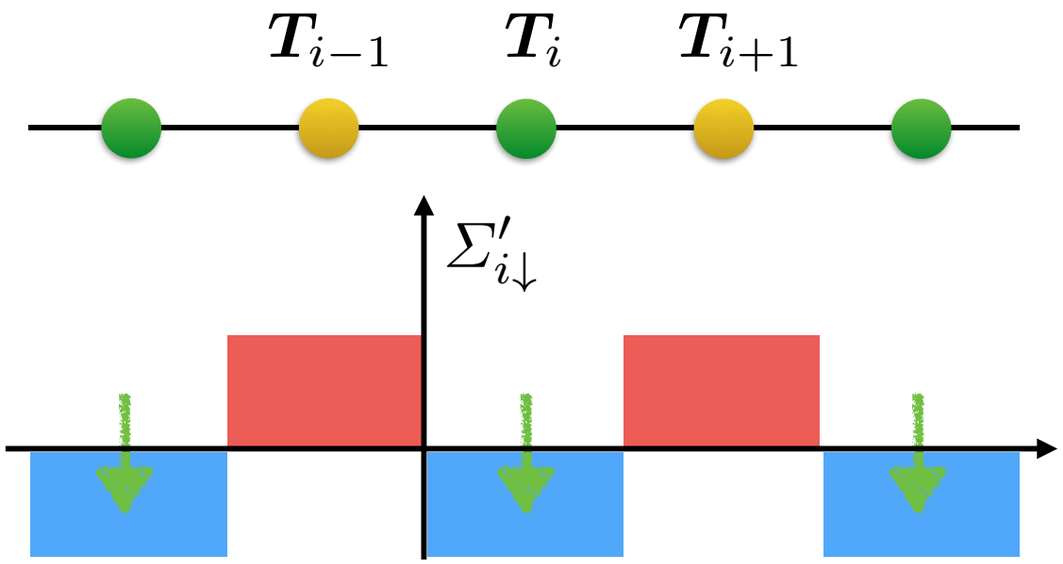


Mott transition: HF vs DMFT

LDA+*U*

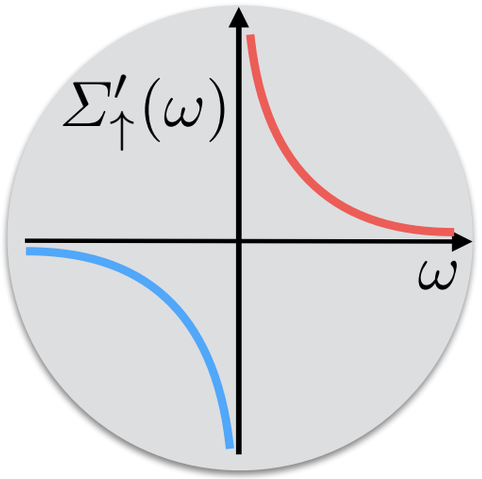
Hartree-Fock

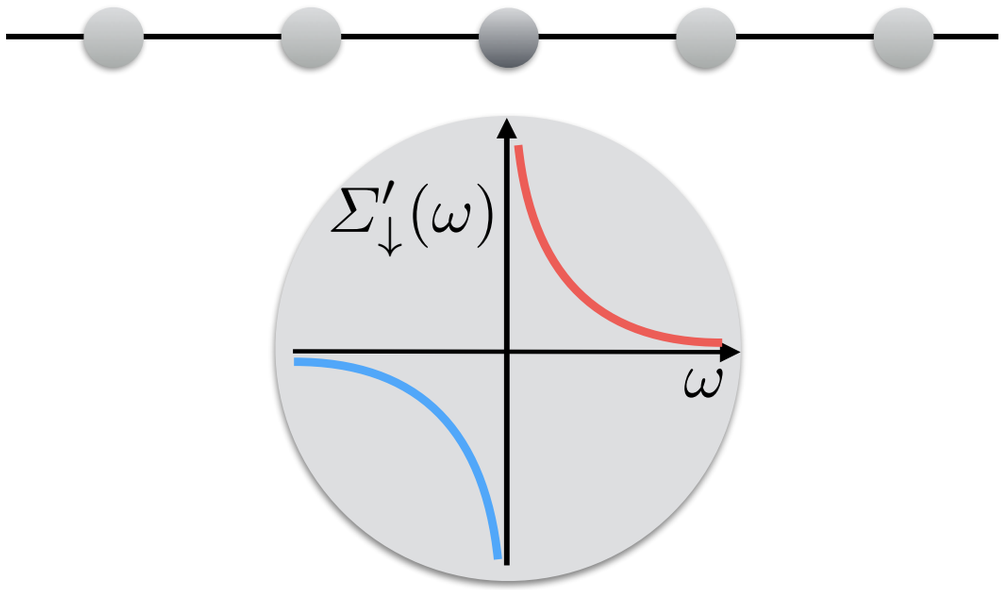




LDA+DMFT

DMFT



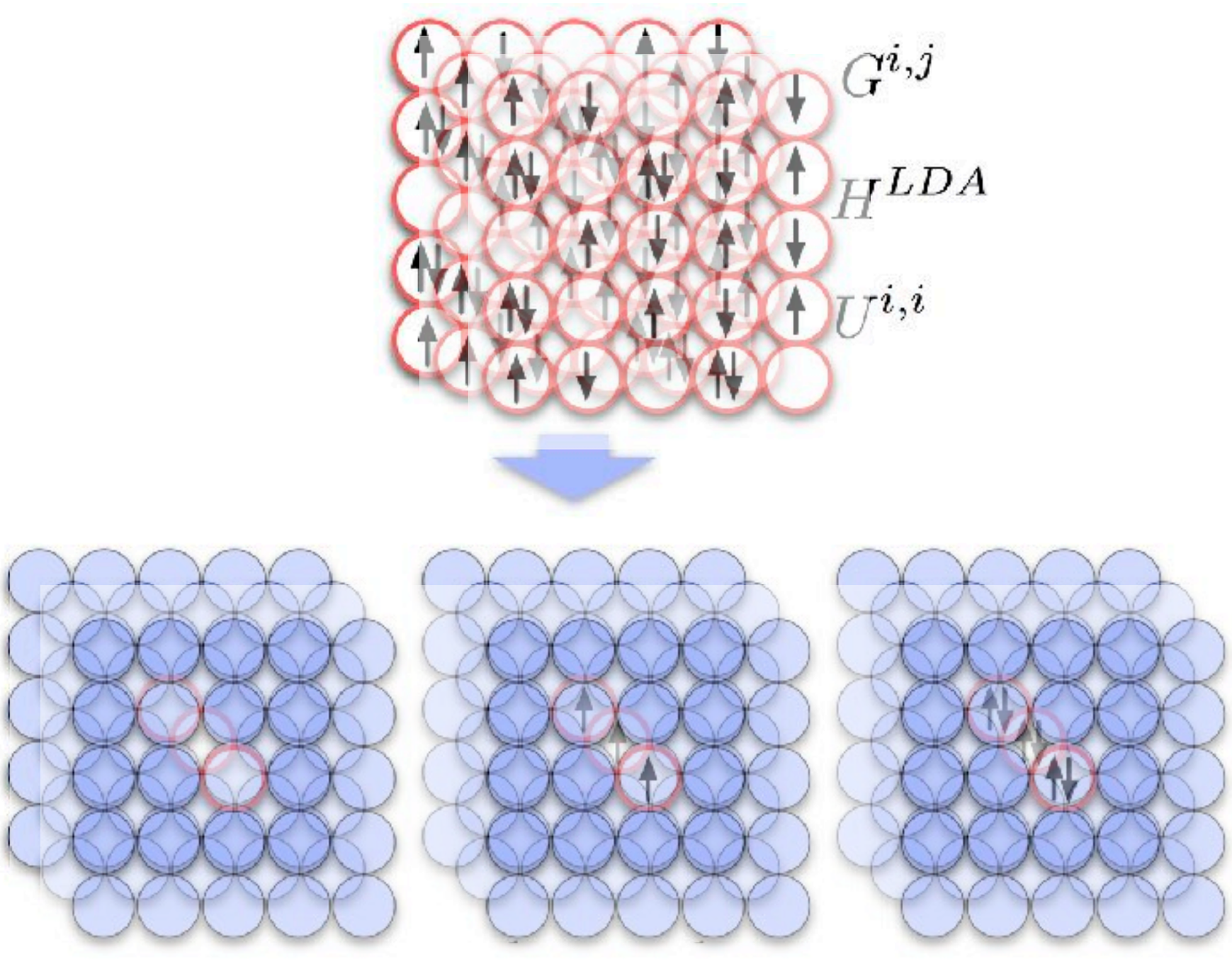


see also my lecture notes in correl17

multi-band Hubbard model

DMFT for multi-band models

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



in theory, more indices

$$H_{\mathbf{k}}^{\mathrm{LDA}} = \begin{pmatrix} H_{\mathbf{k}}^{i_c,i_c} & H_{\mathbf{k}}^{i_c,i'_c} & \cdots \\ H_{\mathbf{k}}^{i'_c,i_c} & H_{\mathbf{k}}^{i'_c,i'_c} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

$$U_{m_\alpha m_\beta m'_\alpha m'_\beta}$$

$$G_{i_c m_\alpha, i'_c m'_\alpha}(i\nu_n) = \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \left[\frac{1}{i\nu_n I - H_{\boldsymbol{k}}^{\mathrm{LDA}} - \Sigma(i\nu_n) + H_{\mathrm{DC}}} \right]_{i_c m_\alpha, i'_c m'_\alpha}$$

$$G_{m_\alpha, m'_\alpha}(i\nu_n) = G_{i_c m_\alpha, i_c m'_\alpha}(i\nu_n)$$
$$\mathcal{G}^{-1}(i\nu_n) = G^{-1}(i\nu_n) + \Sigma^{i_c}(i\nu_n)$$

$\nu_n \rightarrow \tau$ $\quad G(\tau)$

QMC

$G(\tau)$ $\quad \tau \rightarrow \nu_n$

$$\Sigma^{i_c}(i\nu_n) = \mathcal{G}^{-1}(i\nu_n) - G^{-1}(i\nu_n)$$

converged?

NO

$$\Sigma = \begin{pmatrix} \Sigma^{i_c} & 0 & \cdots \\ 0 & \Sigma^{i_c} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

YES

Jolly good show! $\Sigma(i\nu_n)$

You converged $G(i\nu_n)$

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

strongly-correlated systems

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

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

minimal model for a given class of phenomena

as system-specific as possible

build & solve these models

model building

chose the one-electron basis

LDA Wannier(-like) functions

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

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

why LDA Wannier functions?

