LDA+DMFT: Multiorbital Hubbard Models

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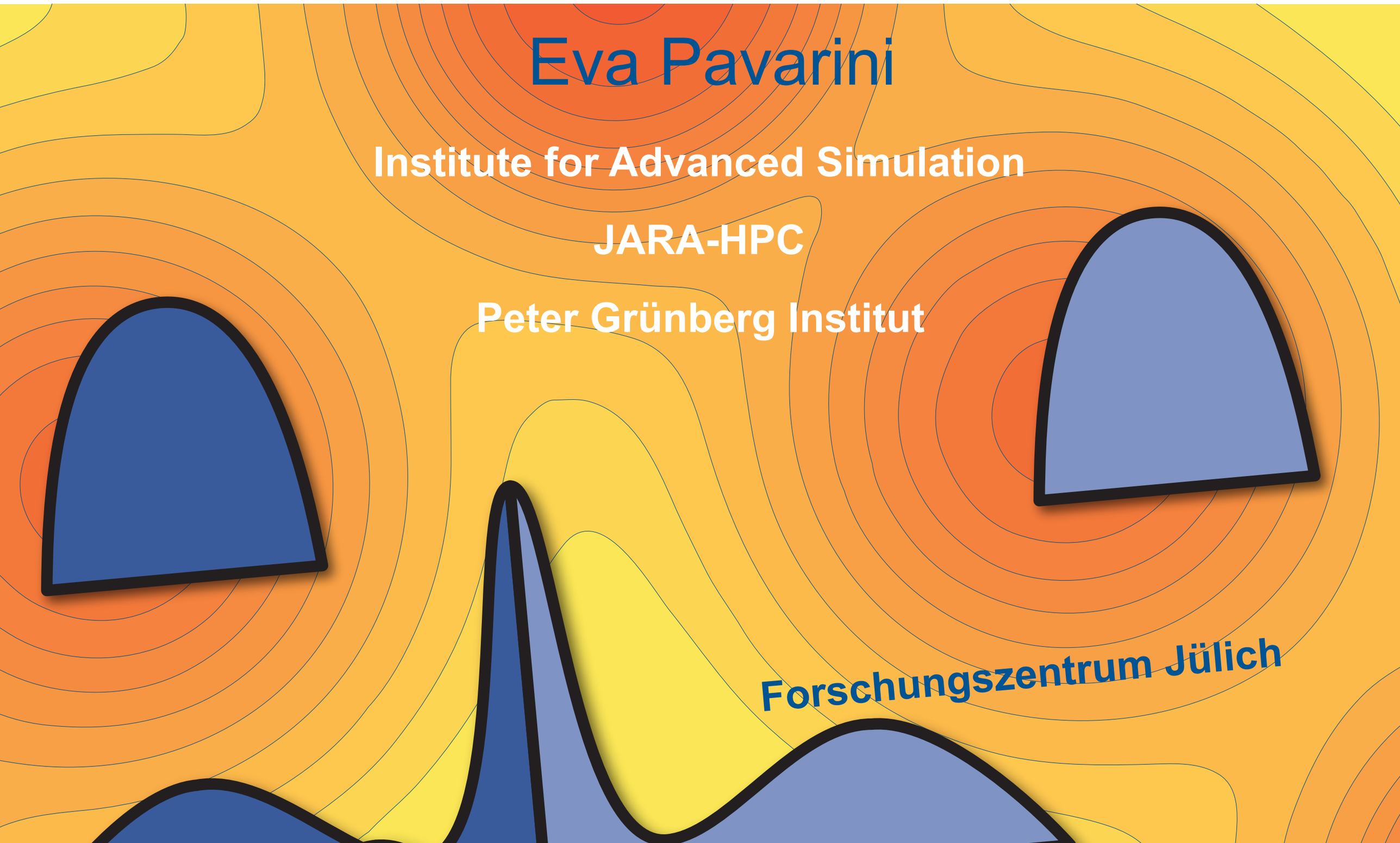


scheme of the lecture

- what is the final goal?
- minimal many-body models & DMFT
  - Hubbard dimer
  - one-band Hubbard model
  - multi-band Hubbard model
- building material-specific many-body models
- what is special in multi-orbital models?

what is the final goal?

the interacting quantum N-body problem

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**

more is different

Philip Warren Anderson

4 August 1972, Volume 177, Number 4047

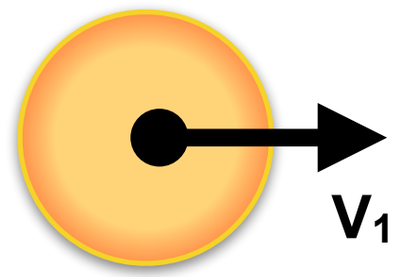
SCIENCE

the classical case

1-body, no interaction

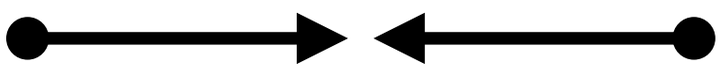
$$E = \frac{1}{2} m_1 \dot{\mathbf{r}}_1^2$$

$$m_1 \ddot{\mathbf{r}}_1 = 0$$

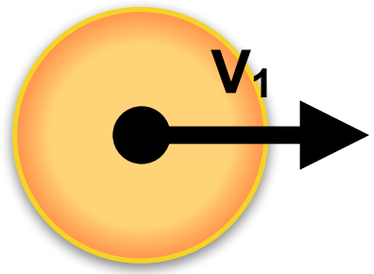


2-bodies, no interaction

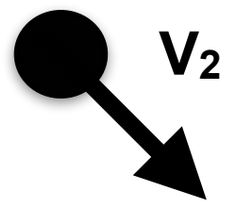
$$E = \frac{1}{2} m_1 \dot{\mathbf{r}}_1^2 + \frac{1}{2} m_2 \dot{\mathbf{r}}_2^2$$



$$m_1 \ddot{\mathbf{r}}_1 = 0$$



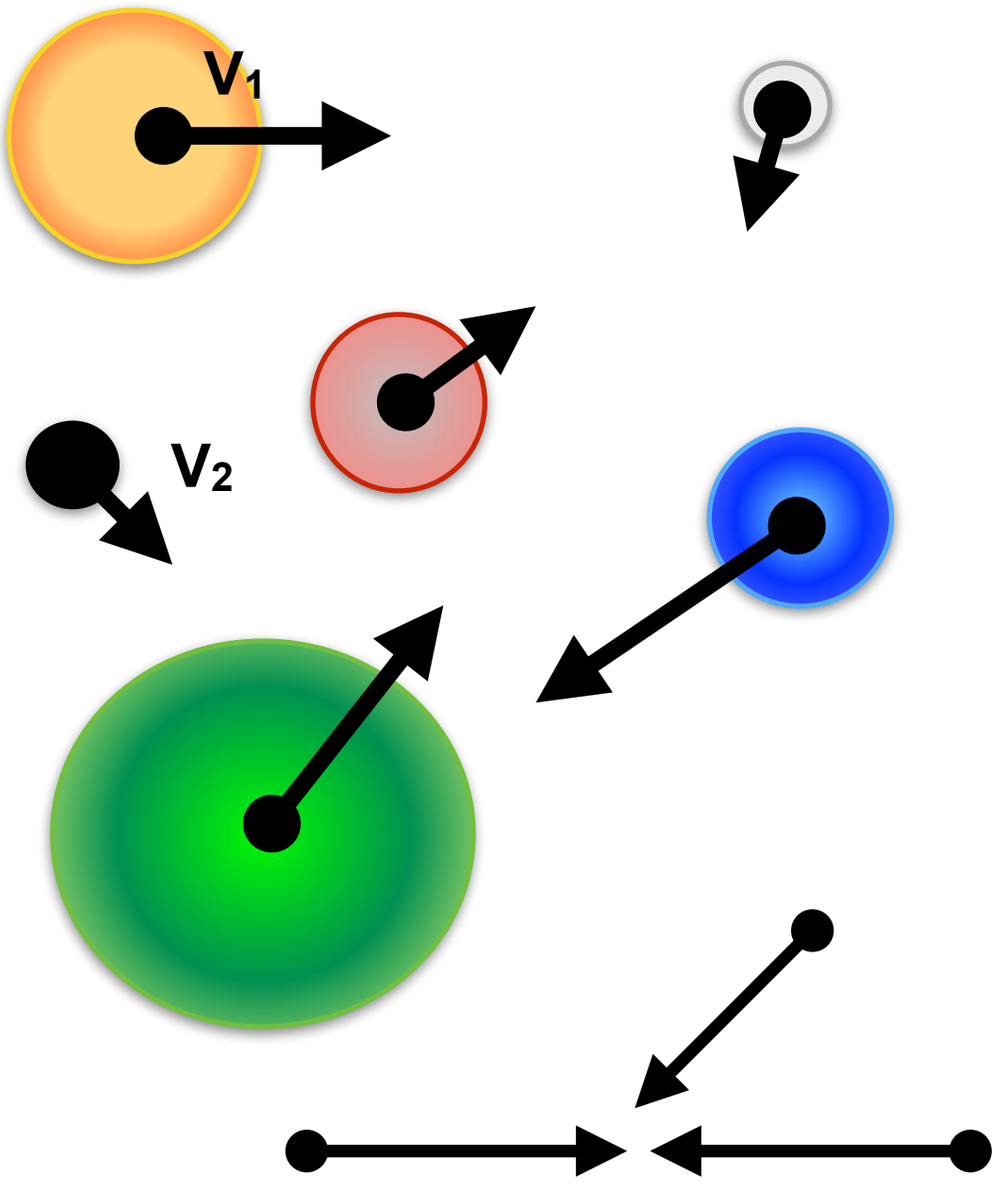
$$m_2 \ddot{\mathbf{r}}_2 = 0$$

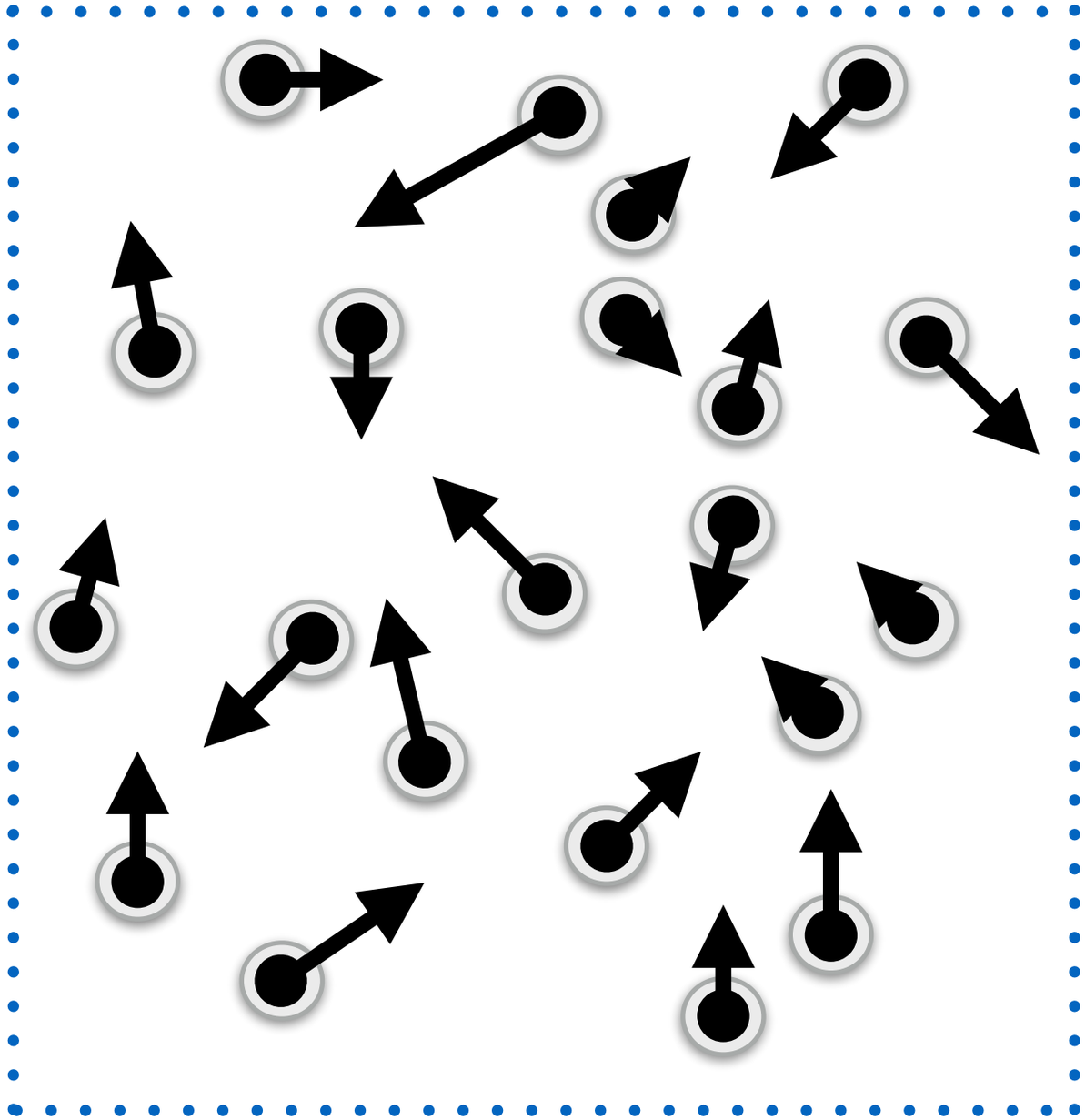


N-bodies, no interaction

$$E = \sum_i \frac{1}{2} m_i \dot{\mathbf{r}}_i^2$$

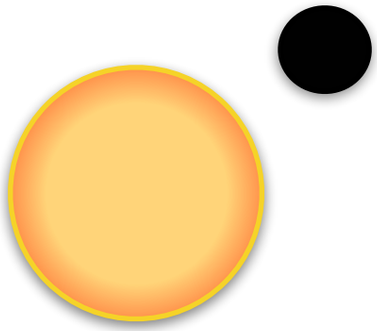
$PV=Nk_BT$



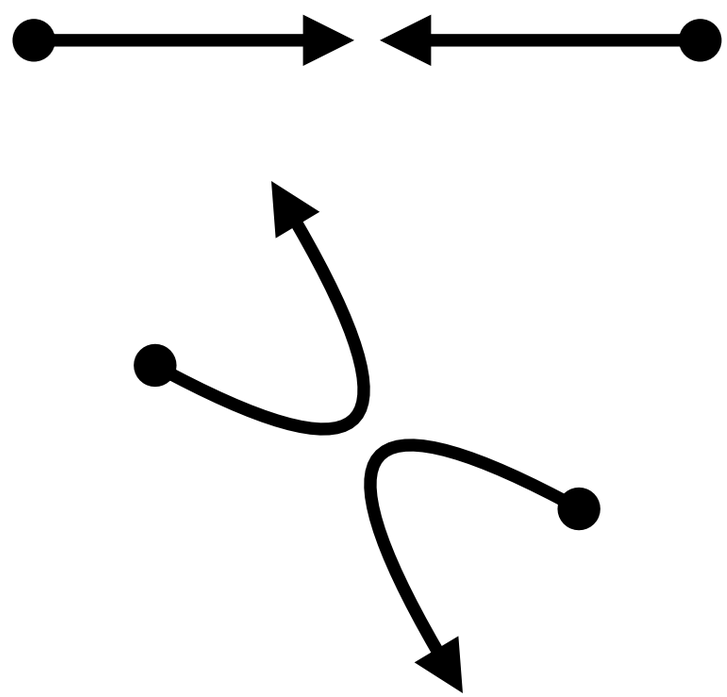


interacting classical 2-body problem

two bodies: analytically solvable problem



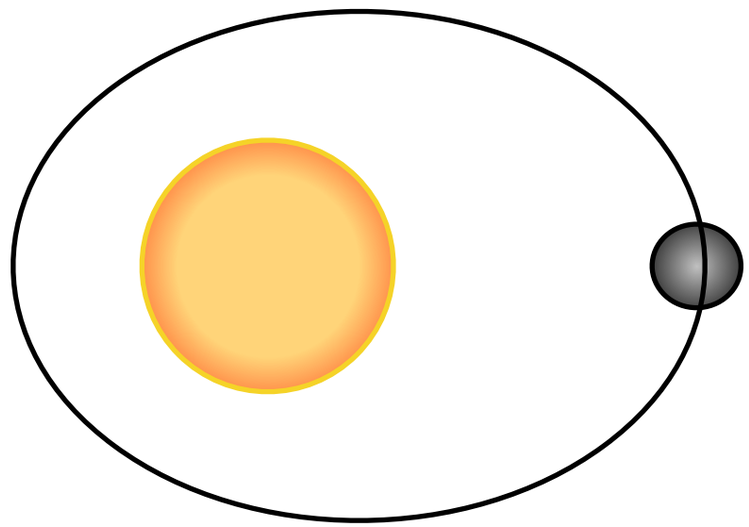
$$\begin{cases} m_1 \ddot{\mathbf{r}}_1 &= \mathbf{F}_{12} \\ m_2 \ddot{\mathbf{r}}_2 &= \mathbf{F}_{21} \end{cases}$$



center of mass and relative coordinates

$$\mathbf{R} = \frac{\mathbf{r}_1 m_1 + \mathbf{r}_2 m_2}{m_1 + m_2} \qquad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

$$M = m_1 + m_2 \qquad \mu = \frac{m_1 m_2}{m_1 + m_2}$$



classical 3-body problem

Oscar II's Prize Competition and the Error in Poincaré's Memoir on the Three Body Problem

JUNE BARROW-GREEN

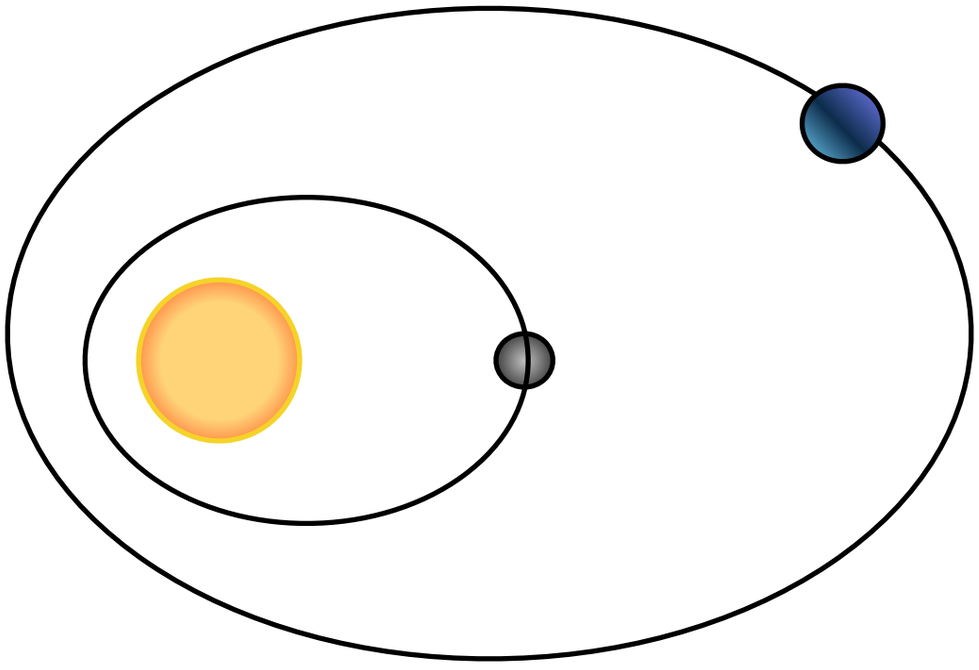
Communicated by JESPER LÜTZEN

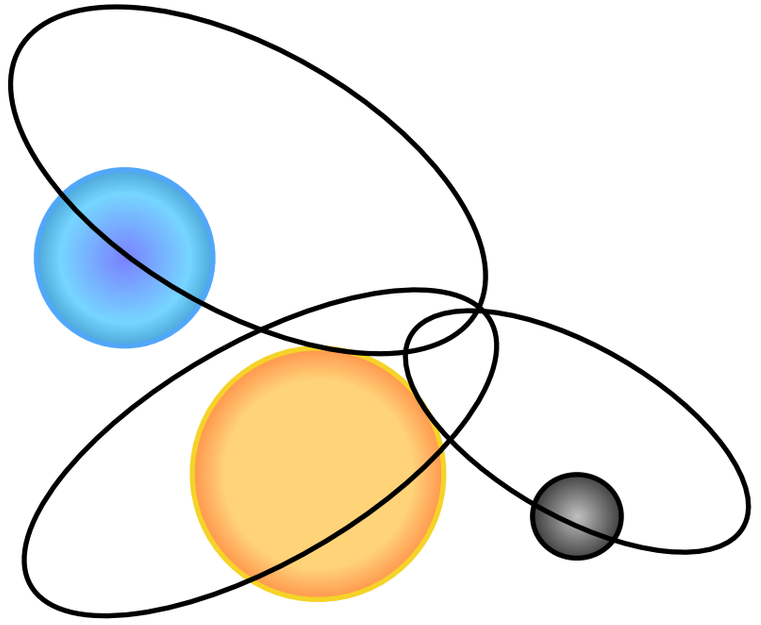
Introduction

In the autumn of 1890 HENRI POINCARÉ's memoir on the three body problem [1] was published in the journal *Acta Mathematica* as the winning entry in the international prize competition sponsored by OSCAR II, King of Sweden and Norway, to mark his 60th birthday on January 21, 1889. Today POINCARÉ's published memoir is renowned both for providing the foundations for his celebrated three-volume *Méthodes Nouvelles de la Mécanique Céleste* [2] and for containing the first mathematical description of chaotic behavior in a dynamical system.