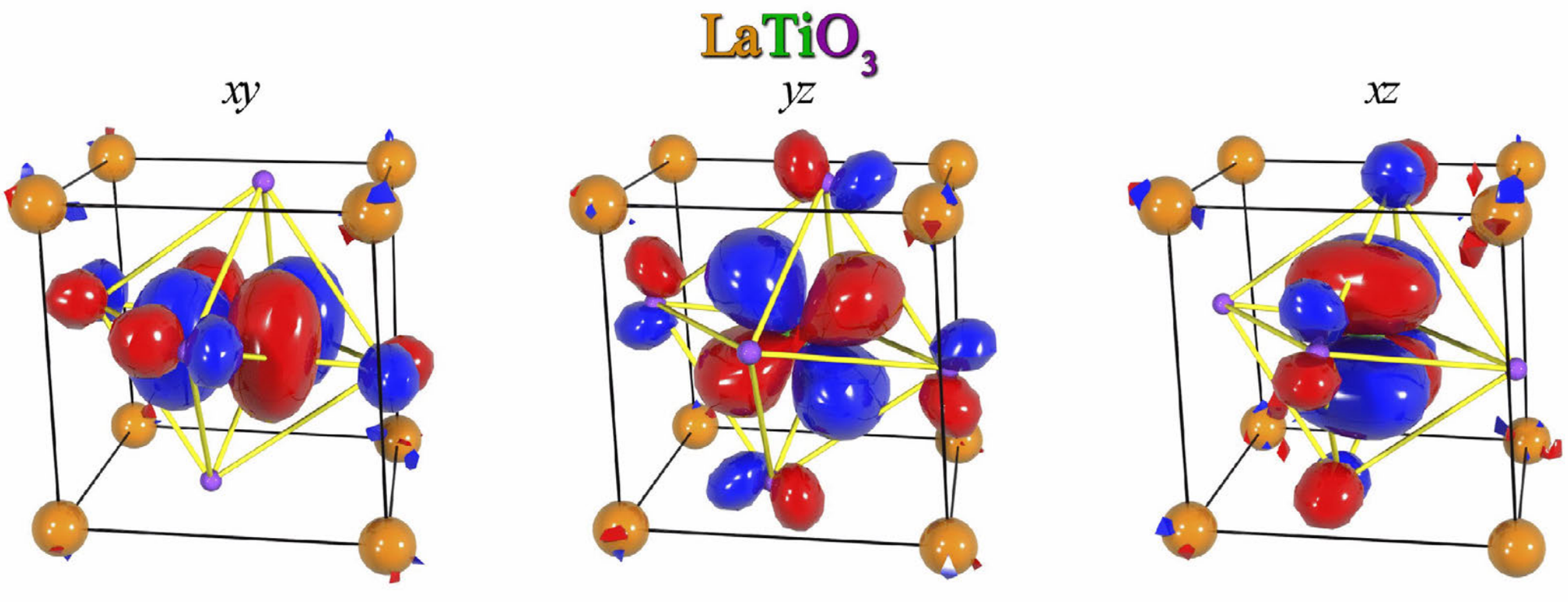
span exactly the one-electron Hamiltonian

can be constructed site-centered & orthogonal & localized

natural basis for **local** Coulomb terms

very good for weakly correlated systems

information on lattice and chemistry

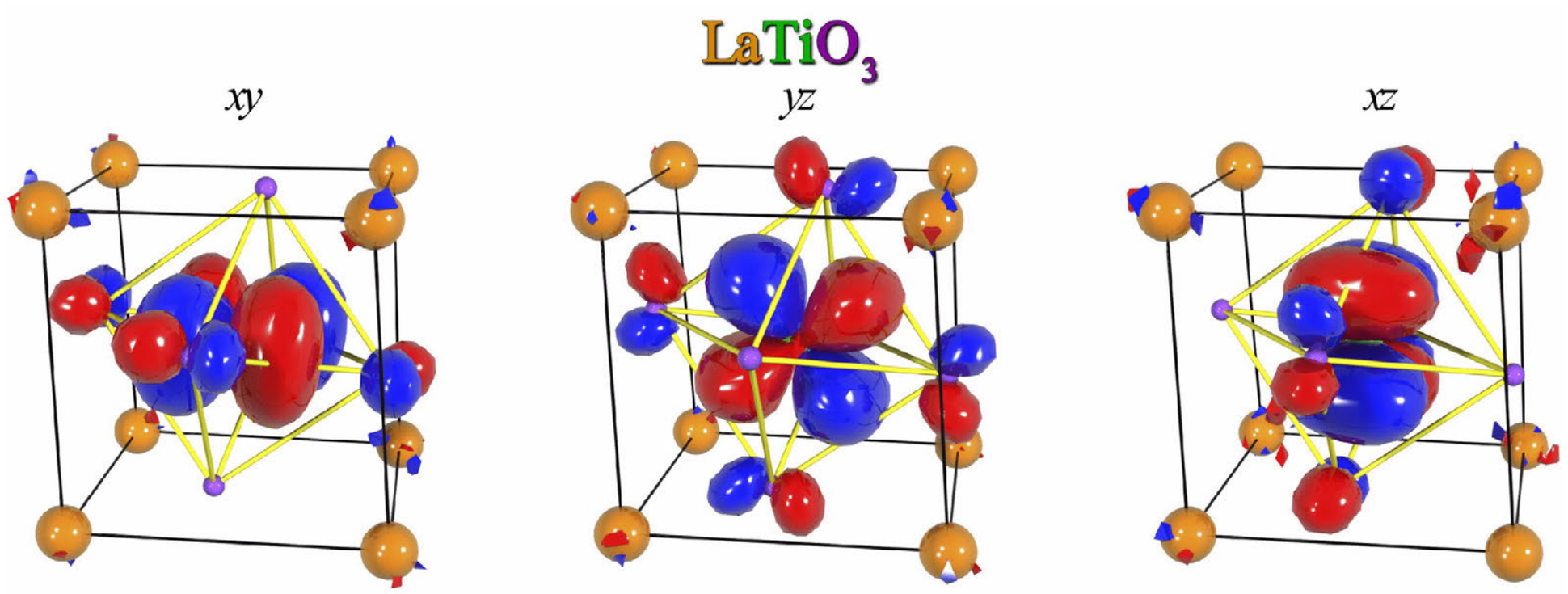


why LDA Wannier functions?

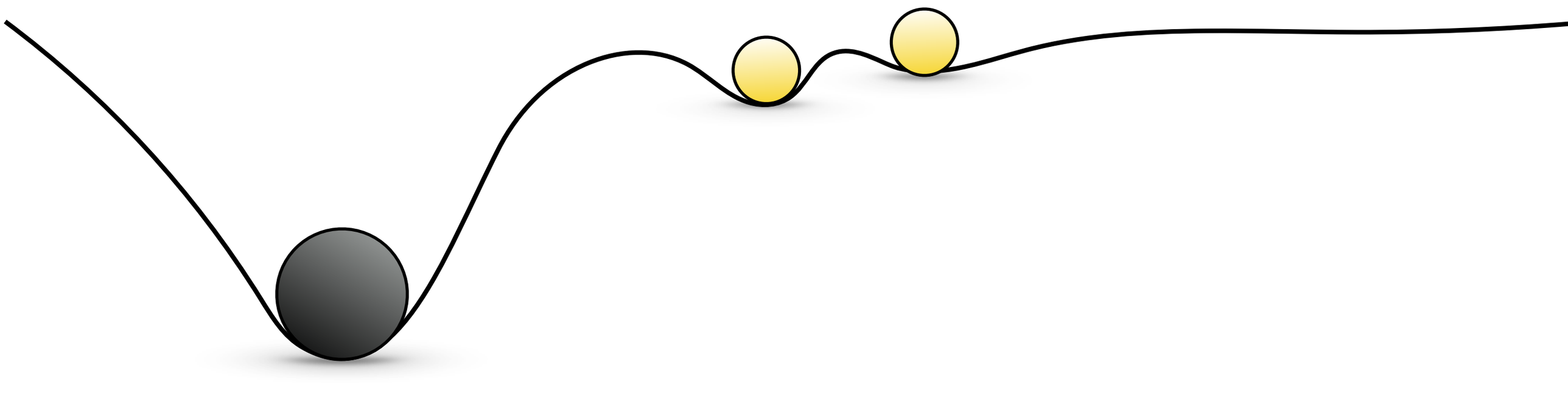
$$\hat{H}_e = \hat{H}_0 + \hat{H}_U \longrightarrow \hat{H}^{\mathrm{LDA}} + \hat{H}_U - \hat{H}_{dc}$$

ΔU

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



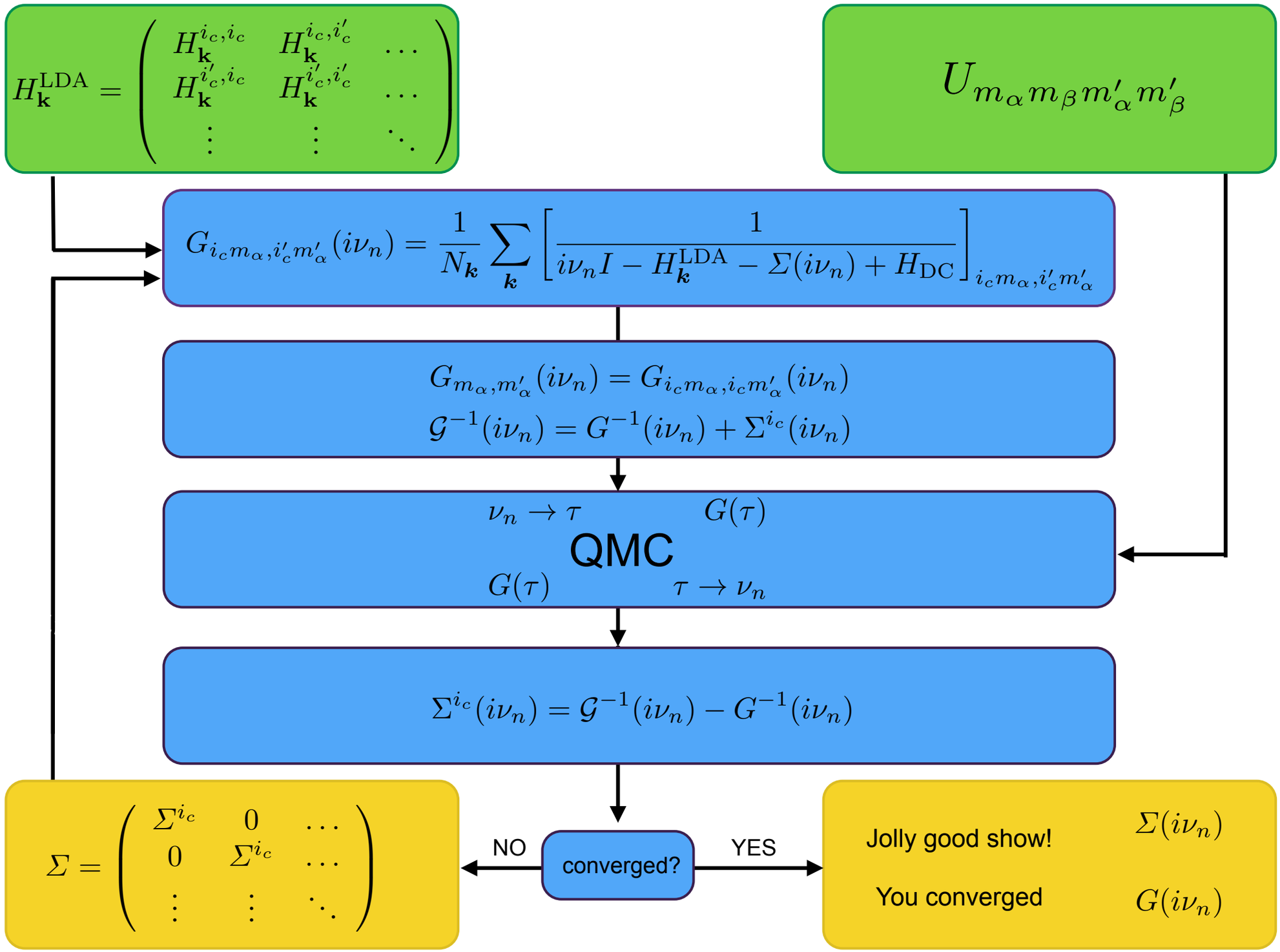
heavy electrons, light electrons



light electrons → DFT (LDA, GGA,…)

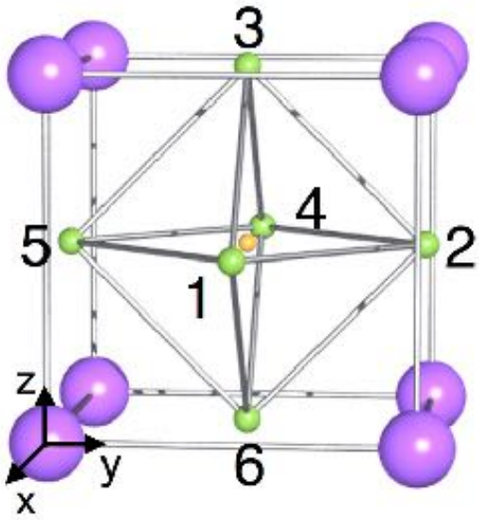
heavy electrons → ΔU correction, DMFT

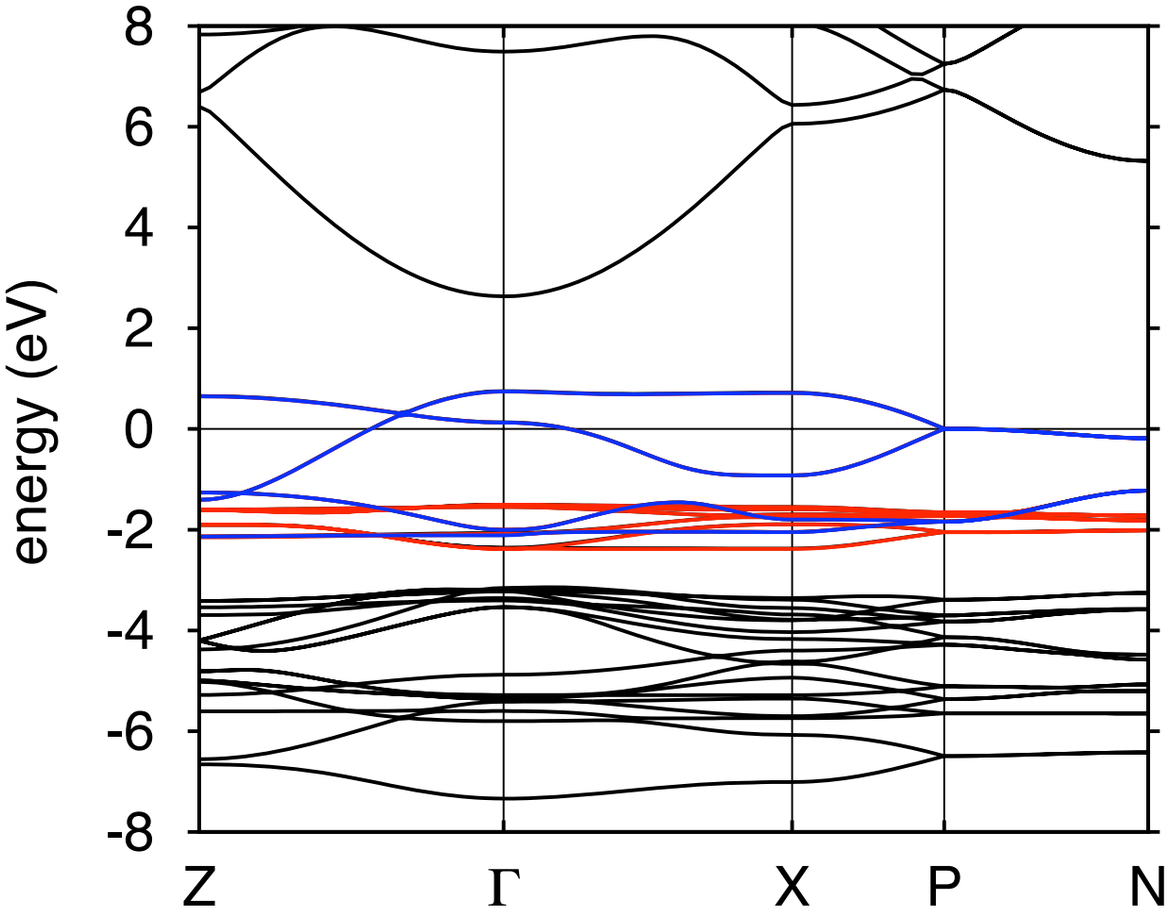
self-consistency loop



to downfold or not to downfold?

$KCuF_3$





e_g

t_{2g}

integrate out light electrons

massive downfolding: no DC correction

around mean-field approximation

$$\hat{H}_U = U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

$$\hat{H}_{\mathrm{DC}} = U \sum_i \left(\hat{n}_{i\uparrow}\bar{n}_{i\downarrow} + \bar{n}_{i\uparrow}\hat{n}_{i\downarrow} - \bar{n}_{i\uparrow}\bar{n}_{i\downarrow} \right)$$

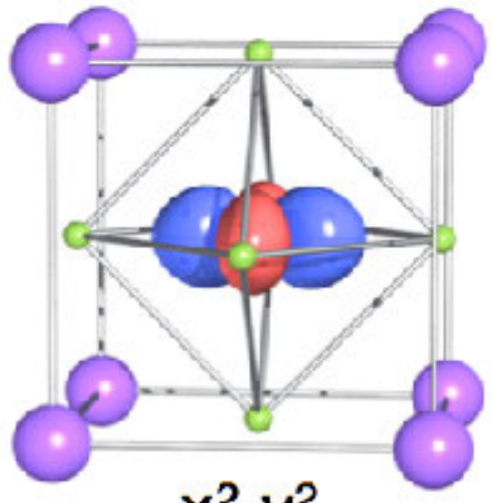
$$\bar{n}_{i\sigma} = n/2$$

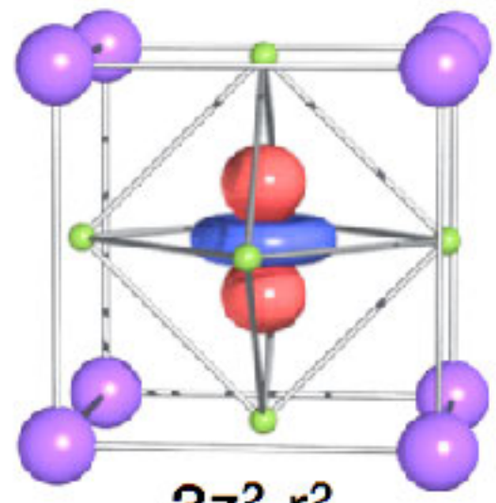
$$\hat{H}_{\mathrm{DC}} = \frac{n}{2} U \sum_i \left(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} - \frac{n}{2} \right) = \delta\mu \hat{N} - \mathrm{const}$$

should we downfold light electrons?

no downfolding

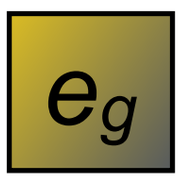
more parameters & H_{DC}

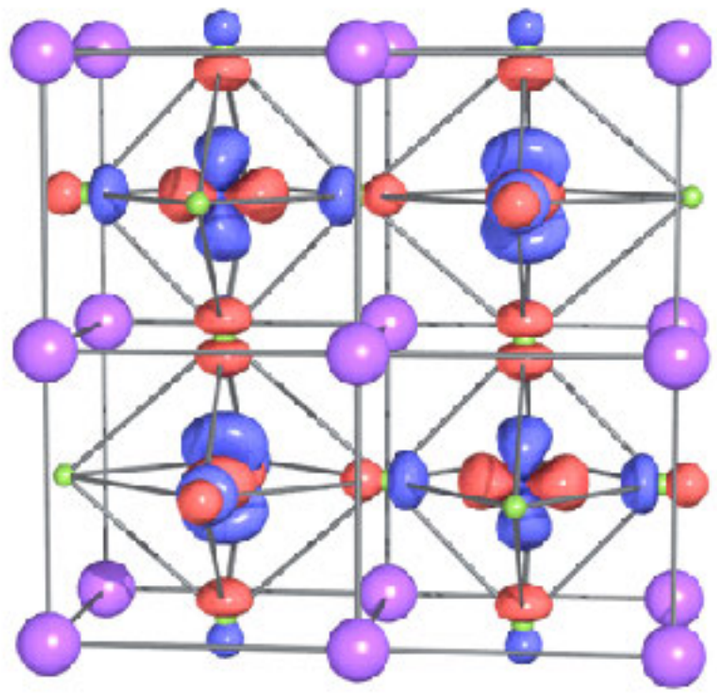




WF more localized

massive downfolding





fewer parameters & no H_{DC}

WF less localized

how important is the basis 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

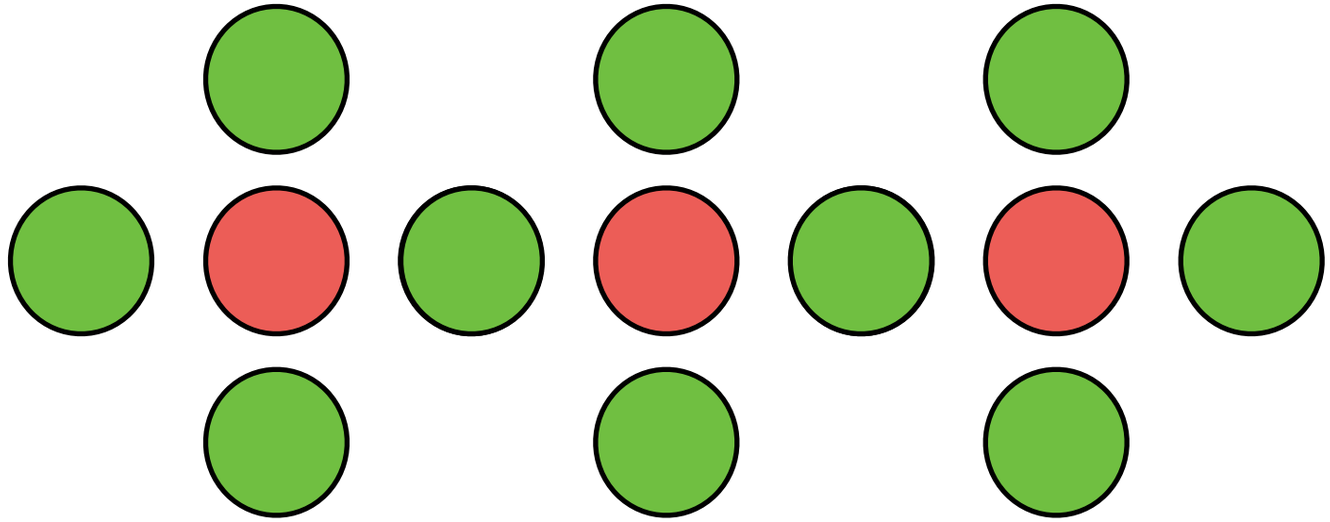
$$U^{iji'j'}_{np\,n'p'} = \int d\mathbf{r}_1 \int d\mathbf{r}_2\, \overline{\psi_{in\sigma}}(\mathbf{r}_1)\overline{\psi_{jp\sigma'}}(\mathbf{r}_2)\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\psi_{j'p'\sigma'}(\mathbf{r}_2)\psi_{i'n'\sigma}(\mathbf{r}_1).$$