interacting classical 3-body problem

chaotic behavior is possible





butterfly effect: behavior highly sensitive to initial conditions

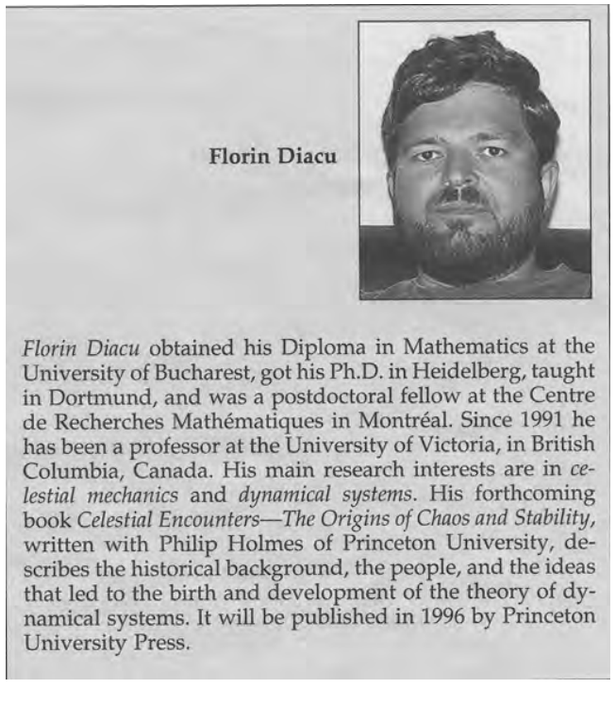
the present determines the future,
but the approximate present does not approximately determine the future
(Edward Lorenz)

Sundmann series solution (1907-1912)

For the 3-body problem there is series solution in powers of $t^{1/3}$ which converges for any $t^{(*)}$

(*) with exception of some initial conditions

Karl Frithiof Sundman



Florin Diacu

Florin Diacu obtained his Diploma in Mathematics at the University of Bucharest, got his Ph.D. in Heidelberg, taught in Dortmund, and was a postdoctoral fellow at the Centre de Recherches Mathématiques in Montréal. Since 1991 he has been a professor at the University of Victoria, in British Columbia, Canada. His main research interests are in *celestial mechanics* and *dynamical systems*. His forthcoming book *Celestial Encounters—The Origins of Chaos and Stability*, written with Philip Holmes of Princeton University, describes the historical background, the people, and the ideas that led to the birth and development of the theory of dynamical systems. It will be published in 1996 by Princeton University Press.

The Solution of the *n*-body Problem*

Florin Diacu

what about N > 3 ?

The Solution of the *n*-body Problem*

Florin Diacu

[...] It took about 7 decades until the general case was solved. In 1991, a Chinese student, Quidong (Don) Wang, published a beautiful paper [Wa], [D1], in which he provided a convergent power series solution of the *n*-body problem.

Did this mean the end of the *n*-body problem? Was this old question—unsuccessfully attacked by the greatest mathematicians of the last 3 centuries—merely solved by a student in a moment of rare inspiration?

[...] Paradoxically [...] not; in fact we know nothing more than before having this solution.

exact solution does not help

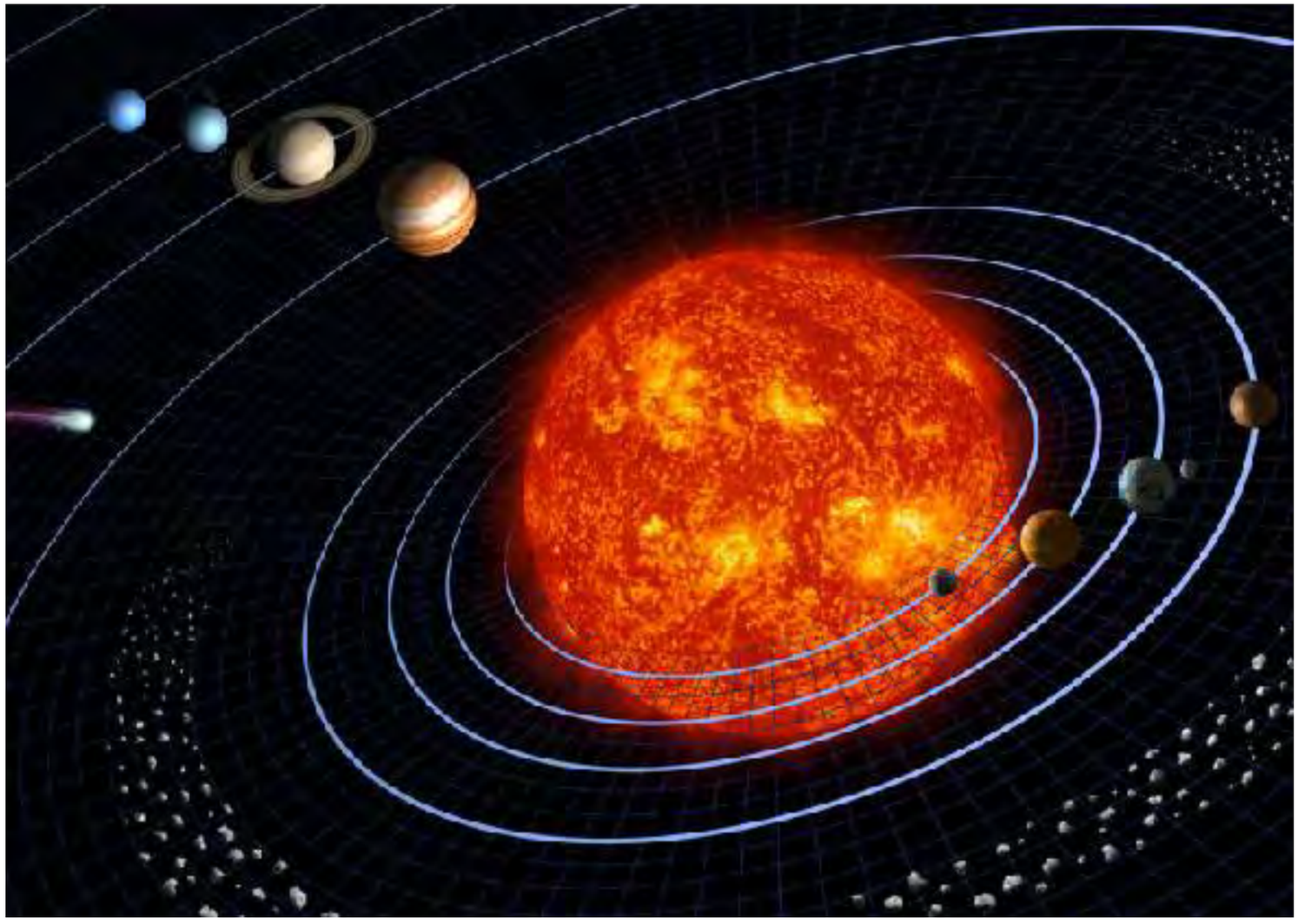
The Solution of the *n*-body Problem*

Florin Diacu

The Foundations of Mathematics

What Sundman and Wang did is in accord with the way solutions of initial value problems are defined; everything is apparently all right; but there is a problem, a big one: these series solutions, though convergent on the whole real axis, have very slow convergence. One would have to sum up millions of terms to determine the motion of the particles for insignificantly short intervals of time. The round-off errors make these series unusable in numerical work. From the theoretical point of view, these solutions add nothing to what was previously known about the *n*-body problem.

emergent behavior



(from NASA website)

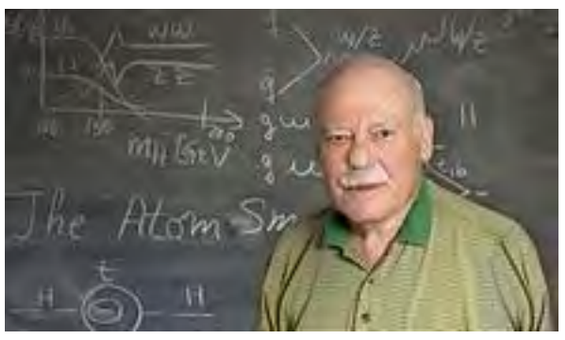
Kolmogorov–Arnold–Moser theorem

If masses, eccentricities, and inclinations of planets are small enough, many initial conditions lead to quasiperiodic planetary trajectories

the quantum case

E. Wigner and F. Seitz

If one had a great calculating machine, one might apply it to the problem of solving the Schrödinger equation for each metal [...] It is not clear, however, that a great deal would be gained by this. Presumably the results would agree with the experimentally determined quantities and nothing vastly new would be learned from the calculation. [. . .].



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

… and the exact solution would be useless

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 Practical Great Dream Machine ?

... It would indeed be remarkable if Nature fortified herself against further advances in knowledge behind the analytical difficulties of the many-body problem.

Max Born (1960)

why do atom exist? how can we explain the periodic table?

what is the mechanism of high-Tc superconductivity?

why are some systems metals and other insulators?

what is the mechanism of orbital ordering?

no two samples are identical: **generic** features only

what is the final goal?

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

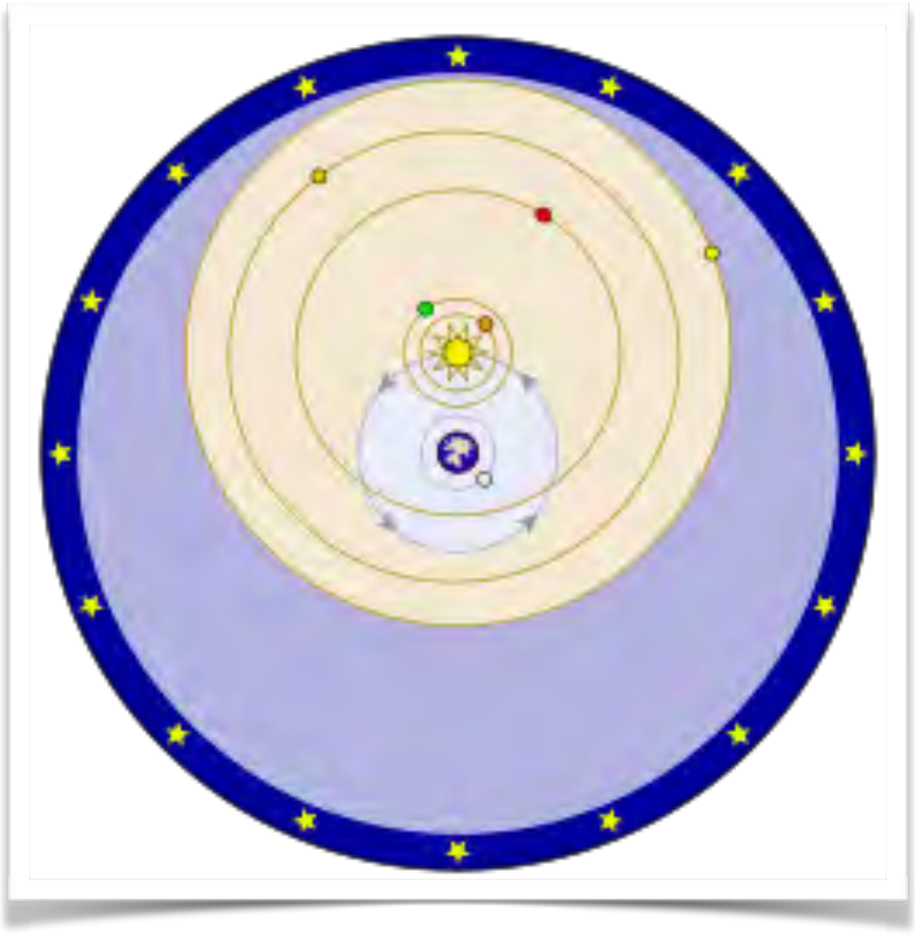
minimal model for a given class of phenomena

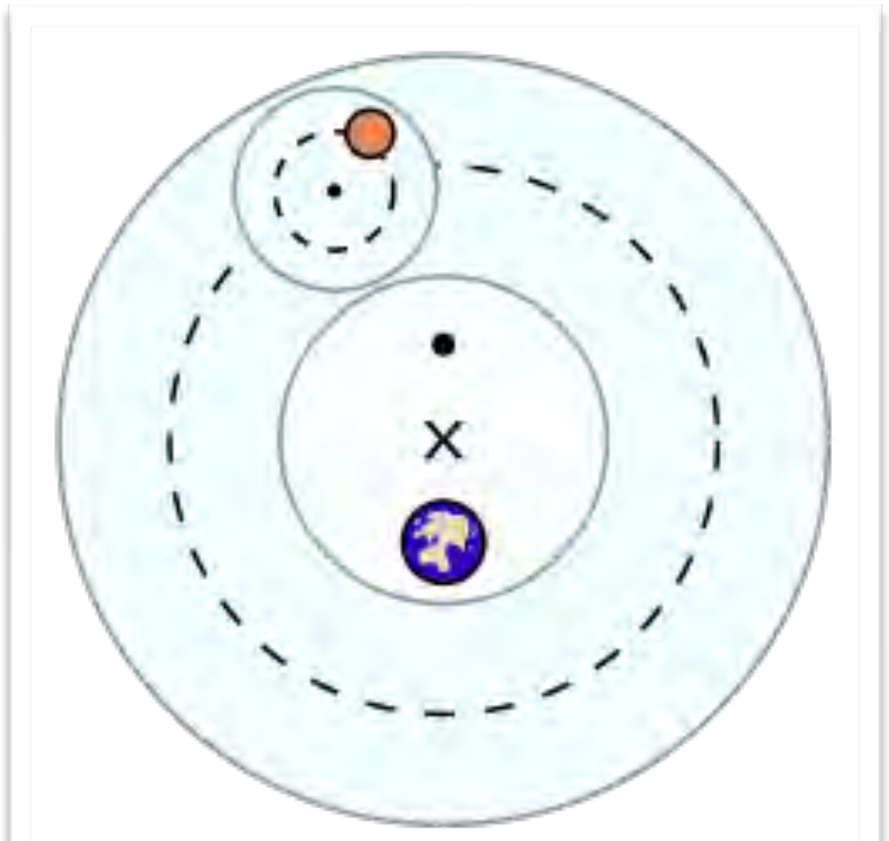
as system-specific as possible

& find approximate methods that work

how good should we fit experiments?

Copernican vs Ptolemaic model





figures from wikipedia

how do we do this?

0. electronic Hamiltonian in 2nd quantization

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

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

complete one-electron basis set!

1. build minimal models

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

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

DFT Kohn-Sham *ab-initio* Hamiltonian

very good approach for weakly correlated systems

density-functional theory

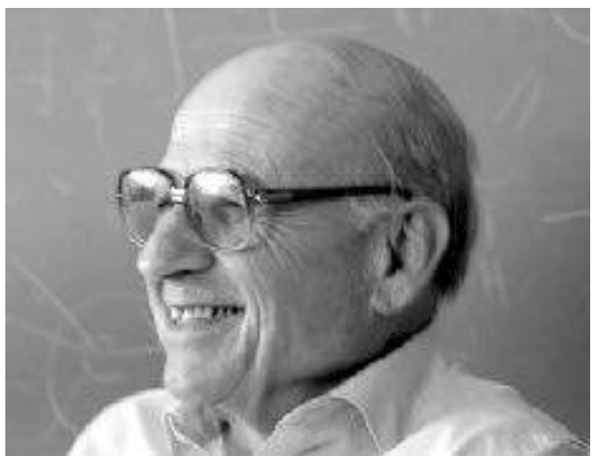
$$\hat{H} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} - \sum_\alpha \frac{1}{2M_\alpha}\nabla_\alpha^2 + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha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

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,…)



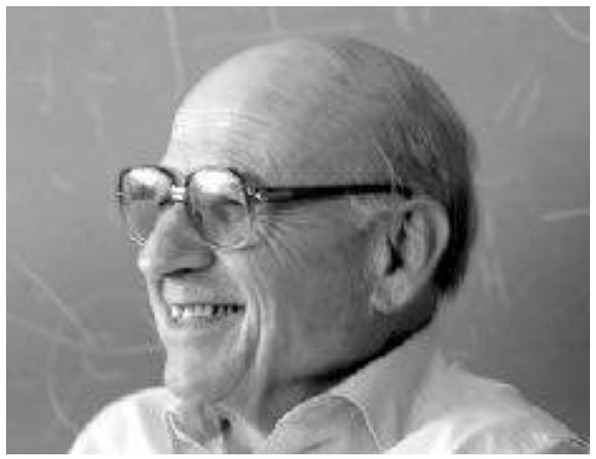
Walter Kohn

Nobel Prize in Chemistry (1998)

Kohn-Sham equations

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

density functional theory



Walter Kohn

Nobel Prize in Chemistry (1998)

$$E_{xc}[n] = \int d\mathbf{r} \epsilon_{xc}^{\mathrm{LDA}}(n(\mathbf{r}))n(\mathbf{r})$$

homogeneous electron gas

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

The practical DFT-based Great Dream Machine

weakly correlated systems

what do the parameters contain?

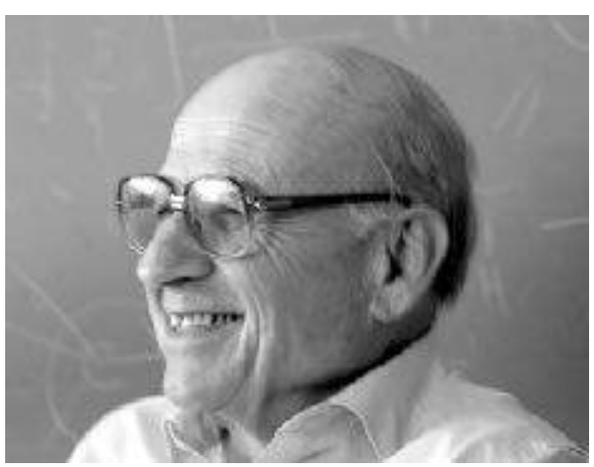
$$t_{a,b} = -\int d\mathbf{r}\, \overline{\psi_a}(\boldsymbol{r}) \left[-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r})\right] \psi_b(\boldsymbol{r}),$$

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...

The Great Solid State Physics Dream Machine

"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)**

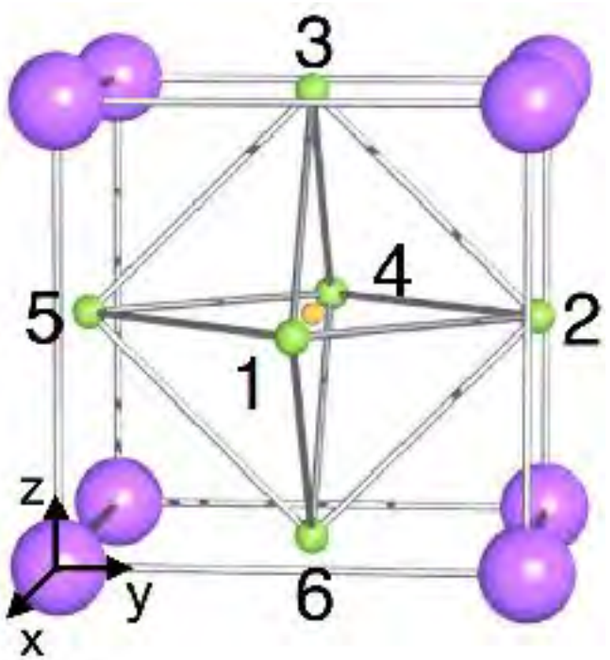
origin of failures: one-electron picture

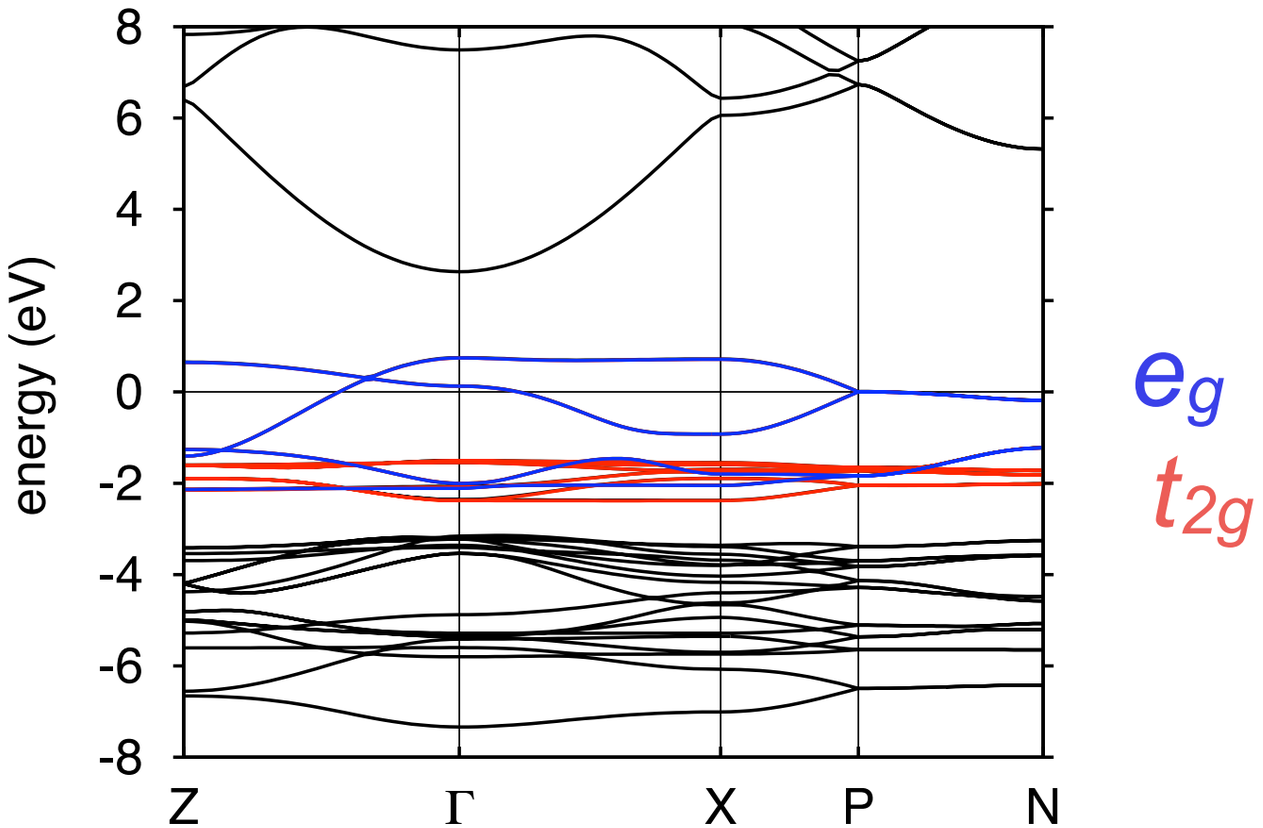
(RO Jones, *DFT for emergents*, Autumn School on Correlated Electrons 2013)

when does this approach fail?

$KCuF_3$

experimentally: above 40 K **paramagnetic** insulator

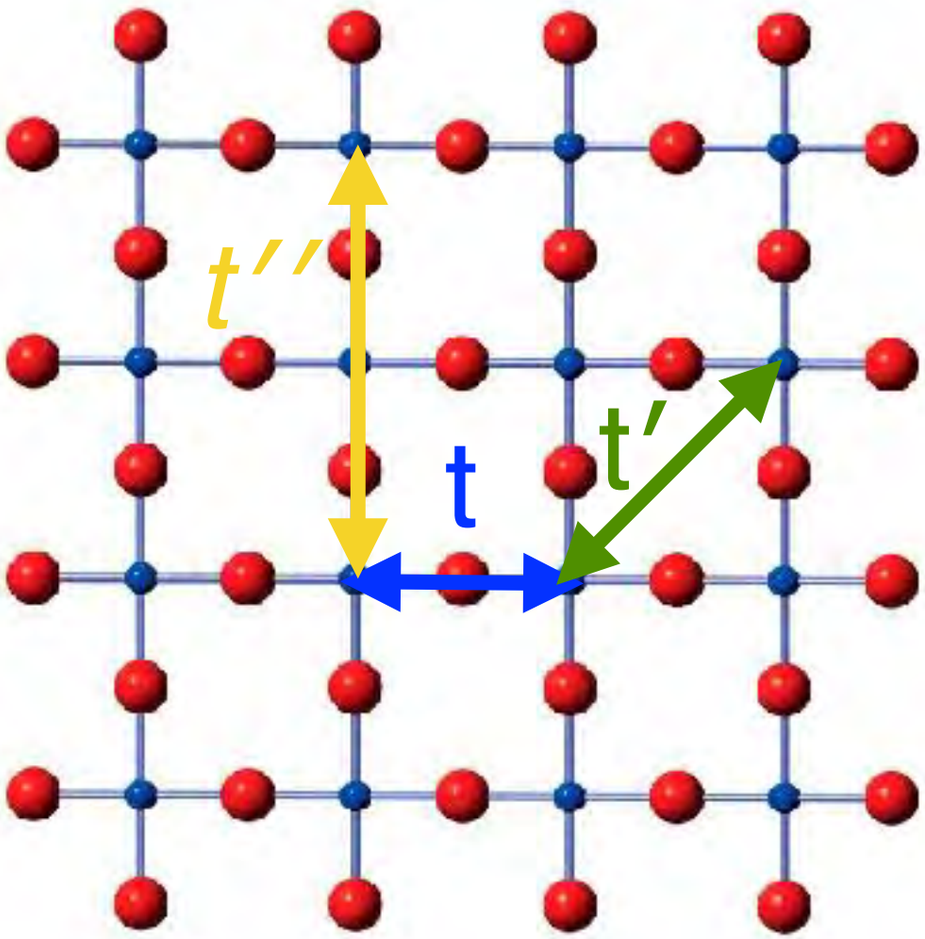




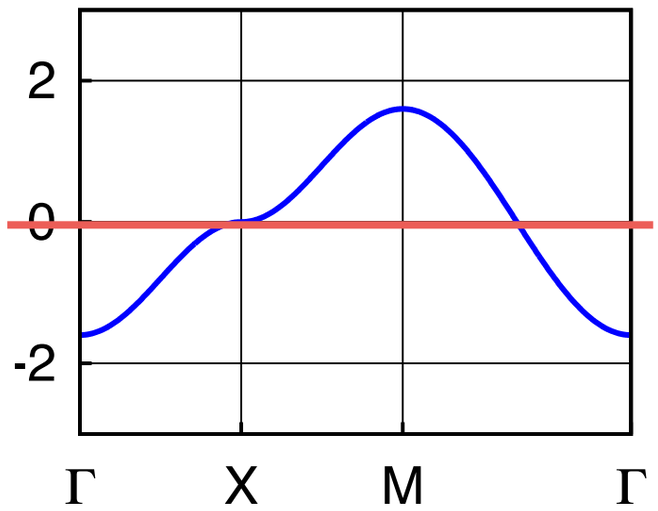
$$\hat{\tilde{H}}_e = \sum_{ab} \tilde{t}_{ab} c_a^\dagger c_b$$

electron counting argument

one electron per site

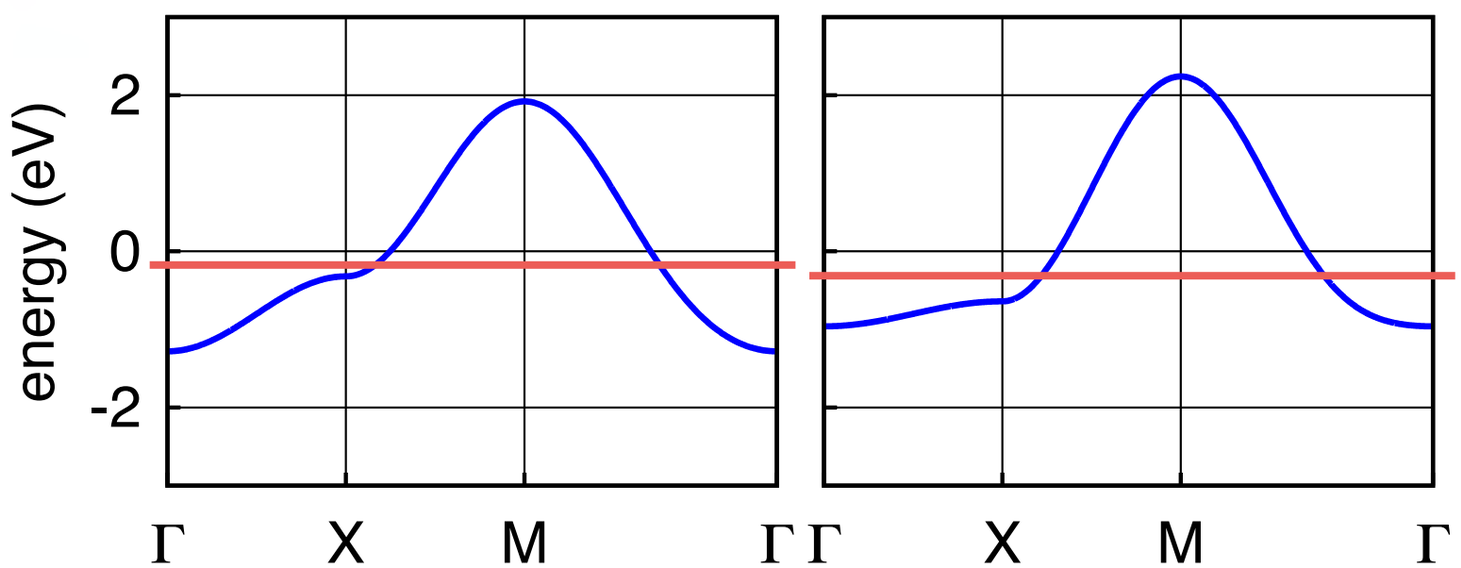


$$\varepsilon_{\boldsymbol{k}} = -2t[\cos k_x + \cos k_y]$$

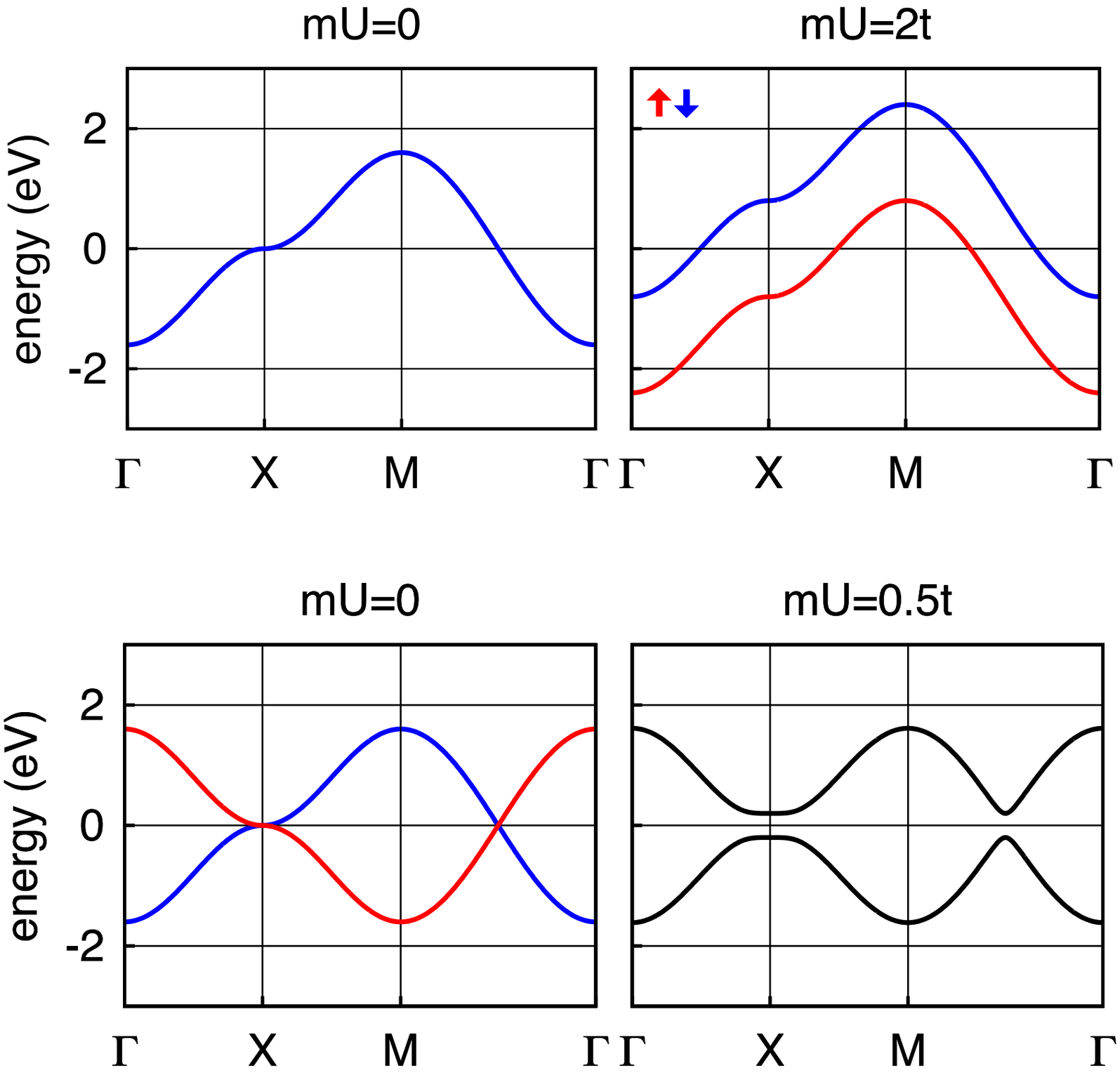


t′/t= =0.2

t′/t= =0.4



how could I open a gap?



$KCuF_3$

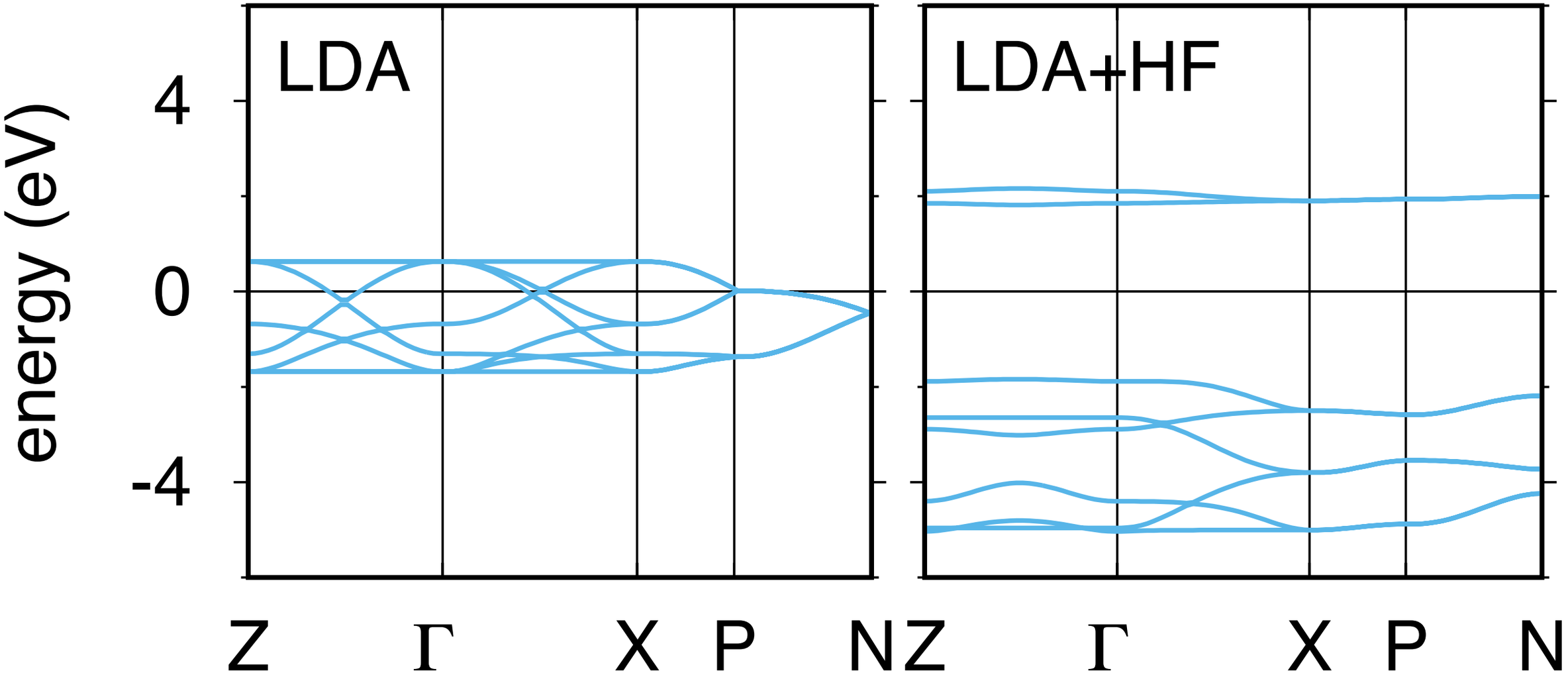
shown e_g bands only

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

LDA: metal

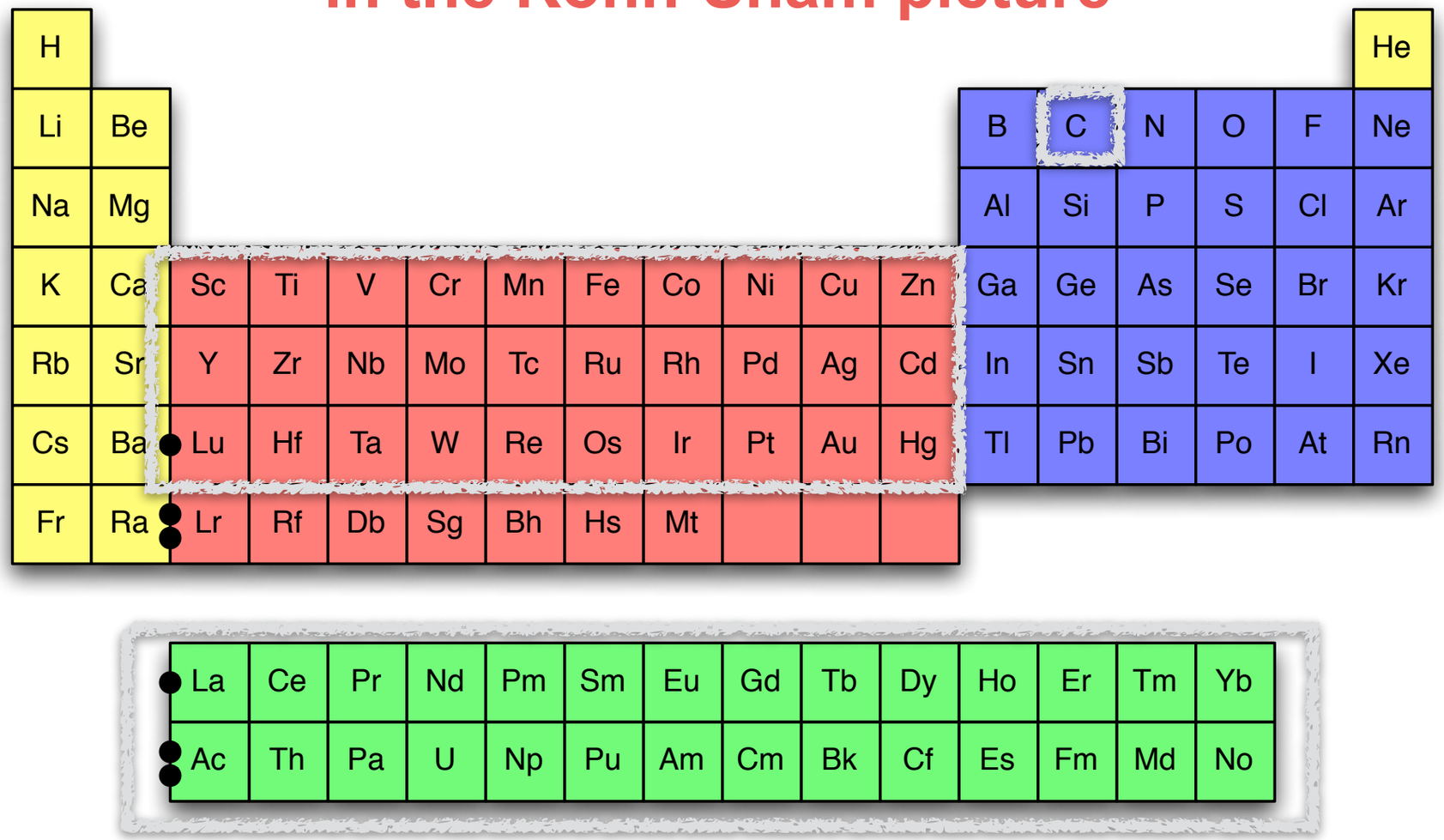
LDA+*U*: insulator BUT only with orbital AND spin order