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

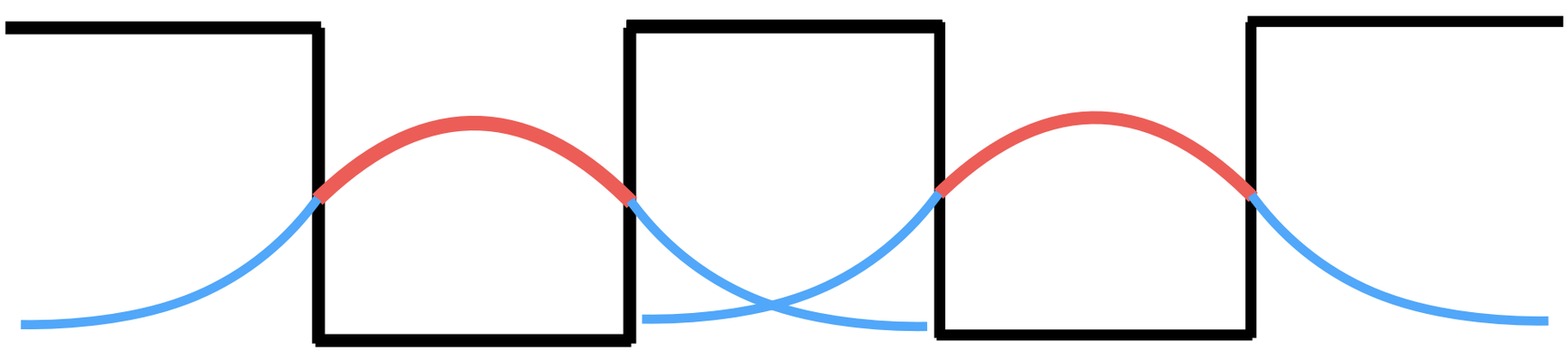
$$U^{iji'j'}_{mp\,m'p'} \propto \frac{\delta_{i,i'}\delta_{j,j'}}{|\boldsymbol{T}_i - \boldsymbol{T}_j|},$$

extreme localization

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

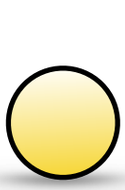


methods based on space tiling functions inside the sphere?



screening effects

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



light electrons → DFT (LDA, GGA,…)

heavy electrons → ΔU correction, DMFT

screening: **approximate** schemes such as cRPA, cLDA

LDA+DMFT

$$H_{\mathbf{k}}^{\mathrm{LDA}} = \begin{pmatrix} H_{\mathbf{k}}^{i_c,i_c} & H_{\mathbf{k}}^{i_c,i'_c} & \cdots \\ H_{\mathbf{k}}^{i'_c,i_c} & H_{\mathbf{k}}^{i'_c,i'_c} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

$$U_{m_\alpha m_\beta m'_\alpha m'_\beta}$$

$$G_{i_c m_\alpha, i'_c m'_\alpha}(i\nu_n) = \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \left[\frac{1}{i\nu_n I - H_{\boldsymbol{k}}^{\mathrm{LDA}} - \Sigma(i\nu_n) + H_{\mathrm{DC}}} \right]_{i_c m_\alpha, i'_c m'_\alpha}$$

$$G_{m_\alpha, m'_\alpha}(i\nu_n) = G_{i_c m_\alpha, i_c m'_\alpha}(i\nu_n)$$
$$\mathcal{G}^{-1}(i\nu_n) = G^{-1}(i\nu_n) + \Sigma^{i_c}(i\nu_n)$$

$\nu_n \rightarrow \tau$ $\quad G(\tau)$

QMC

$G(\tau)$ $\quad \tau \rightarrow \nu_n$

$$\Sigma^{i_c}(i\nu_n) = \mathcal{G}^{-1}(i\nu_n) - G^{-1}(i\nu_n)$$

converged?

NO

$$\Sigma = \begin{pmatrix} \Sigma^{i_c} & 0 & \cdots \\ 0 & \Sigma^{i_c} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

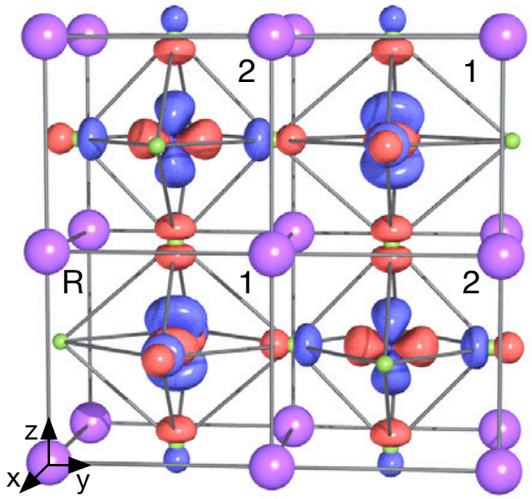
YES

Jolly good show! $\quad \Sigma(i\nu_n)$

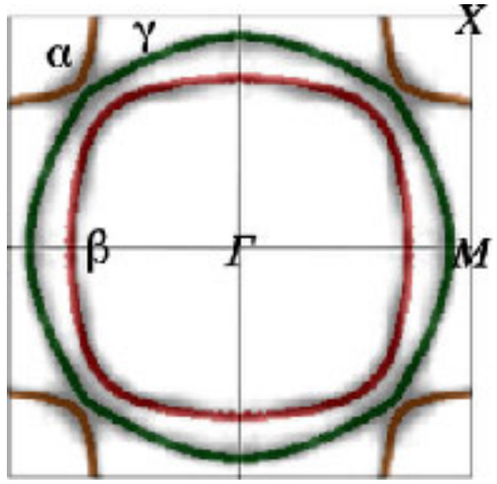
You converged $\quad G(i\nu_n)$

what can we be done?