non-magnetic (Pauli paramagnet) **AF-magnetic order**



strongly correlated systems

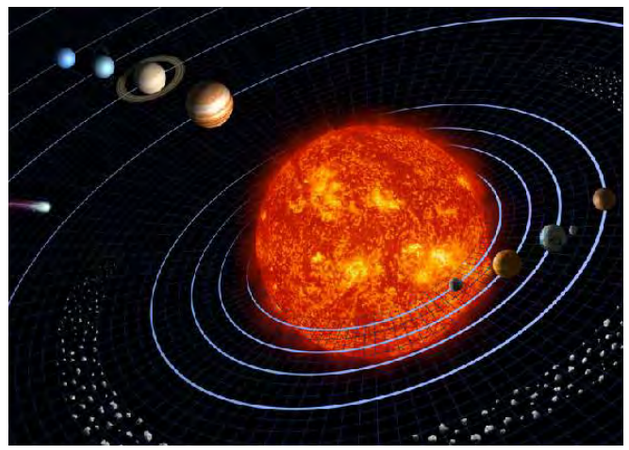
paramagnetic Mott insulators are either metals or magnetically ordered insulators
in the Kohn-Sham picture



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

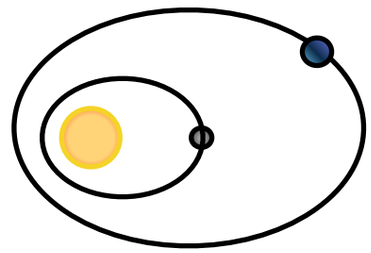
1. minimal models that capture the phenomenon

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



minimal model for metal-insulator transition

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



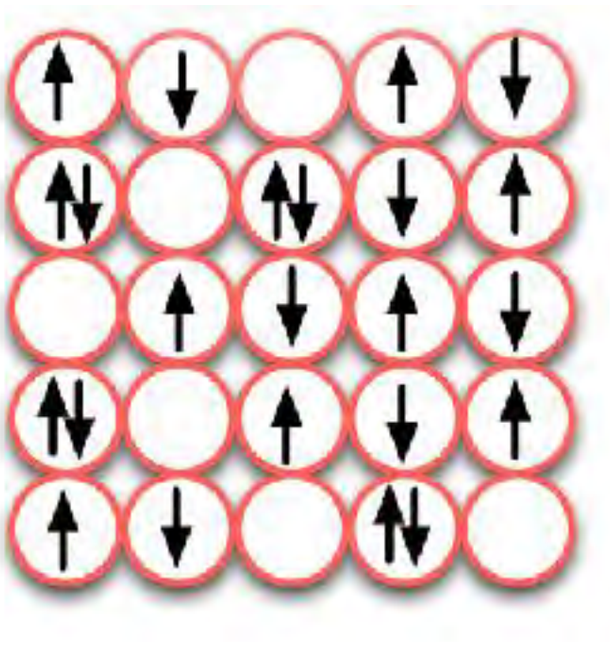
Hubbard model at half filling

local Coulomb produce strong correlation effects

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**

high-T_c superconducting cuprates

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

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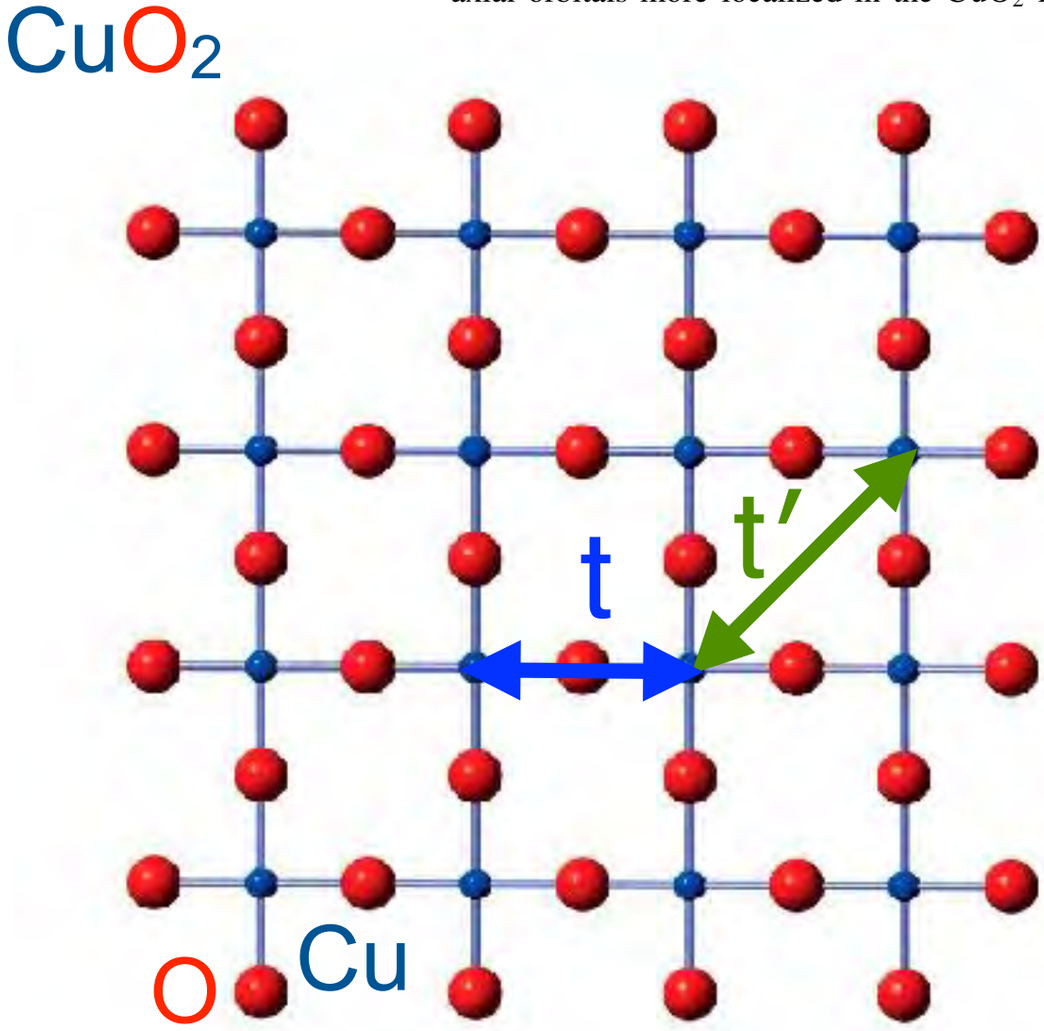
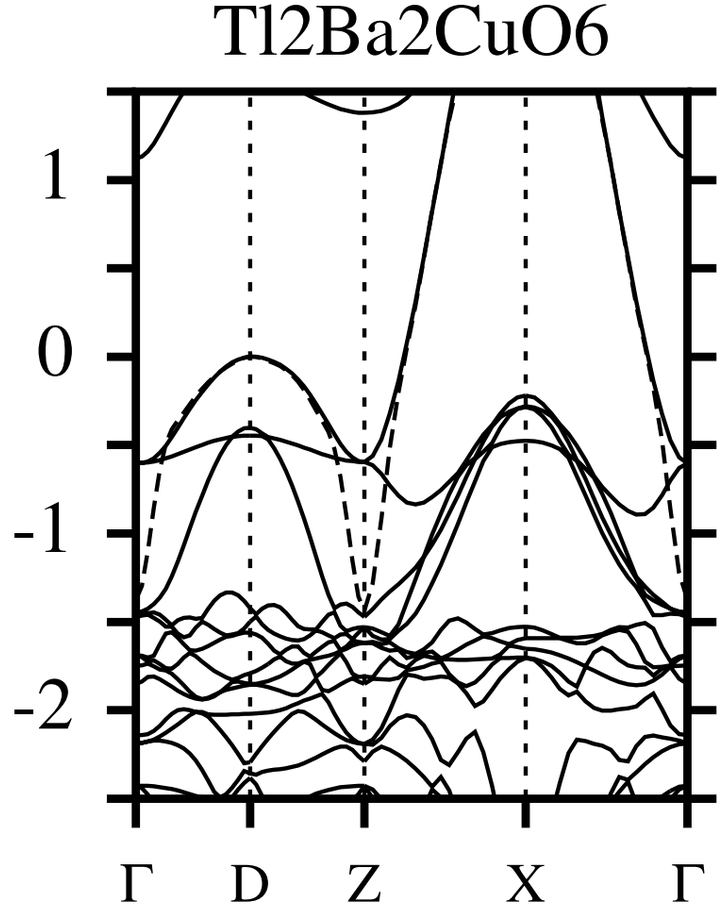
By calculation and analysis of the bare conduction bands in a large number of hole-doped high-temperature superconductors, we have identified the range of the intralayer hopping as the essential, material-dependent parameter. It is controlled by the energy of the axial orbital, a hybrid between Cu 4*s*, 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.

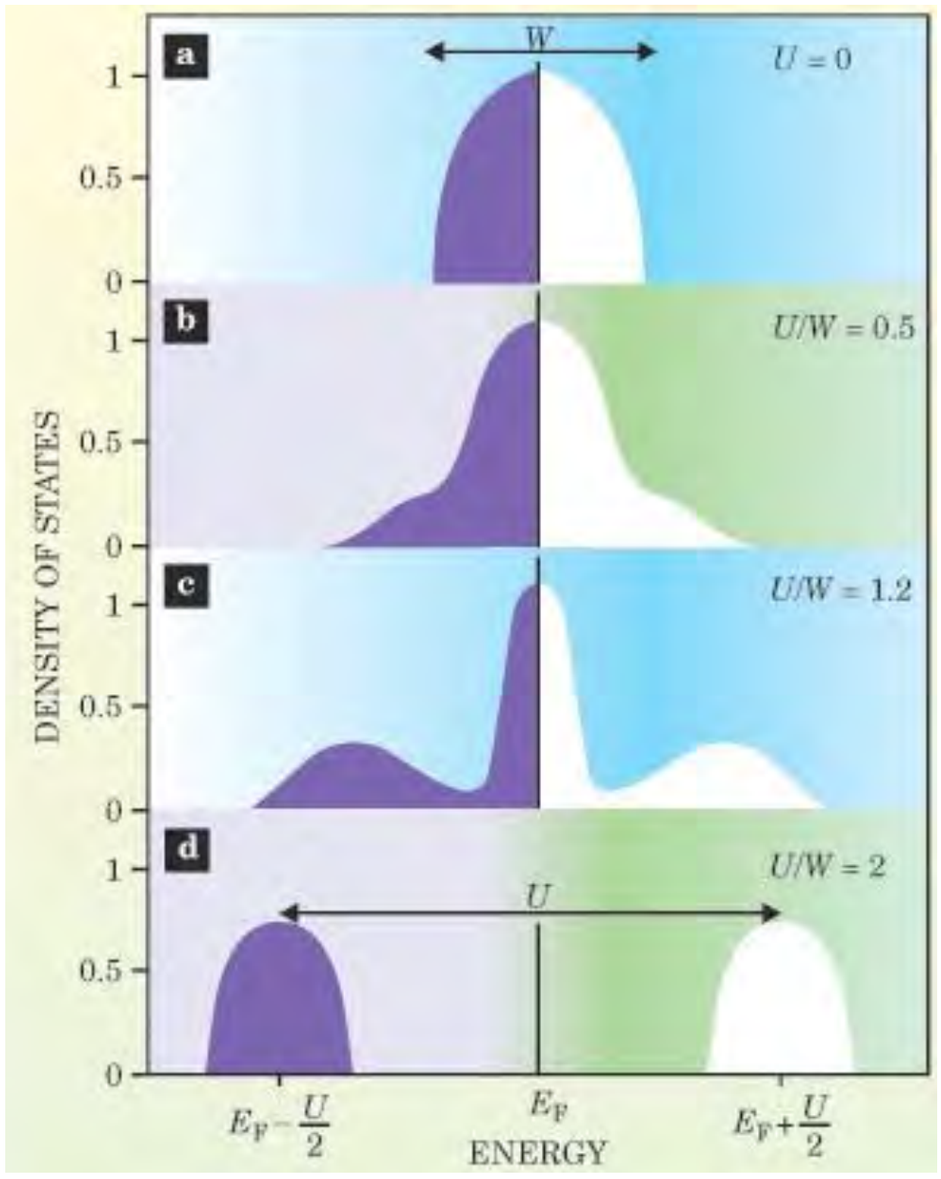




2. find approximate methods that work

DMFT

local self energy approximation



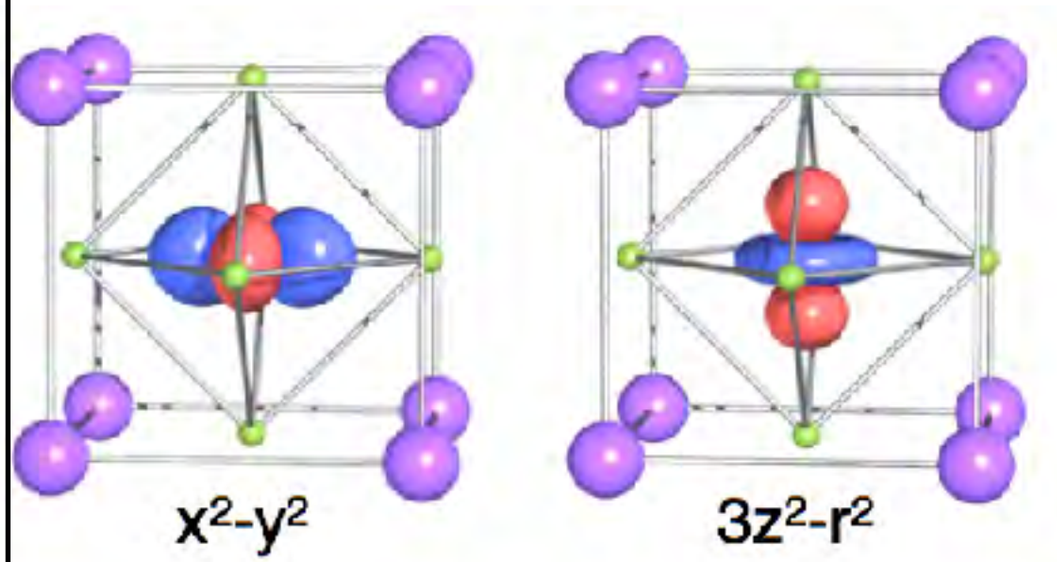
$$H = -t \sum_{\sigma} \sum_{\langle ii' \rangle} c^{\dagger}_{i\sigma} c_{i'\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow}$$

Bethe lattice W: band width

exact for t=0, U=0 & infinite dimension limit

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

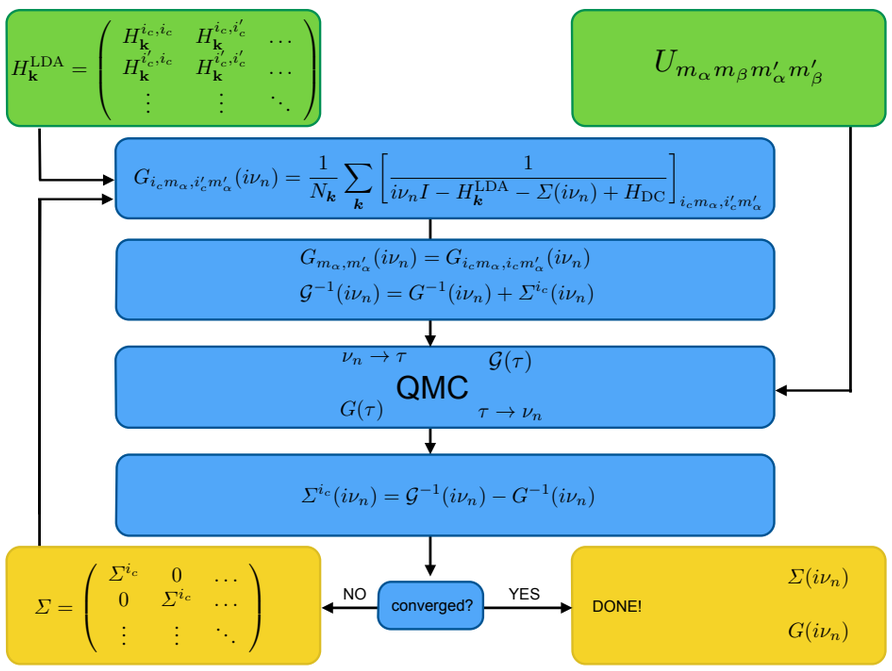
3. make it more realistic: LDA+DMFT



basis

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

models



method extensions

scheme of the lecture

- what is the final goal?
- minimal many-body models & DMFT
  - Hubbard dimer
  - one-band Hubbard model
  - multi-band Hubbard model
- building material-specific many-body models
- what is special in multi-orbital models?

minimal models & DMFT

DMFT for the Hubbard dimer

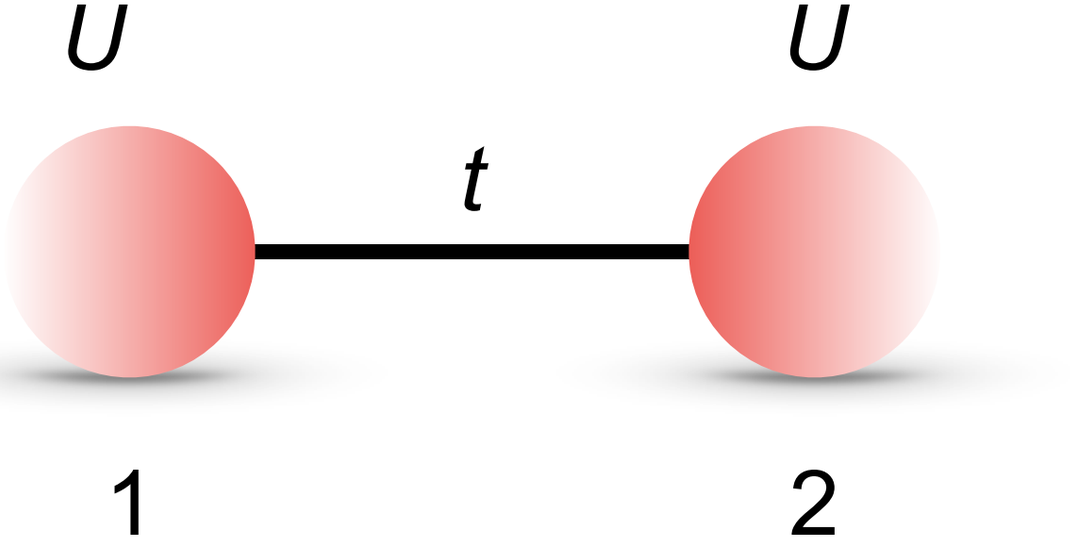
this is a **toy** model: coordination number is one