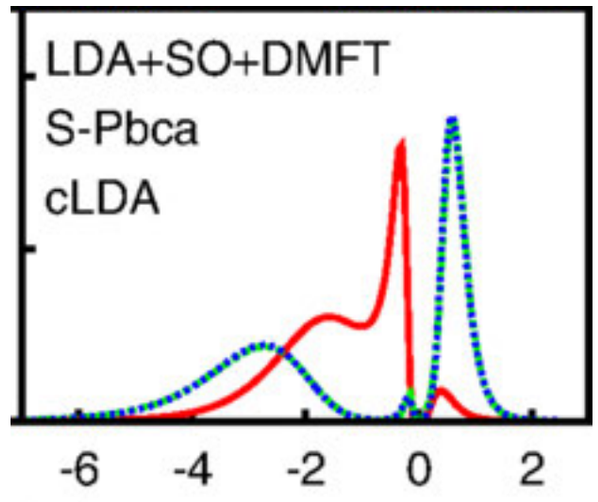
orbital order



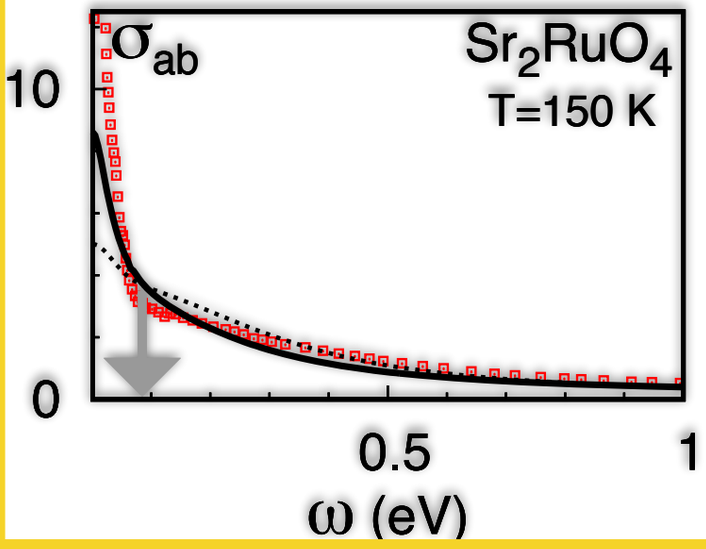
Fermi surface



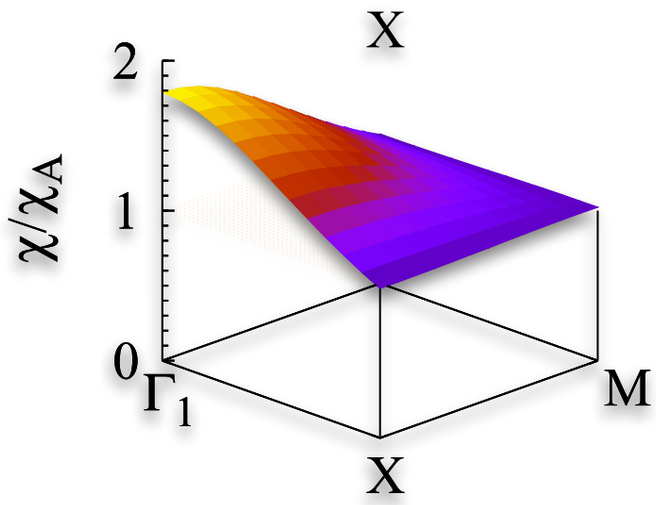
spin-orbit



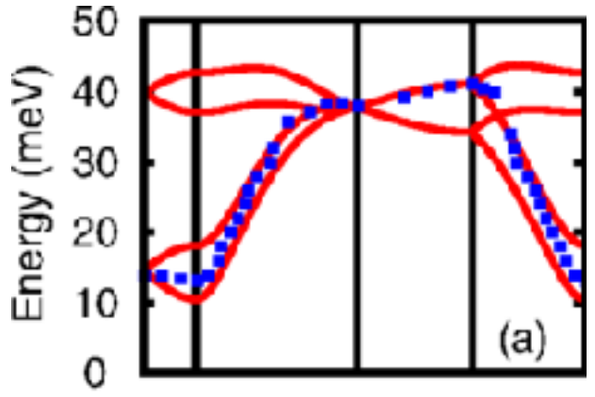
conductivity



response functions



spin waves



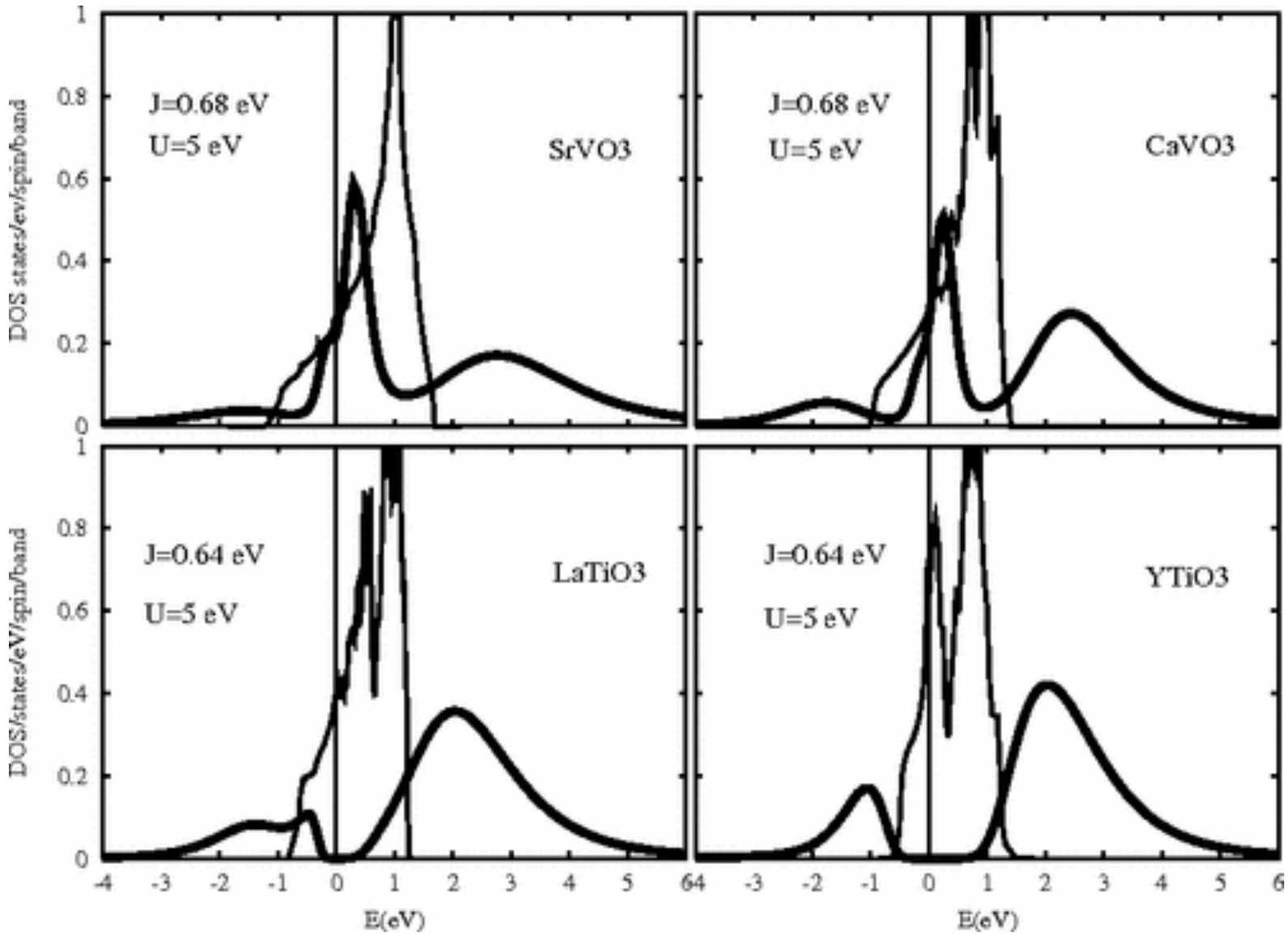
do we need it ?

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]



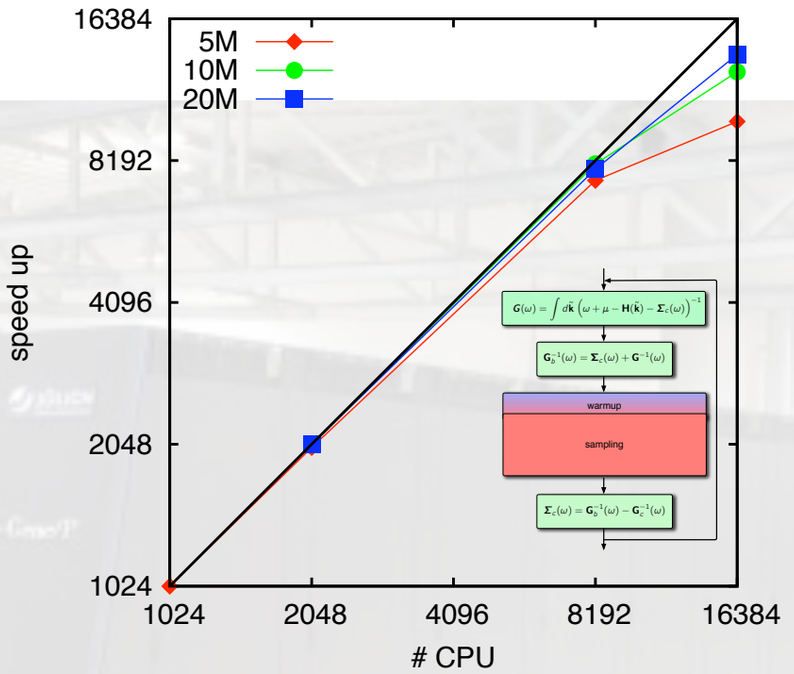
t_{2g}^1

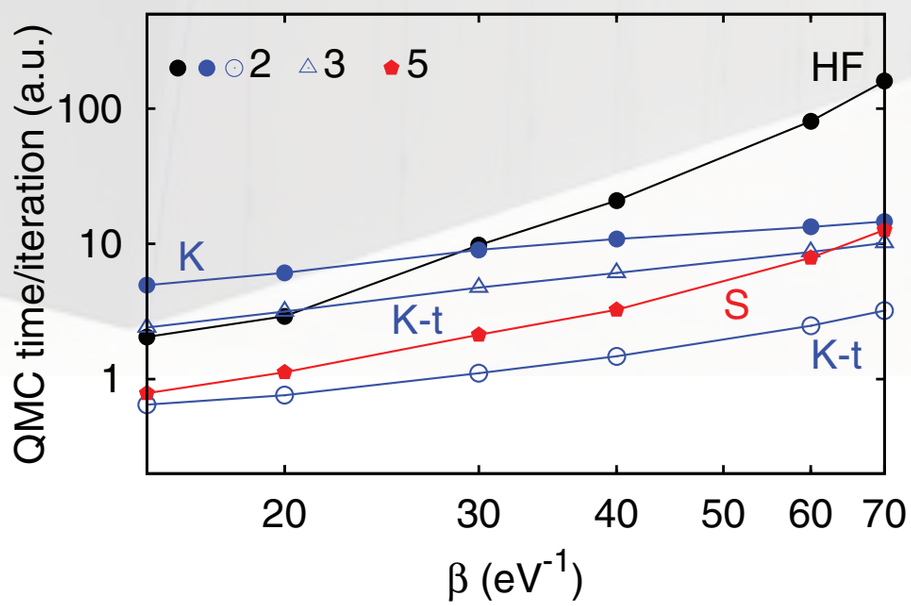
Δ=200-300 meV

a small crystal field plays a key role

our DMFT codes for materials

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





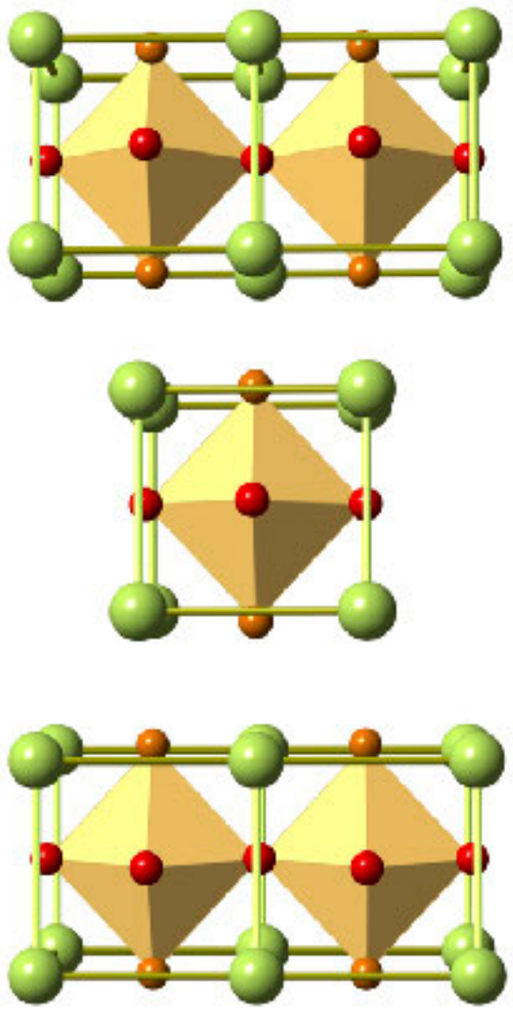
DMFT and cDMFT

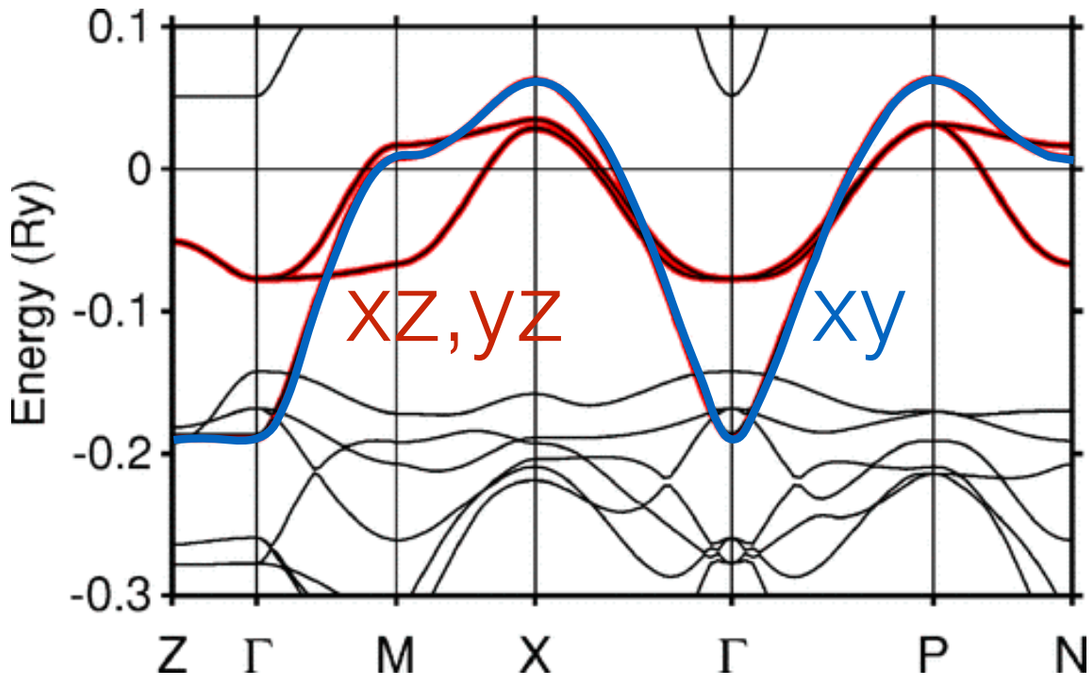
quantum impurity solvers:

general HF QMC
general CT-INT QMC
general CT-HYB QMC

an example:
Sr_2RuO_4
and its Fermi surface

the case of Sr_2RuO_4



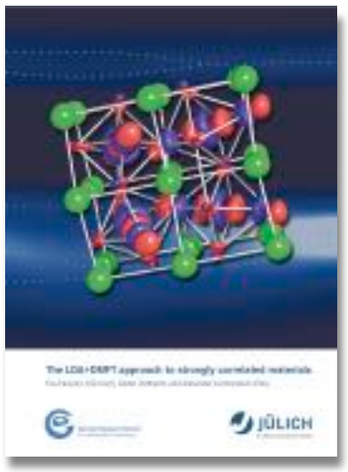


G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)

t_{2g} or e_g only models

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

QI size: 3x3



$$\hat{H} = -\sum_{\sigma} \sum_{i \neq i'} \sum_{mm'} t^{i,i'}_{m,m'}\, c^\dagger_{im\sigma} c_{i'm'\sigma}$$

$$+ U \sum_{i\ m} \hat{n}_{im\uparrow} \hat{n}_{im\downarrow} + \frac{1}{2} \sum_{\substack{i\sigma\sigma' \\ m \neq m'}} \left(U - 2J - J\delta_{\sigma,\sigma'}\right) \hat{n}_{im\sigma} \hat{n}_{im'\sigma'}$$

$$- J \sum_{i\ m \neq m'} \left(c^\dagger_{im\uparrow} c^\dagger_{im\downarrow} c_{im'\uparrow} c_{im'\downarrow} + c^\dagger_{im\uparrow} c_{im\downarrow} c^\dagger_{im'\downarrow} c_{im'\uparrow} \right)$$

derivation: www.cond-mat.de/events/correl11/manuscripts/pavarini.pdf

however, spin-orbit interaction important

QI size: 6x6

$$H = -\sum_{ii'}\sum_{mm'}\sum_{\sigma\sigma'} t^{i,i'}_{m\sigma,m'\sigma'} c^{\dagger}_{im\sigma} c_{i'm'\sigma'}$$

$$+\frac{1}{2}\sum_{i}\sum_{mm'pp'}\sum_{\sigma\sigma'} U_{mm'pp'} c^{\dagger}_{im\sigma} c^{\dagger}_{im'\sigma'} c_{ip'\sigma'} c_{ip\sigma}$$

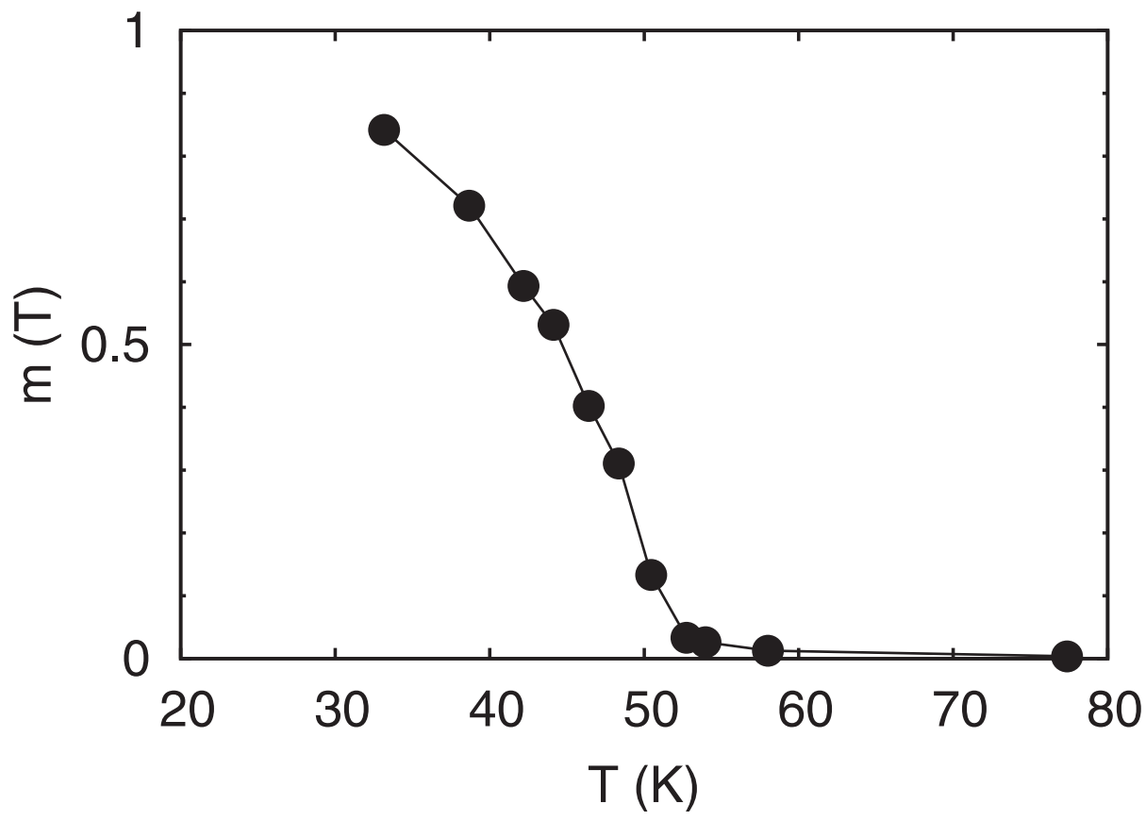
local spin-orbit interaction

$$H_{\mathrm{SO}} = \sum_{i\mu} H^{i\mu}_{\mathrm{SO}} = \sum_{i\mu}\sum_{m\sigma m'\sigma'} \lambda^{i}_{\mu} \xi^{i\mu}_{m\sigma m'\sigma'} c^{\dagger}_{im\sigma} c_{im'\sigma'}$$

with SO, everything more difficult

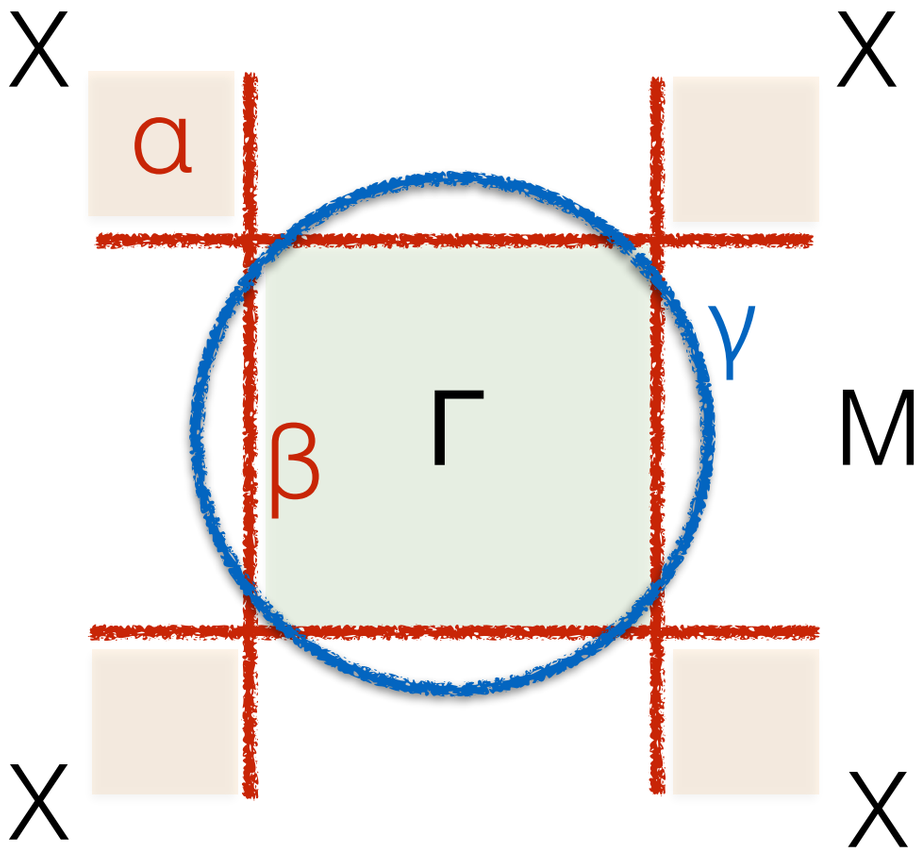
larger (6x6) Green function matrices, QMC sign problem

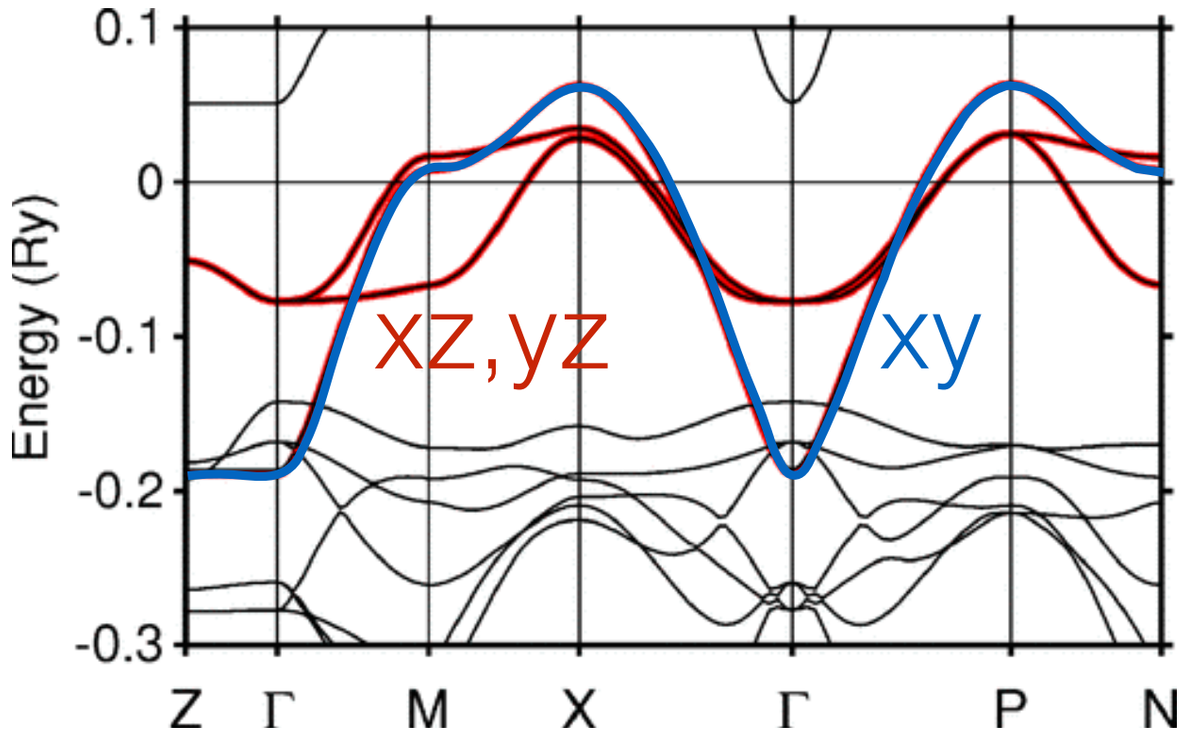
basis that diagonalizes on-site Hamiltonian/Green function
reduces sign problem



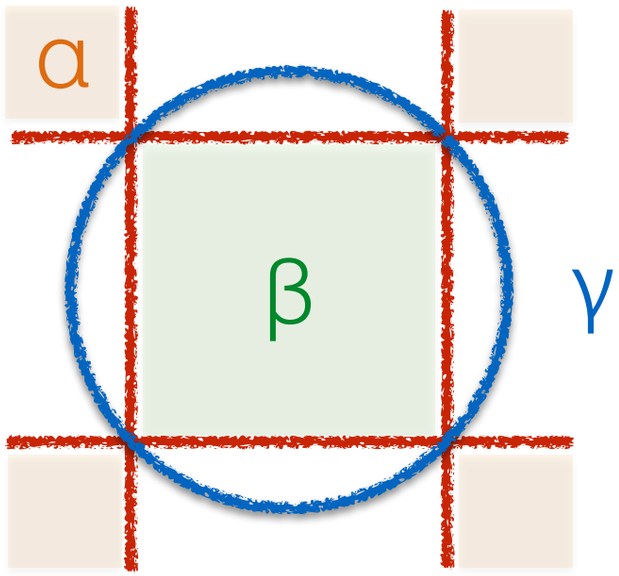
A. Flesch *et al.,* Phys. Rev. B **87**, 195141 (2013)