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

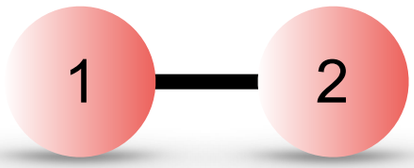
the Hubbard dimer

the Hubbard dimer

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



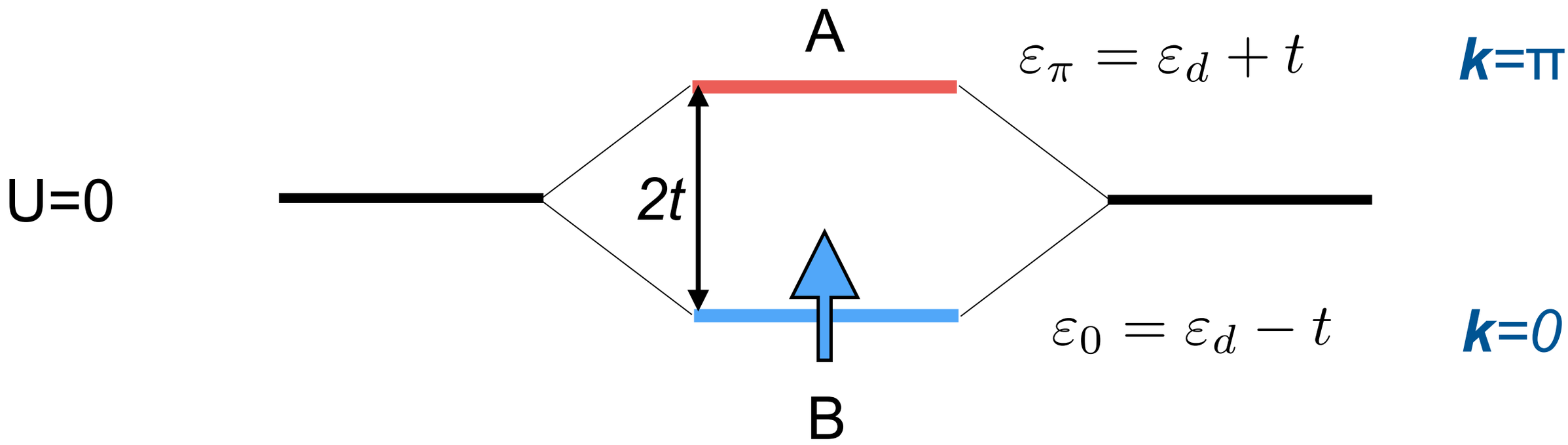
https://www.cond-mat.de/events/correl17/manuscripts/pavarini.pdf



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

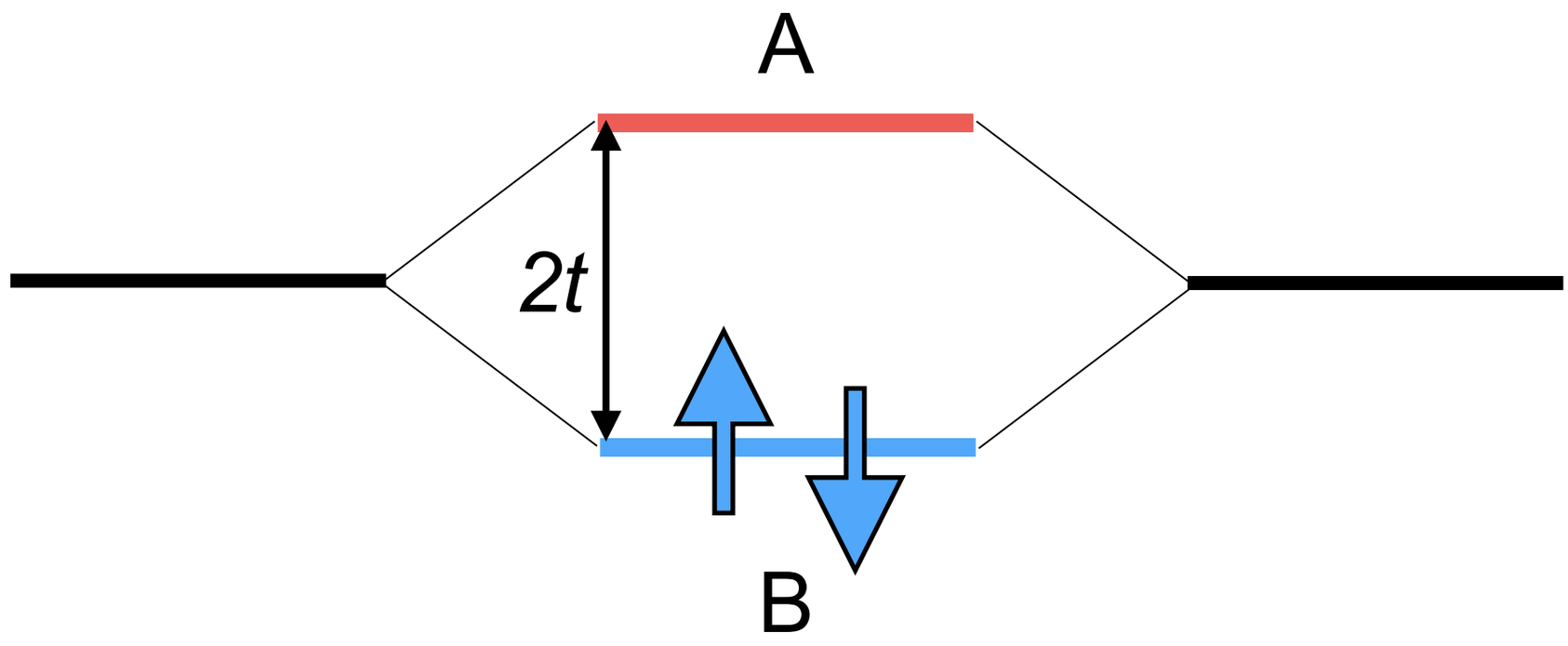


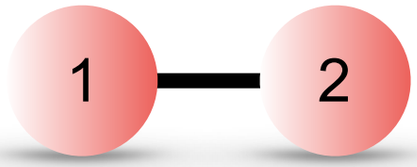
finite *t*: exact diagonalization

half filling (N=2)

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

U=0

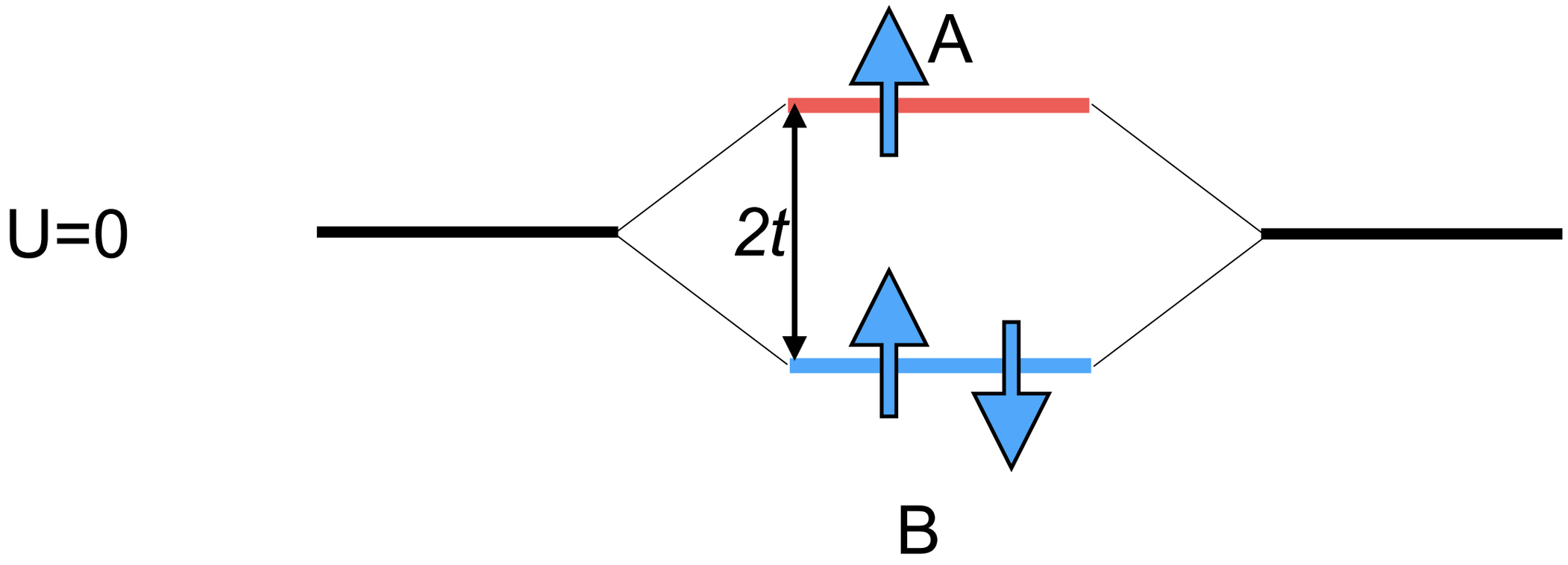


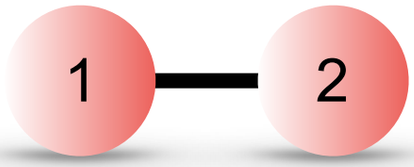


finite *t*: exact diagonalization

N=3

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





the local Green function

Lehmann representation

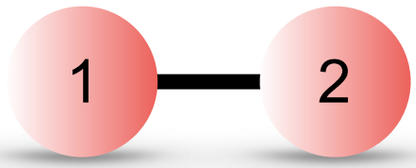
$$G_{ii,\sigma}(i\nu_n) = \frac{1}{Z}\sum_{nn'N} e^{-\beta(E_n(N)-\mu N)} \left[\frac{|\langle n'N-1|c_{i\sigma}|nN\rangle|^2}{i\nu_n - [E_n(N) - E_{n'}(N-1) - \mu]} + \frac{|\langle n'N+1|c^\dagger_{i\sigma}|nN\rangle|^2}{i\nu_n - [E_{n'}(N+1) - E_n(N) - \mu]} \right],$$

change basis

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

local Green function: k-point average

$$G^\sigma_{11}(i\nu_n) = \frac{1}{2}\left[G^\sigma(0, i\nu_n) + G^\sigma(\pi, i\nu_n)\right]$$



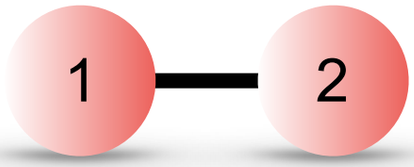
U=0 vs finite *U*

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

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

hybridization function

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



the *local* self-energy

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

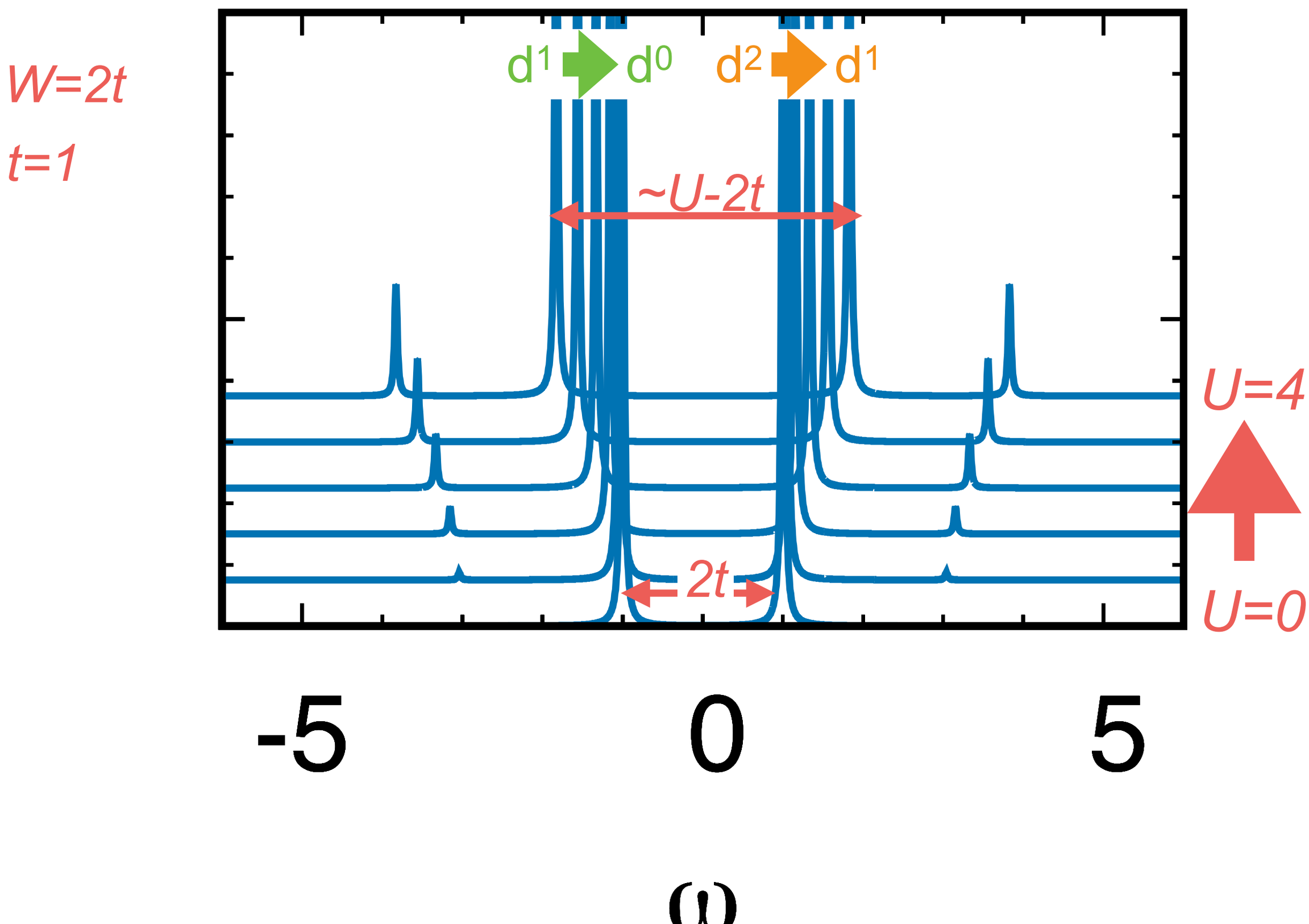
$$\Sigma_l^{\sigma}(i\nu_n) = \frac{1}{2}\left(\Sigma^{\sigma}(\pi, i\nu_n) + \Sigma^{\sigma}(0, i\nu_n)\right)$$ local

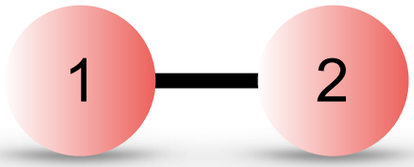
$$\Delta\Sigma_l^{\sigma}(i\nu_n) = \frac{1}{2}\left(\Sigma^{\sigma}(\pi, i\nu_n) - \Sigma^{\sigma}(0, i\nu_n)\right)$$ non-local

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 spectral function





spectral function *U=4*

only **local** self-energy

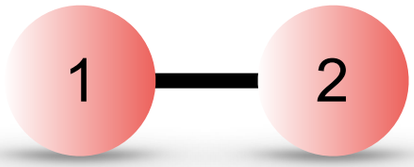
exact

-5 0 5

ω

-5 0 5

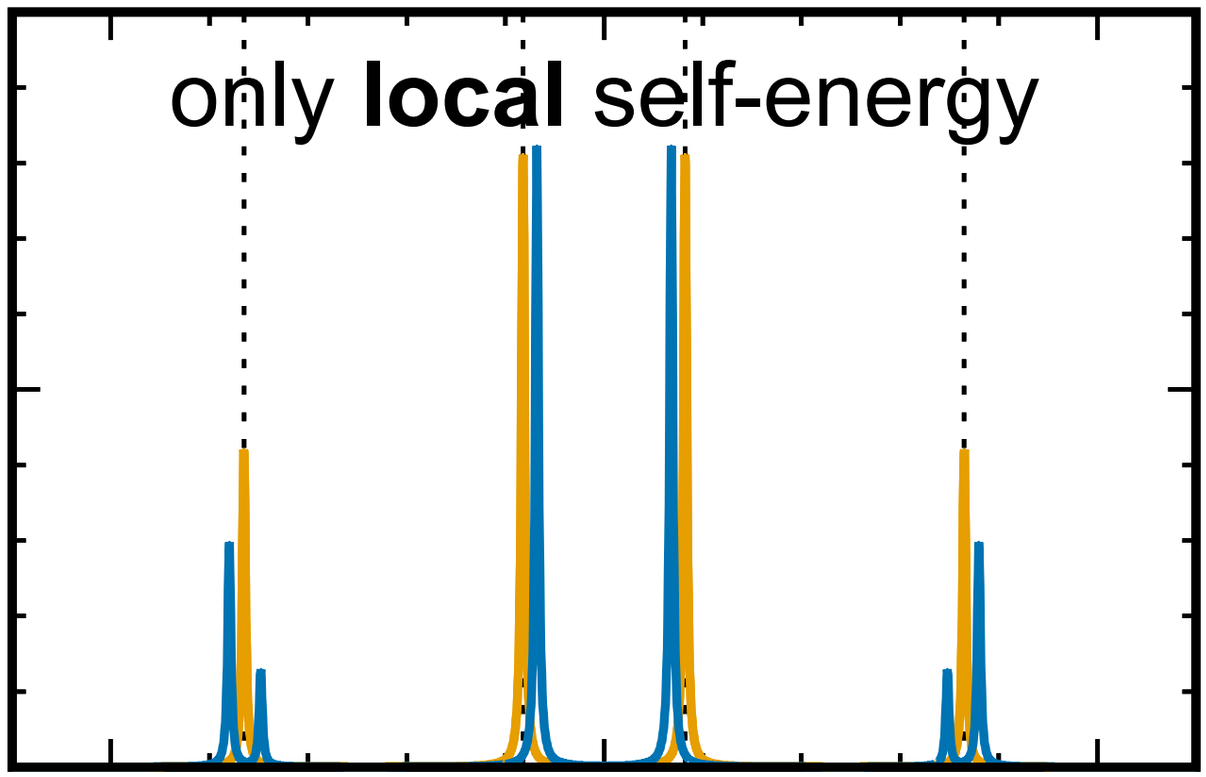
ω



local Dyson equation

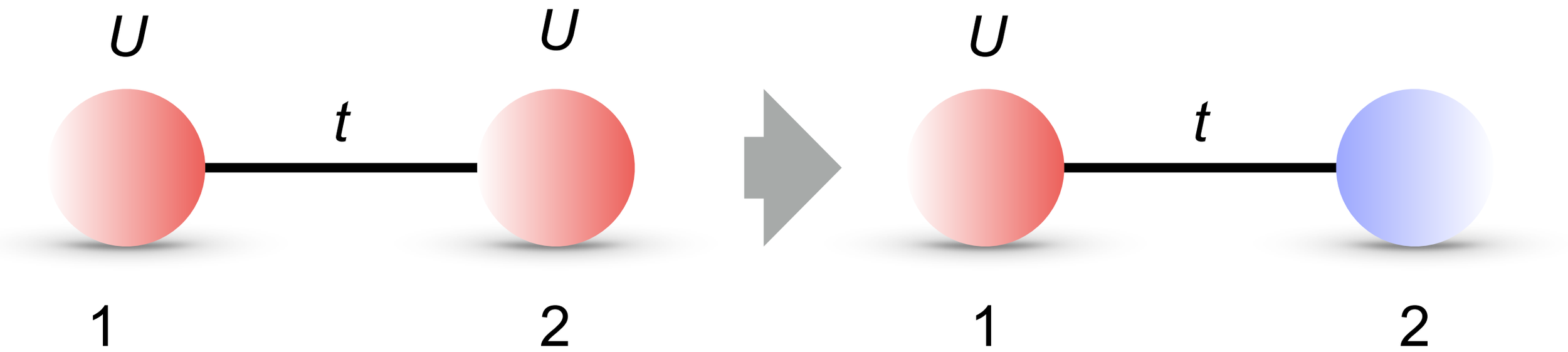
$$\Sigma_l^\sigma(i\nu_n) = \frac{1}{\mathfrak{G}_{i,i}^\sigma(i\nu_n)} - \frac{1}{G_{i,i}^\sigma(i\nu_n)},$$

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

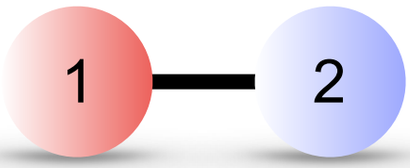


map to a quantum impurity model ?

the Anderson molecule



$$\hat{H} = \varepsilon_d \hat{n}_{1\sigma} + \varepsilon_s \hat{n}_{2\sigma} - t \sum_{\sigma} \left[c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right] + U \hat{n}_{1\uparrow} \hat{n}_{1\downarrow}.$$



self-consistency

N=2

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

same occupations of Hubbard dimer

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

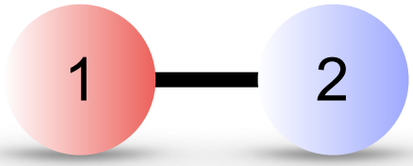
solution: Hubbard vs Anderson

Hubbard dimer

$$G_{11}^{\sigma}(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma_l^{\sigma}(i\nu_n) + F^{\sigma}(i\nu_n))}$$

Anderson molecule

$$G_{d}^{\sigma}(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma_l^{\sigma}(i\nu_n) + F^{0}(i\nu_n))}.$$

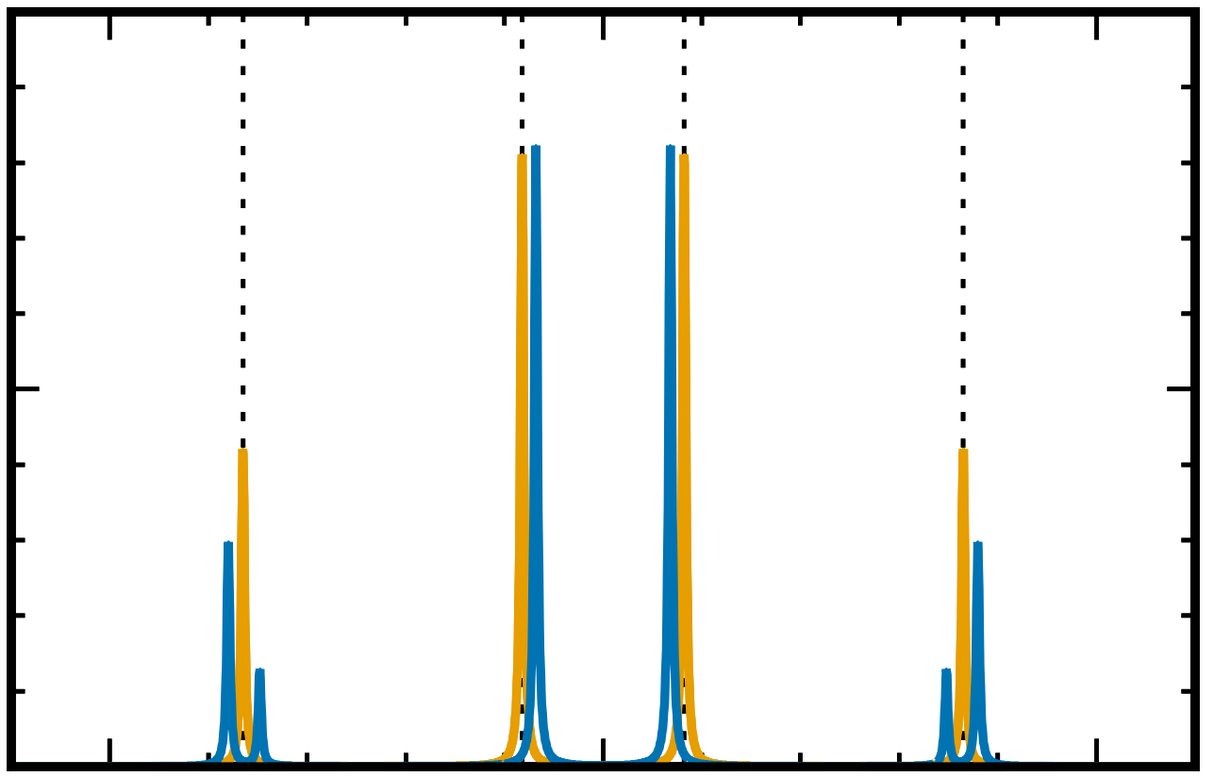


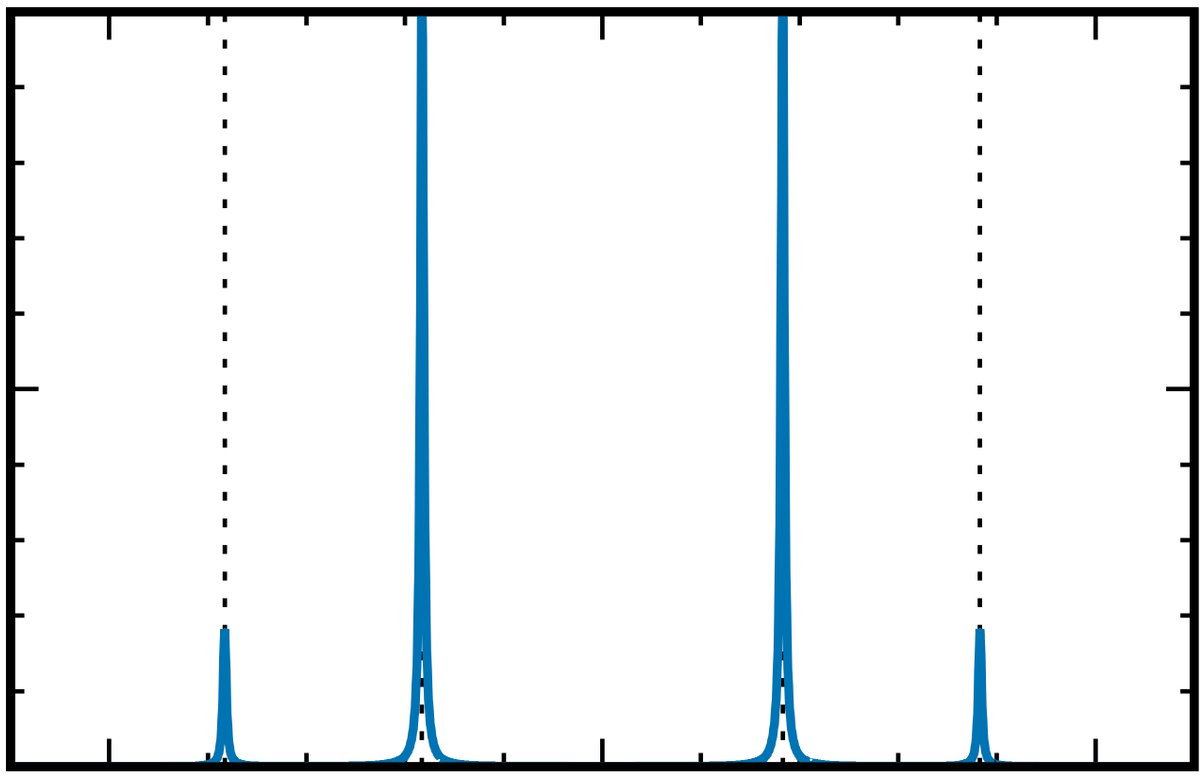
Green function *U=4t*

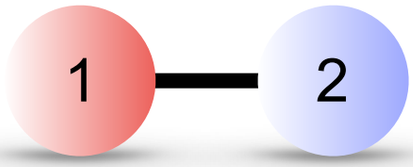
Anderson vs **Hubbard**

only **local** self-energy

exact

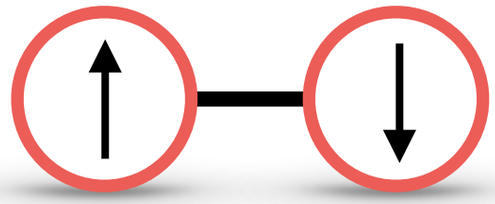






DMFT for the dimer

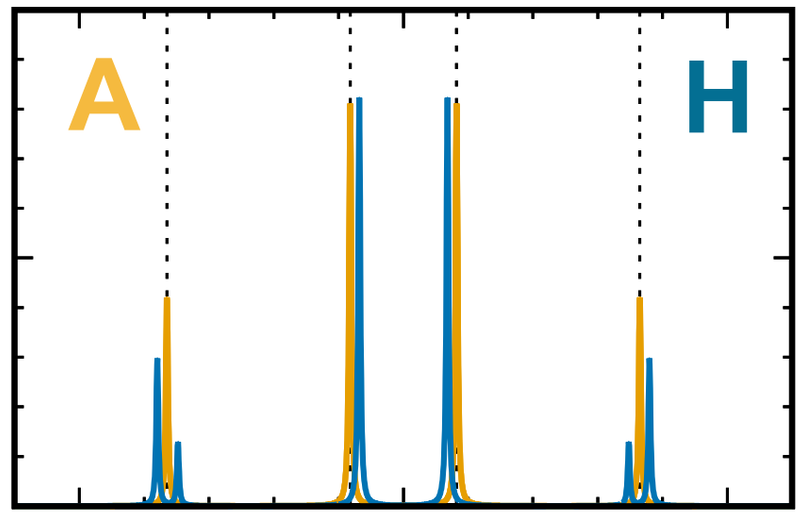
$$\hat{H} = \varepsilon_d \sum_{i\sigma} n_{i\sigma} - t \sum_{\sigma} \left[c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma} \right] + U \sum_{i=1,2} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}.$$



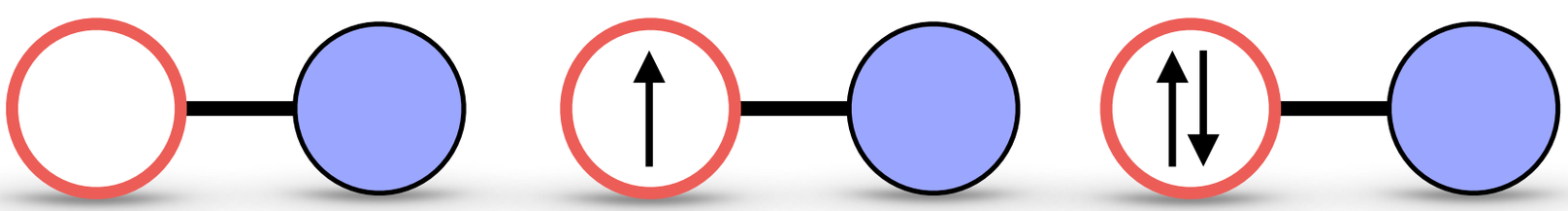
map to quantum impurity model (QIM) in local self-energy approximation

$$\hat{H} = \varepsilon_d \, \hat{n}_{1\sigma} + \varepsilon_s \hat{n}_{2\sigma} - t \sum_{\sigma} \left[c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma} \right] + U \hat{n}_{1\uparrow} \hat{n}_{1\downarrow}.$$

QIM solver



self-consistency loop



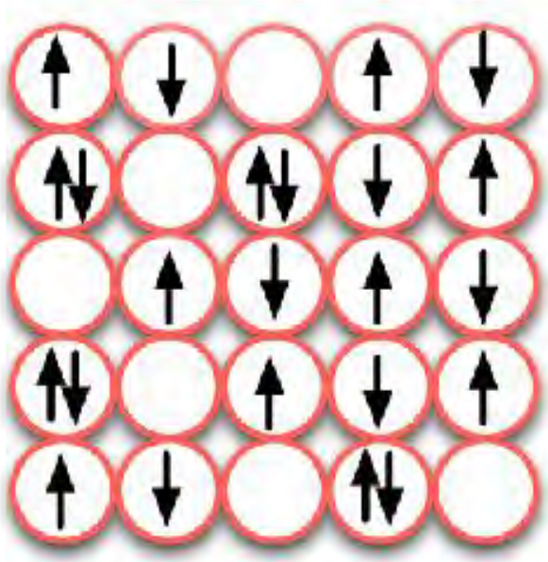
scheme of the lecture

- what is the final goal?
- minimal many-body models & DMFT
  - Hubbard dimer
  - one-band Hubbard model
  - multi-band Hubbard model
- building material-specific models
- what is special in multi-orbital models?

DMFT for the one-band Hubbard model

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

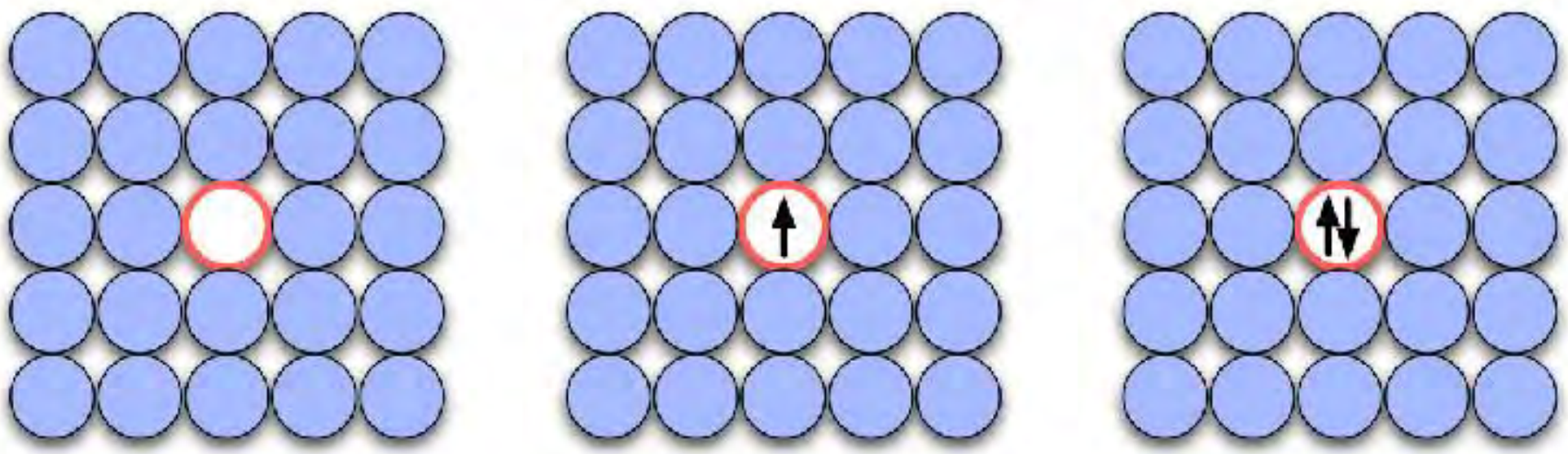
dynamical mean-field theory



$G^{i,j}$

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)

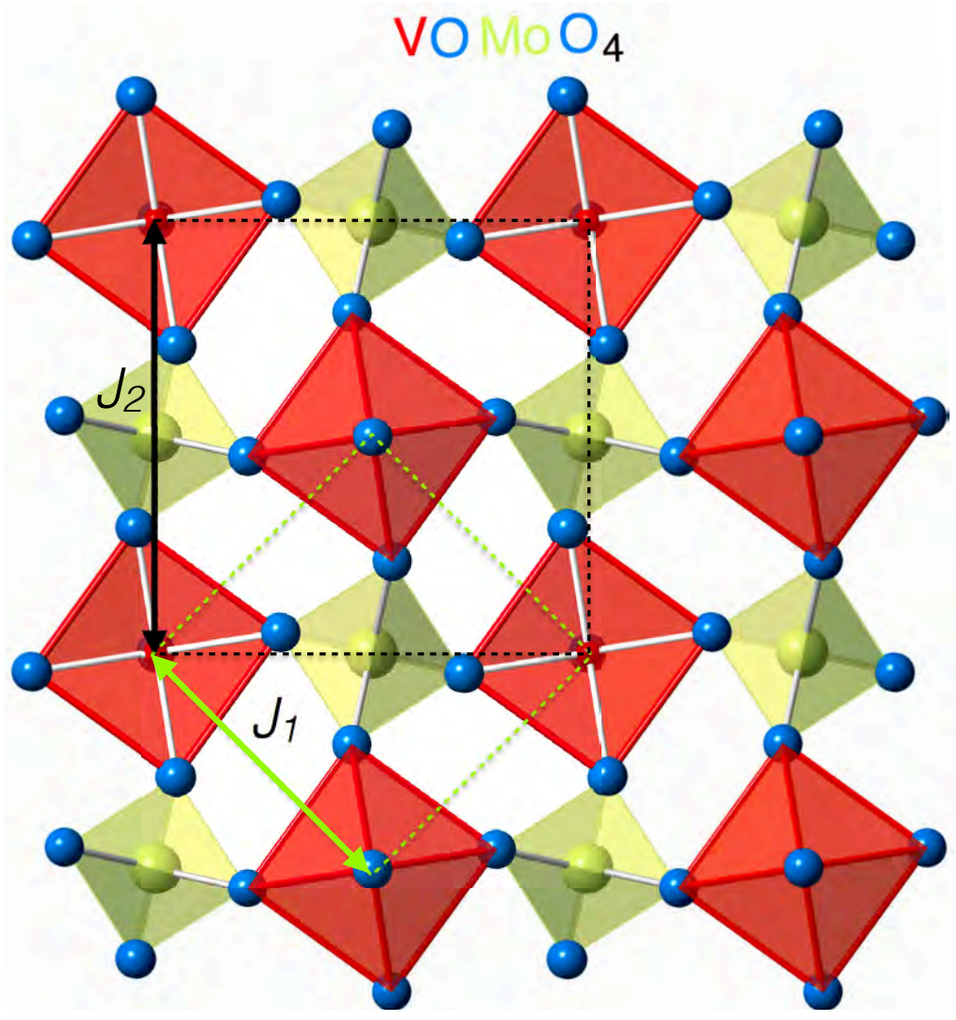
$$H_{\mathrm{A}} = \sum_\sigma \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_\sigma \varepsilon_f n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}$$