Fermi surface Sr_2RuO_4





DMFT — Fermi surface Sr_2RuO_4



$$\hat{\varepsilon} = \begin{pmatrix} \varepsilon_{xy} & 0 & 0 & 0 & \frac{\lambda_{xy}}{2} & \frac{i\lambda_{xy}}{2} \\ 0 & \varepsilon_{yz} & -\frac{i\lambda_z}{2} & -\frac{\lambda_{xy}}{2} & 0 & 0 \\ 0 & \frac{i\lambda_z}{2} & \varepsilon_{xz} & -\frac{i\lambda_{xy}}{2} & 0 & 0 \\ 0 & -\frac{\lambda_{xy}}{2} & \frac{i\lambda_{xy}}{2} & \varepsilon_{xy} & 0 & 0 \\ \frac{\lambda_{xy}}{2} & 0 & 0 & 0 & \varepsilon_{yz} & \frac{i\lambda_z}{2} \\ -\frac{i\lambda_{xy}}{2} & 0 & 0 & 0 & -\frac{i\lambda_z}{2} & \varepsilon_{xz} \end{pmatrix}$$

effective crystal-field

$\varepsilon_{CF}=\varepsilon_{xz/yz}-\varepsilon_{xy}>0$

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

effective spin-orbit coupling

λ_{xy} λ_z

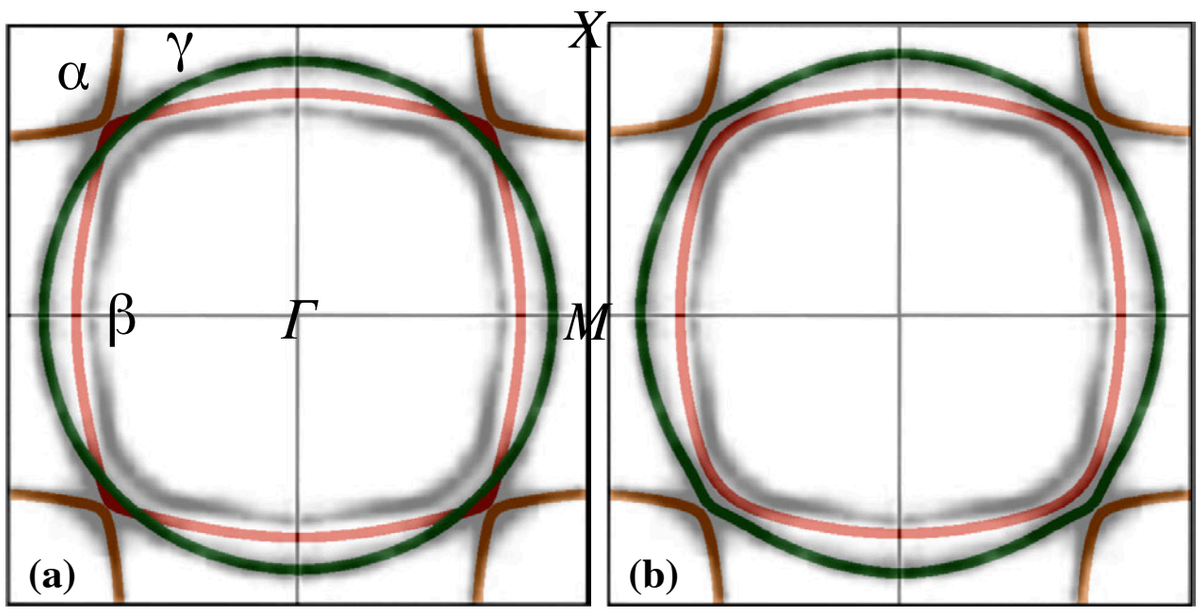
$\lambda \rightarrow \lambda + \Delta\lambda$

Σ(0) changes local Hamiltonian

the LDA+DMFT Fermi surface

LDA

ε_{CF}



LDA+SO

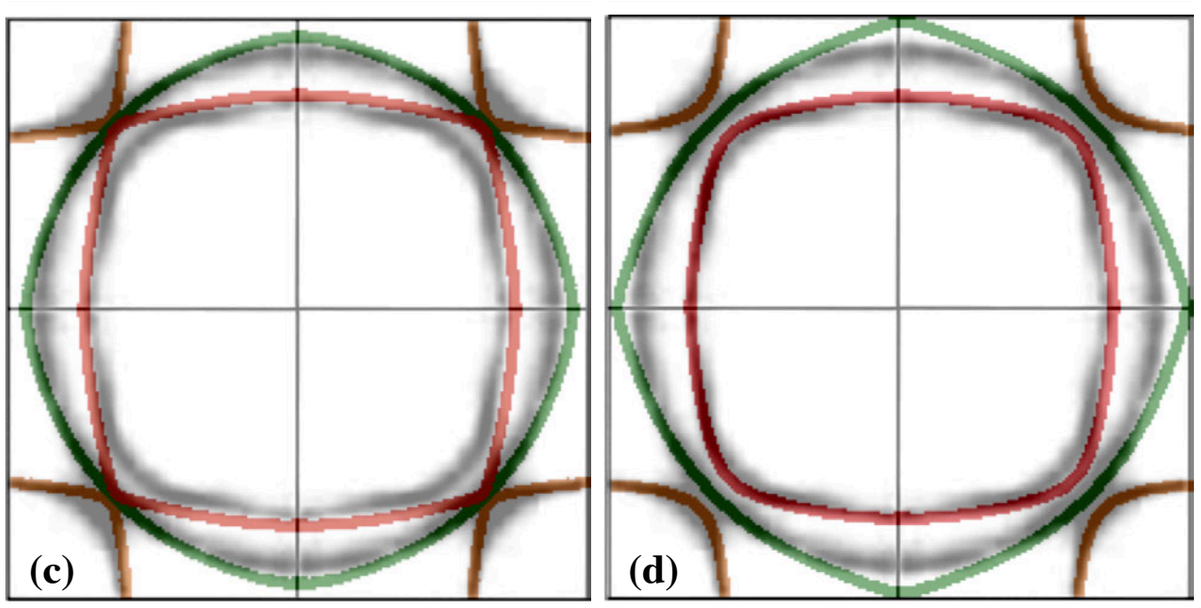
λ

LDA+DMFT

ε_{CF}

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

$\sim 2\varepsilon_{CF}$



LDA+SO+DMFT

λ

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

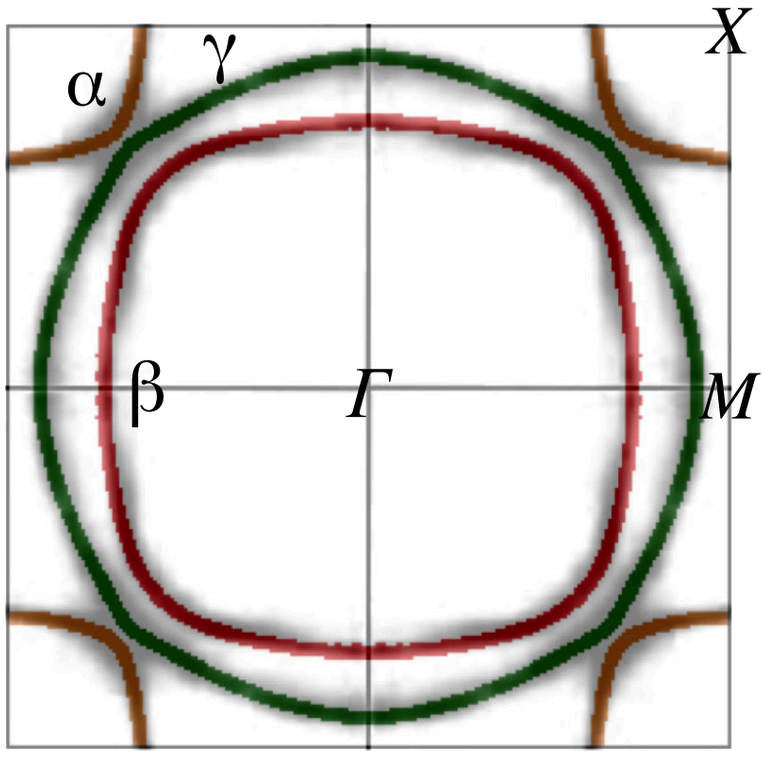
G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)

? 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

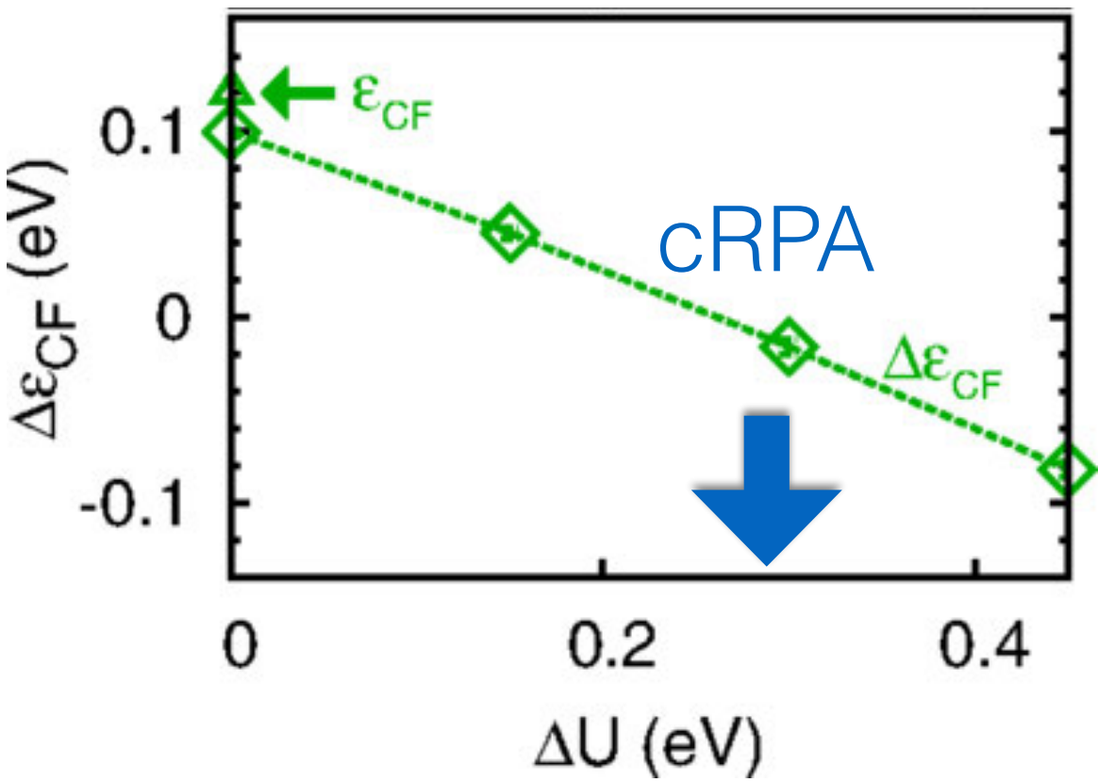
$\varepsilon_{CF} + \Delta' \varepsilon_{CF} \sim \varepsilon_{CF}$