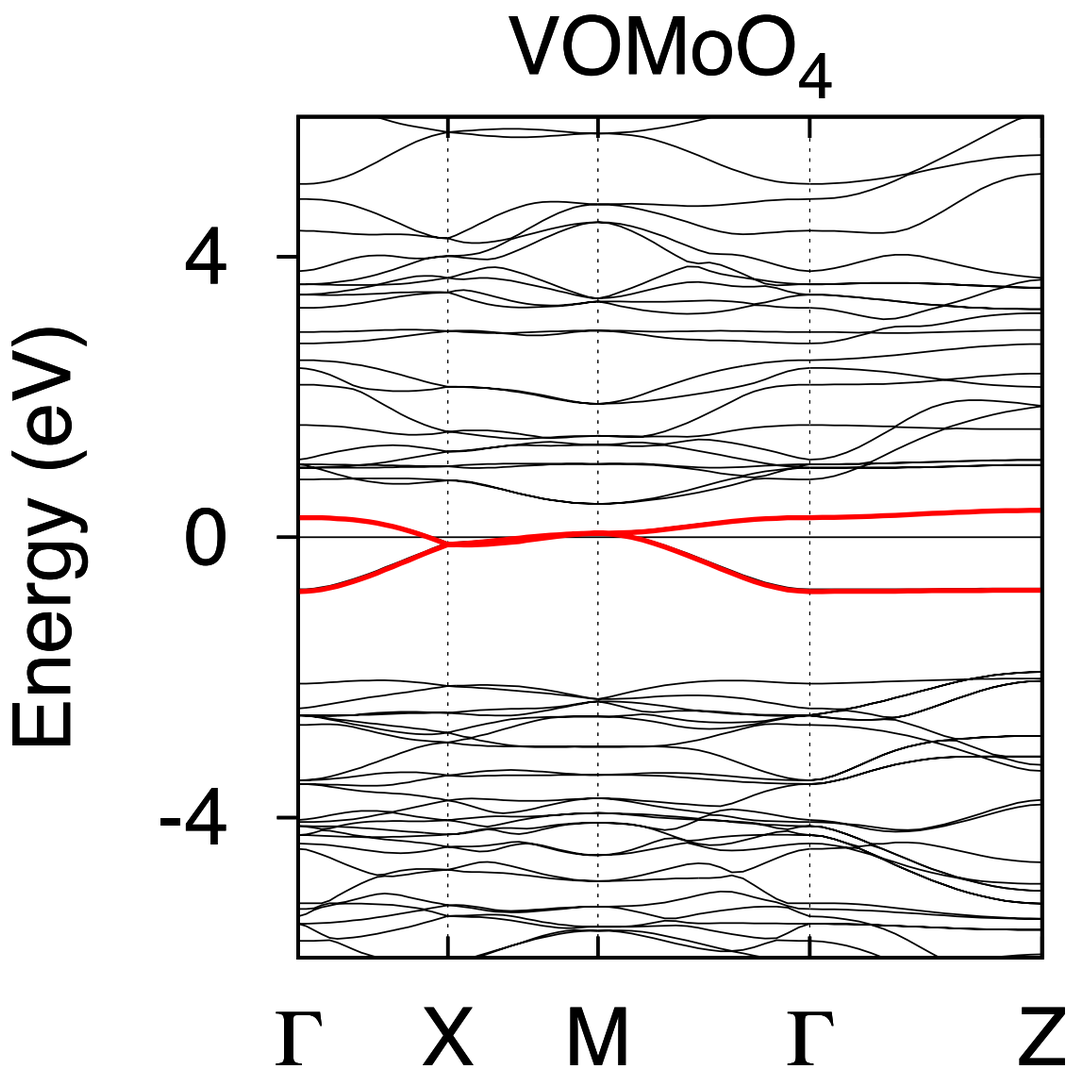
$$+ \sum_\sigma \sum_{\boldsymbol{k}} \left[V_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{f\sigma} + h.c. \right]$$

QIM solver: **QMC**, ED, NRG, DMRG,…

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

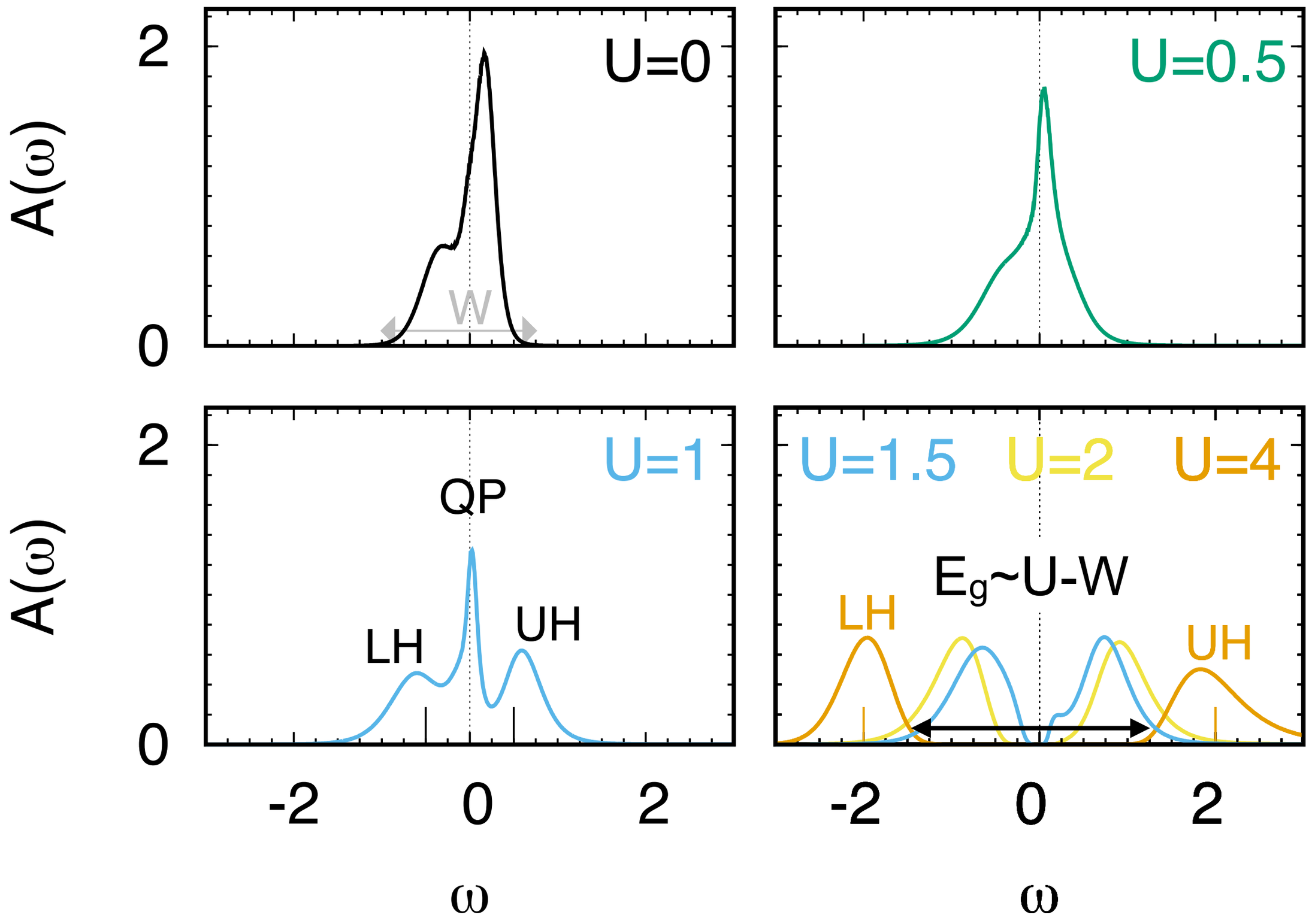
a real-system case: $VOMoO_4$





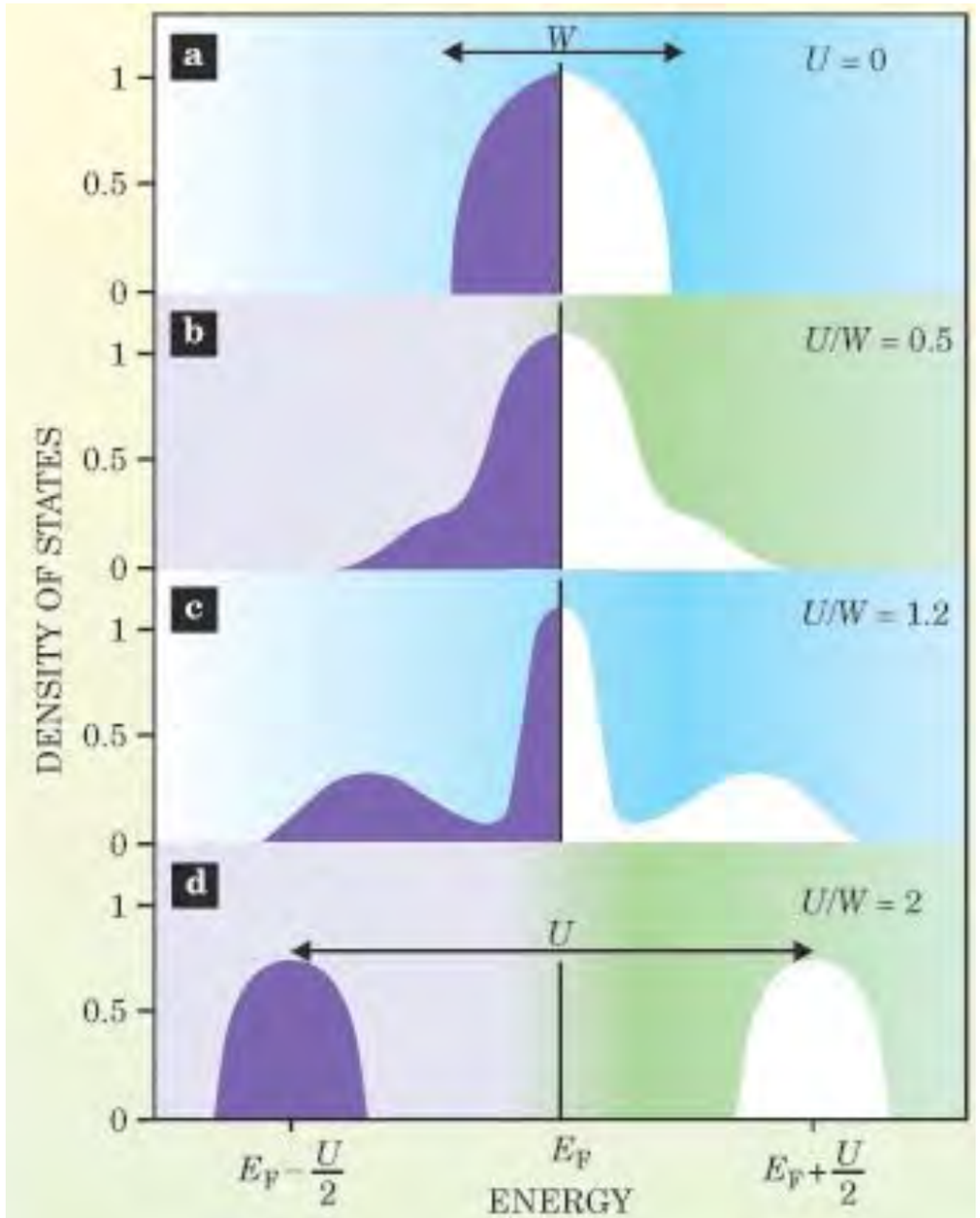
Amin Kiani and Eva Pavarini, Phys. Rev. B **94**, 075112 (2016)

a real-system: $VOMoO_4$



metal-insulator transition

Bethe lattice



insulating phase

$$\mathrm{Im}\Sigma(\omega + i0^+) = -\pi\rho_2\,\delta(\omega) \quad \text{for} \quad \omega \in [-\Delta_g/2, \Delta_g/2] \tag{235}$$

and that $\mathrm{Re}\Sigma$ has the following low-frequency behavior:

$$\mathrm{Re}\Sigma(\omega + i0^+) - U/2 = \frac{\rho_2}{\omega} + O(\omega). \tag{236}$$

A. Georges *et al.*, RMP **63**, 13 (1996)

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

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 case

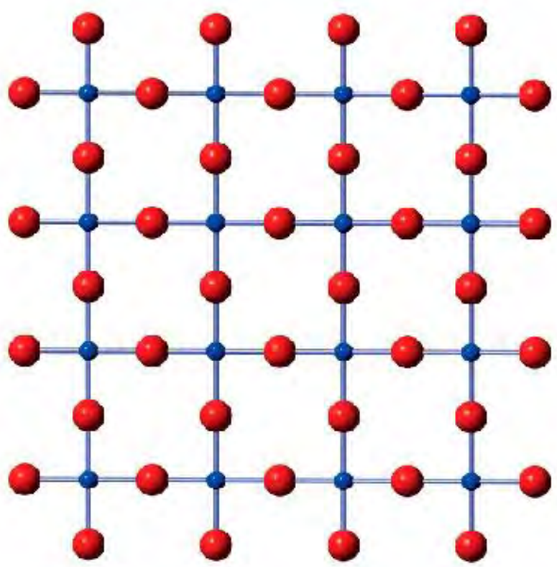
$$\hat{H}_{\mathrm{MF}} = \sum_{\boldsymbol{k}\sigma}\left[\varepsilon_{\boldsymbol{k}} + U\left(\frac{1}{2} - \sigma m\right)\right]\hat{n}_{\boldsymbol{k}\sigma}$$

self-energy

m: magnetization

ferromagnetic Hartree-Fock

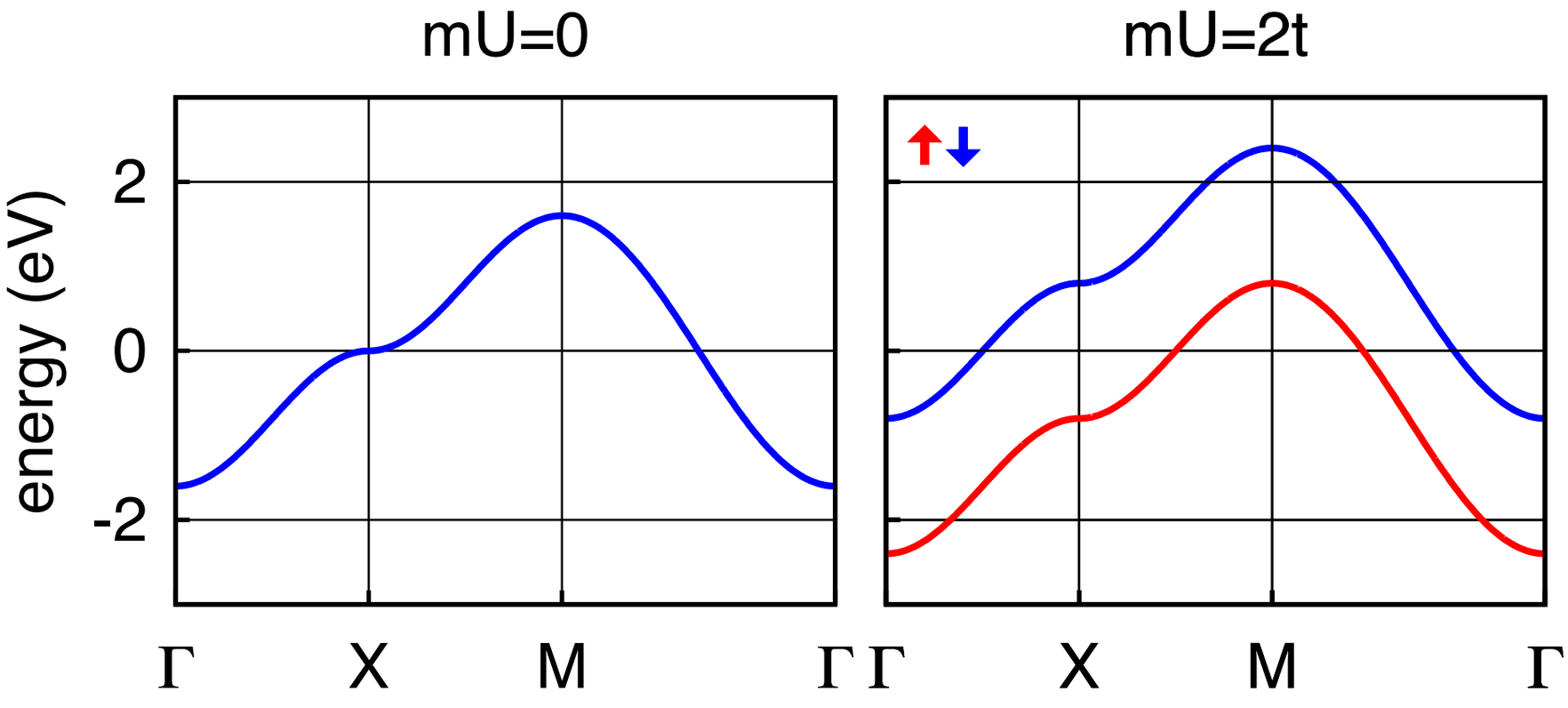
CuO_2



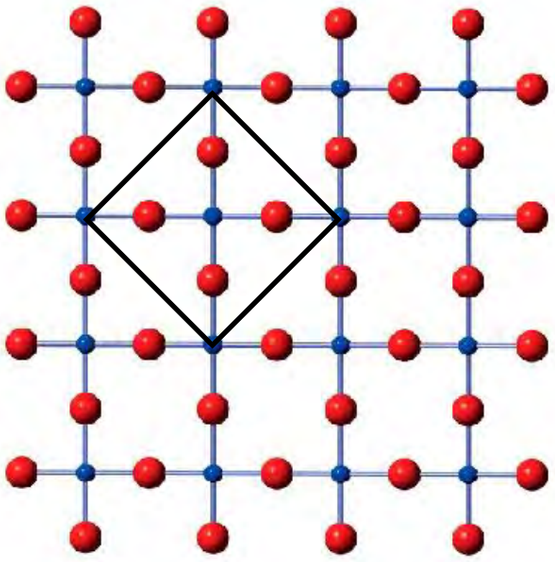
2d-tight binding model

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

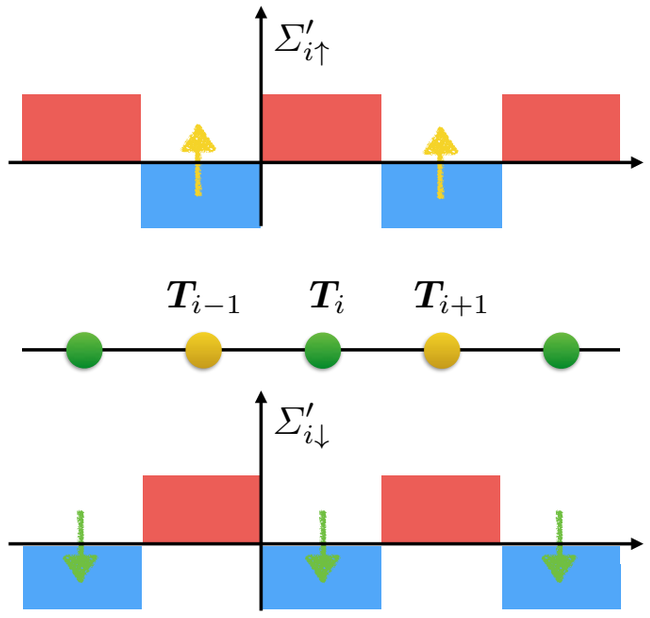
$$\Sigma^{\sigma}(k, i\nu_n) = U\left(\frac{1}{2} - \sigma m\right)$$