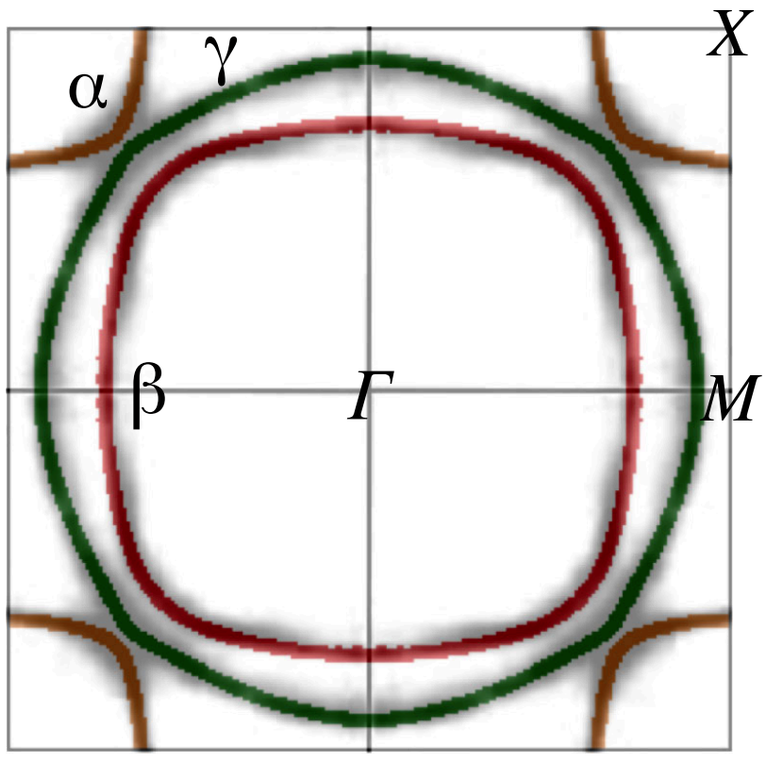
G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)

reduced crystal-field enhancement

- **D_{4h} Coulomb term reduces crystal-field enhancement**



$\Delta U = U_{xy,xy} - U_{xz,xz}$



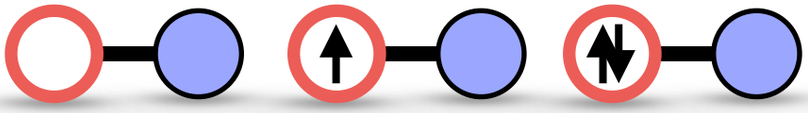
$\varepsilon_{CF} + \Delta'\varepsilon_{CF} \sim \varepsilon_{CF}$

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

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

DMFT

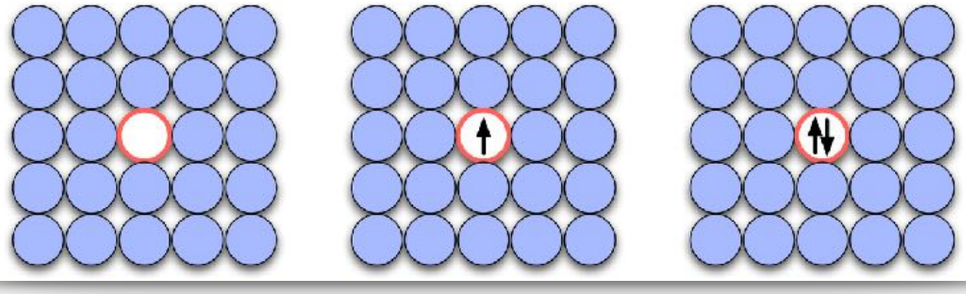
dimer



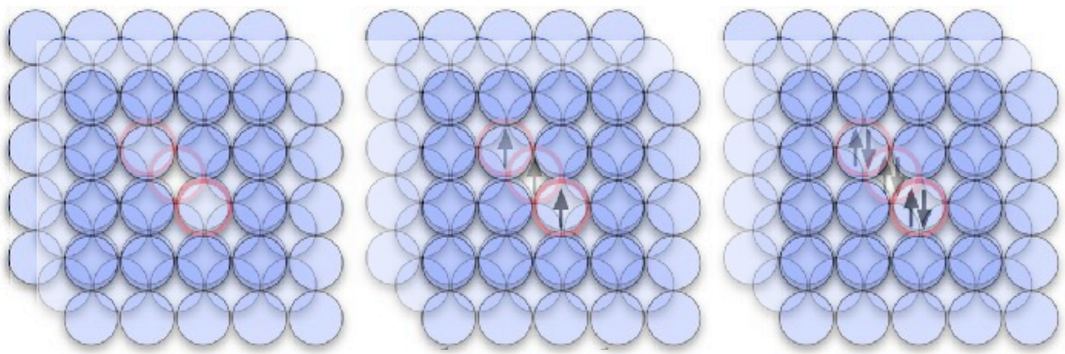
strong-correlations are local

U=V 

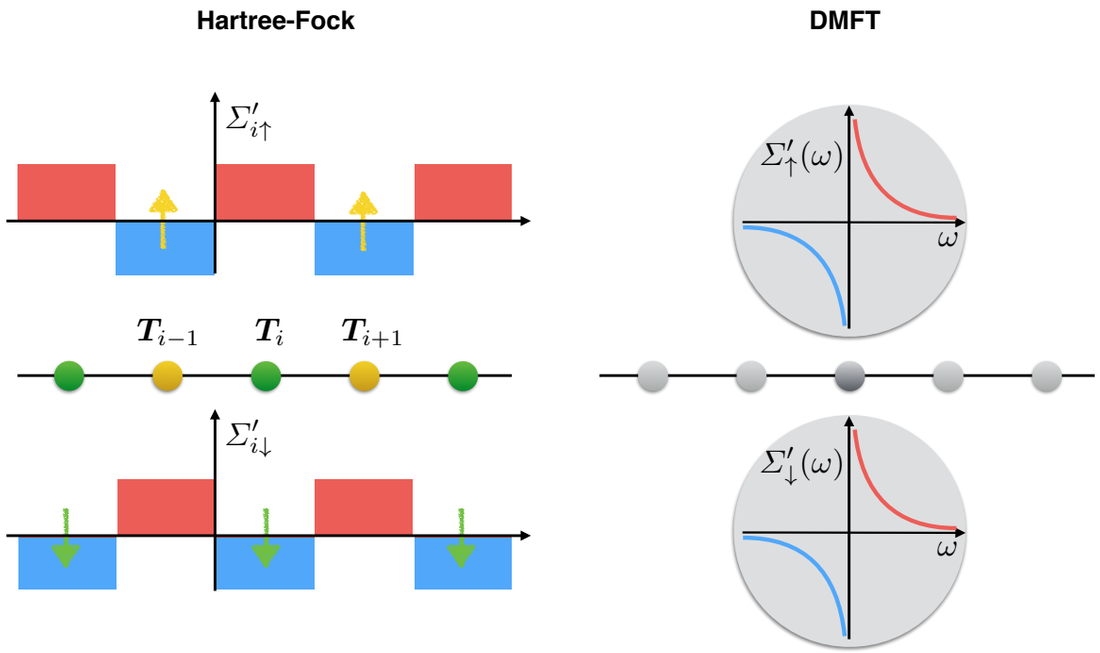
one band



multiband

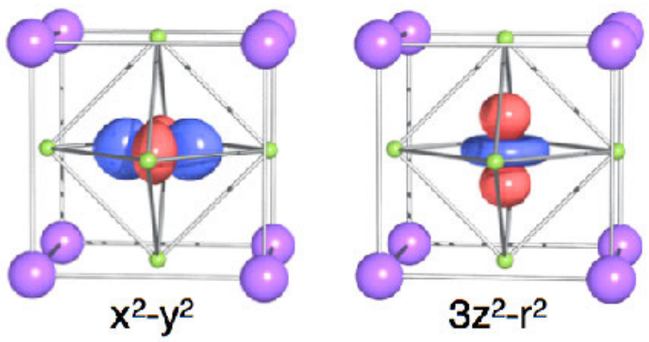


DMFT vs HF

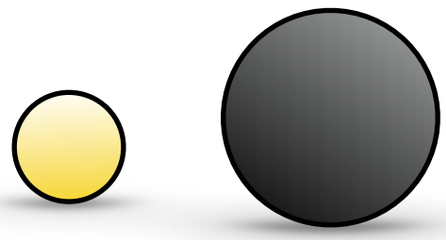


DMFT for materials

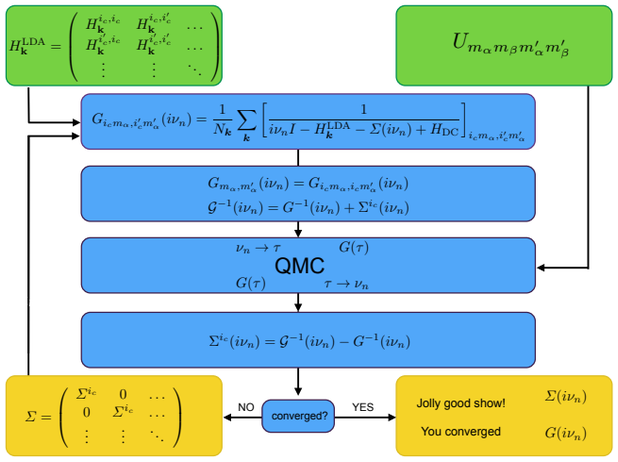
basis choice



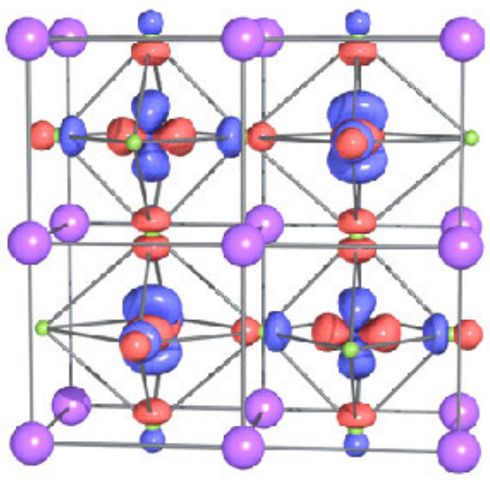
light & heavy electrons



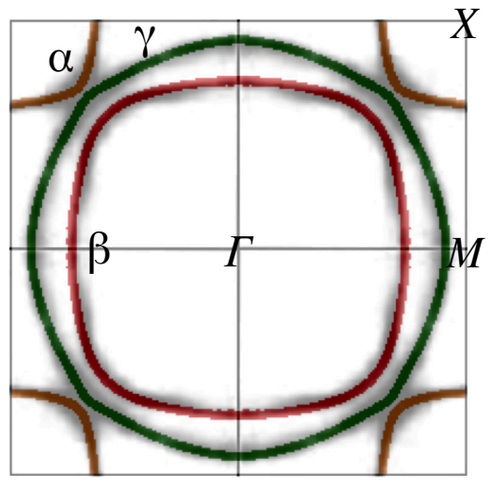
DMFT



downfolding, localization, double counting & screening



spin-orbit coupling & non-spherical U



thank you!