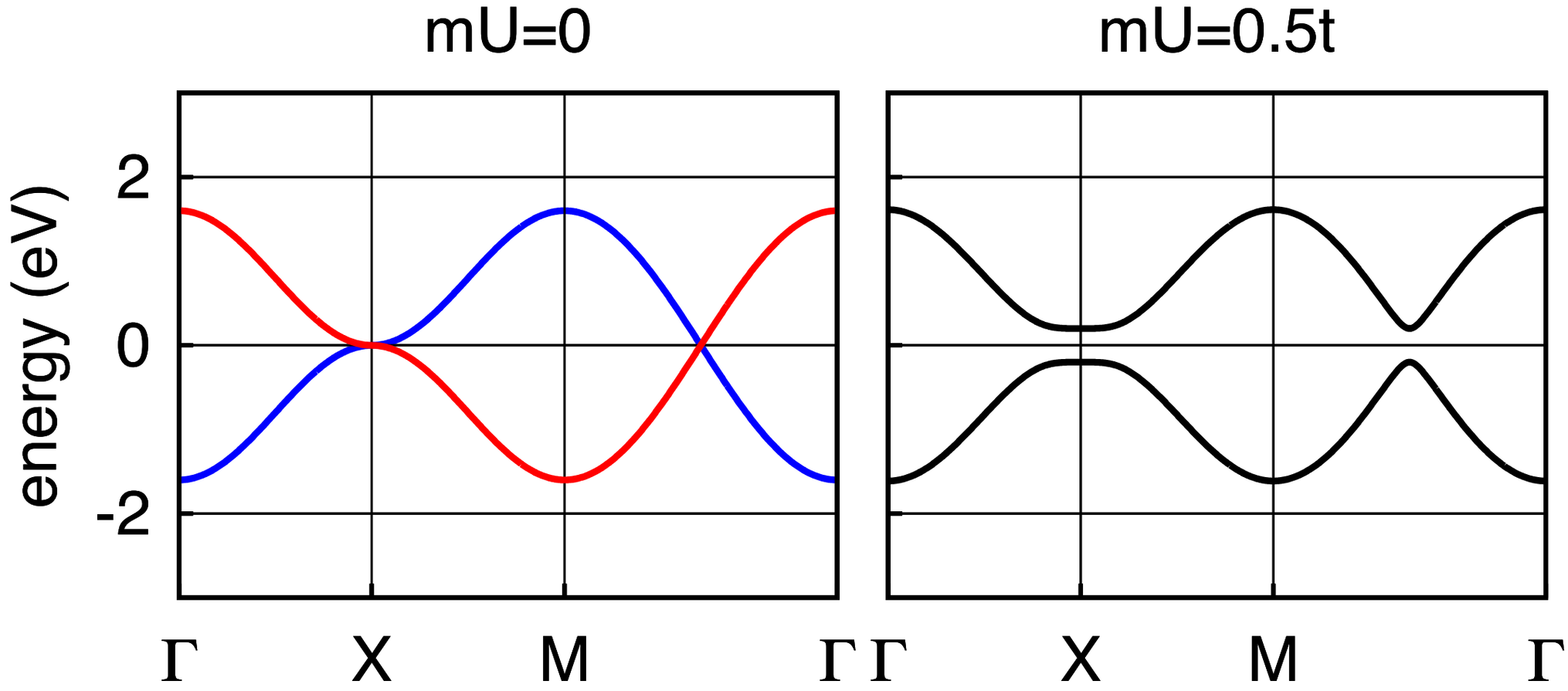


antiferromagnetic case



CuO_2

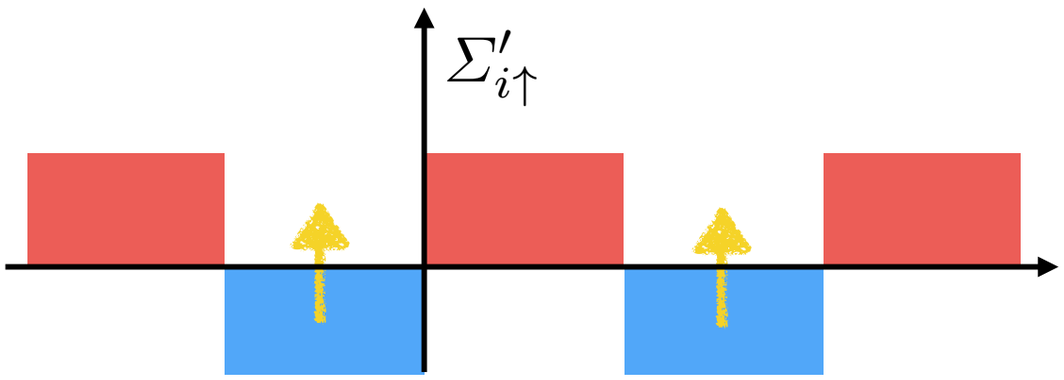


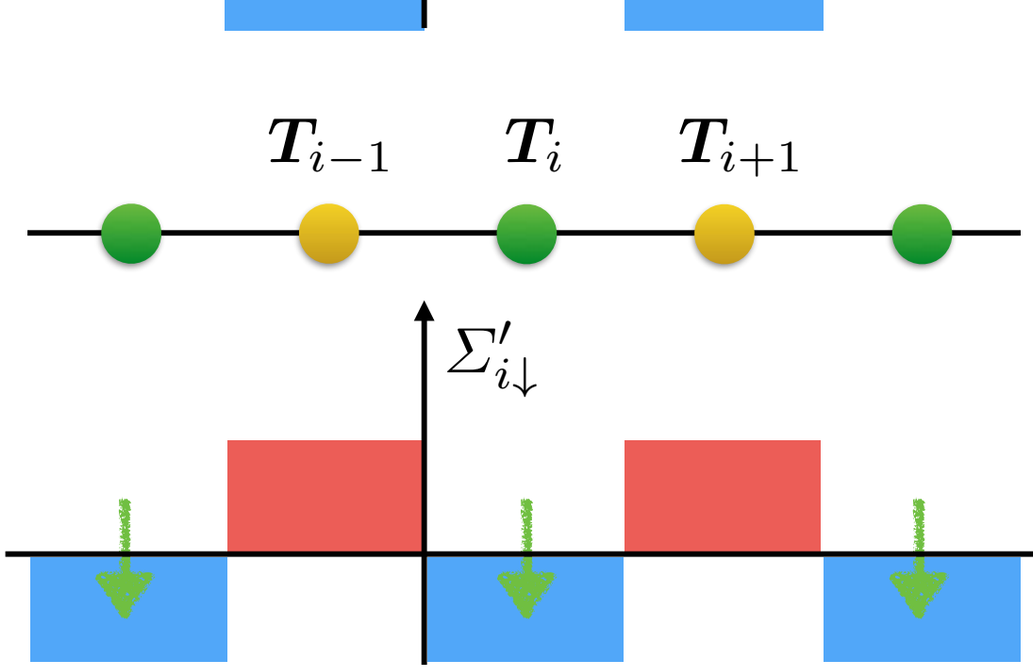


Mott transition: HF vs DMFT

LDA+*U*

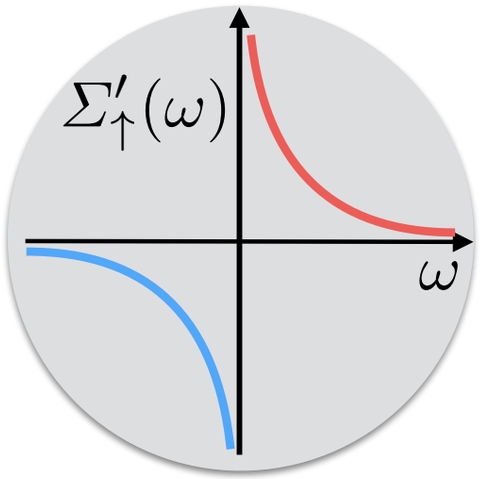
Hartree-Fock

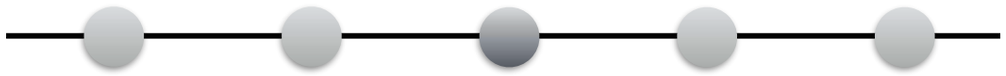


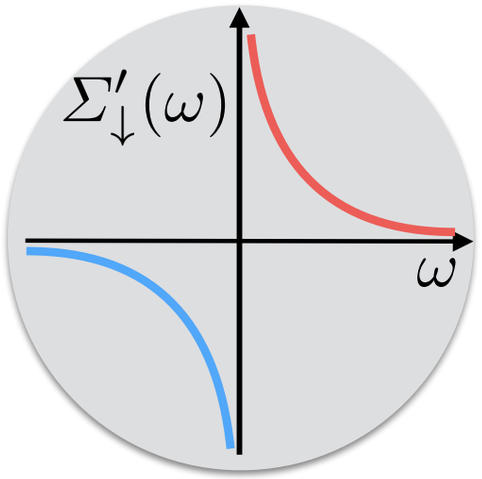


LDA+DMFT

DMFT







see my lecture notes in correl17

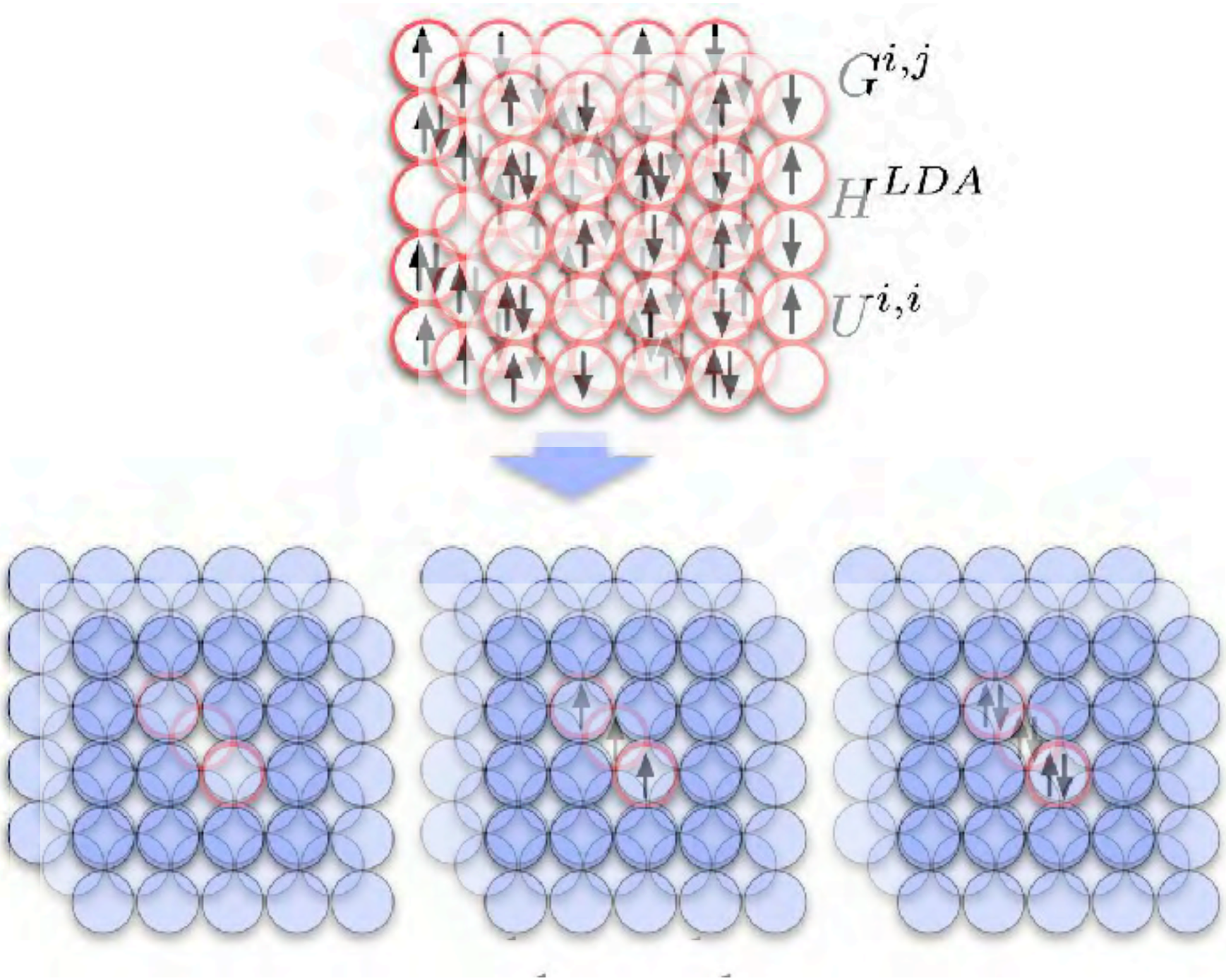
scheme of the lecture

- what is the final goal?
- minimal many-body models & DMFT
  - Hubbard dimer
  - one-band Hubbard model
  - multi-band Hubbard model
- building material-specific models
- what is special in multi-orbital models?

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

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

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

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

$$G_{m_\alpha, m'_\alpha}(i\nu_n) = G_{i_c m_\alpha, i_c m'_\alpha}(i\nu_n)$$

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

$\nu_n \to \tau$ $\quad \mathcal{G}(\tau)$

QMC

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

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

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

NO — converged? — YES

DONE!

$\Sigma(i\nu_n)$

$G(i\nu_n)$

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

scheme of the lecture

- what is the final goal?
- minimal many-body models & DMFT
  - Hubbard dimer
  - one-band Hubbard model
  - multi-band Hubbard model
- building material-specific models
- what is special in multi-orbital models?

0. chose the one-electron basis

LDA Wannier(-like) functions

$$\hat{H}_0 = -\sum_{\sigma} \sum_{ii'} \sum_{nn'} t^{i,i'}_{n,n'} c^{\dagger}_{in\sigma} c_{i'n'\sigma},$$

$$\hat{H}_U = \frac{1}{2} \sum_{ii'jj'} \sum_{\sigma\sigma'} \sum_{nn'pp'} U^{iji'j'}_{np\ n'p'} c^{\dagger}_{in\sigma} c^{\dagger}_{jp\sigma'} c_{j'p'\sigma'} c_{i'n'\sigma}.$$

why LDA Wannier functions?

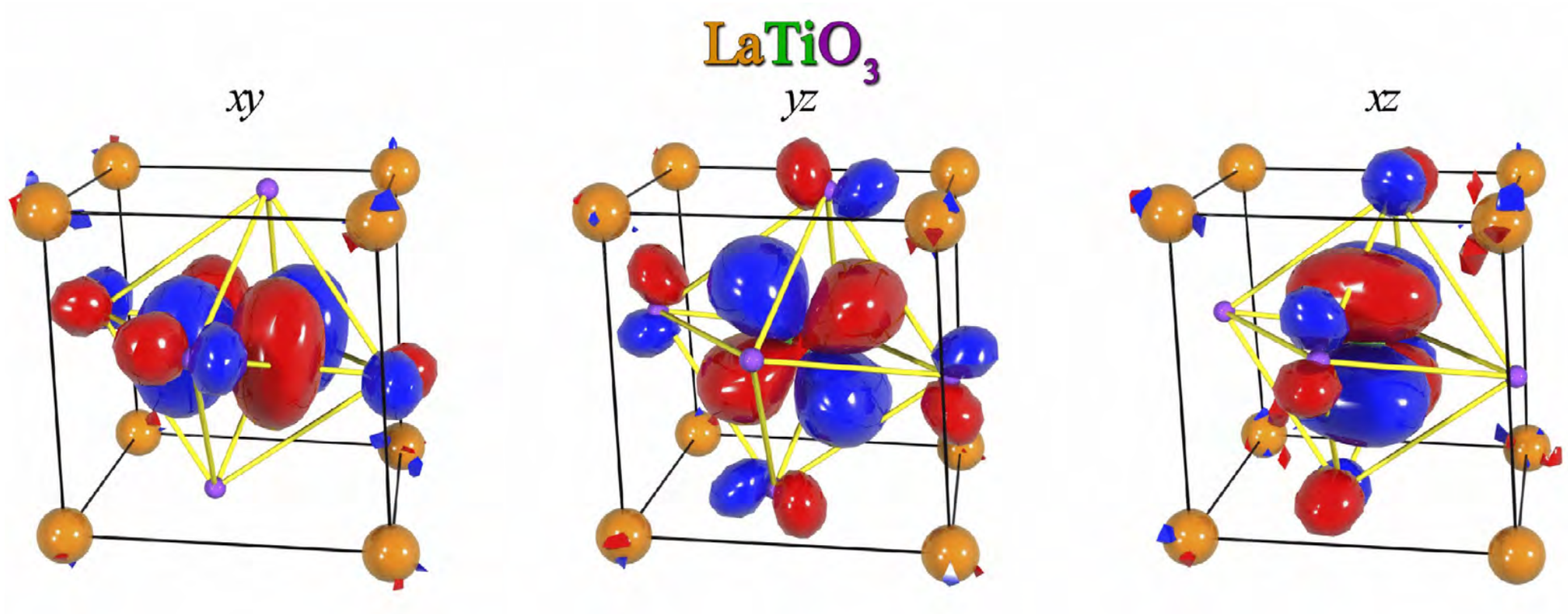
span exactly the one-electron Hamiltonian

can be constructed site-centered & orthogonal & localized

natural basis for **local** Coulomb terms

very good for weakly correlated systems

information on lattice and chemistry

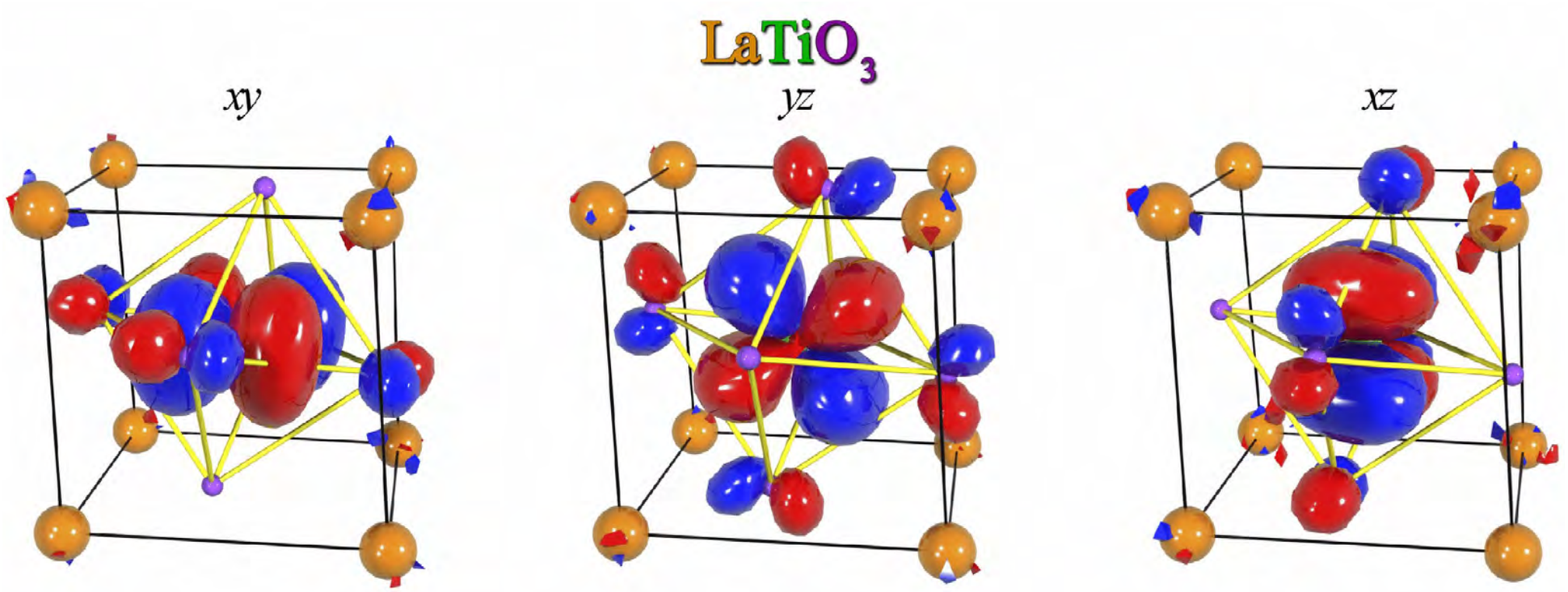


why LDA Wannier functions?

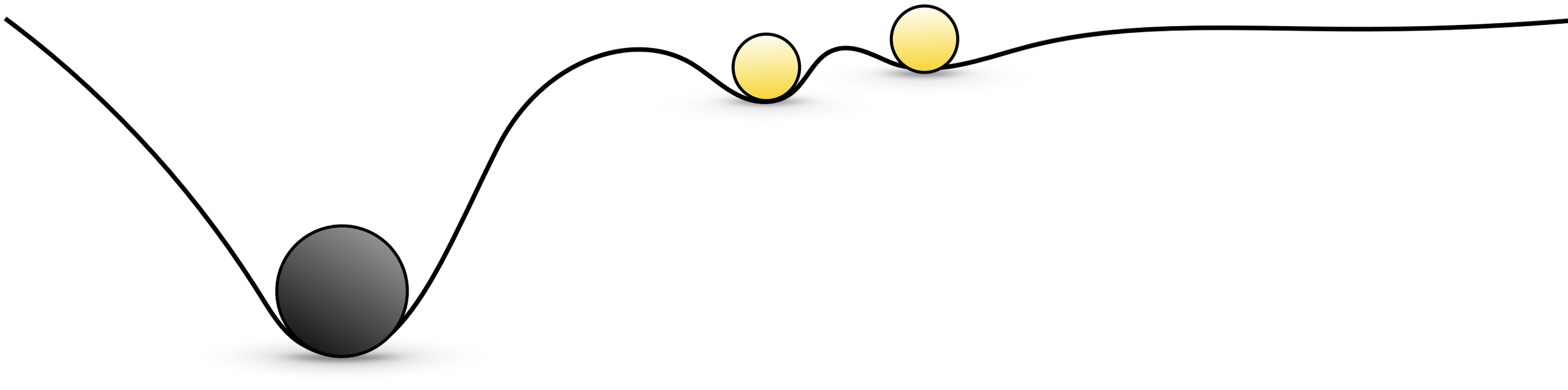
$$\hat{H}_e = \hat{H}_0 + \hat{H}_U \longrightarrow \hat{H}^{\mathrm{LDA}} + \hat{H}_U - \hat{H}_{dc}$$

ΔU

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



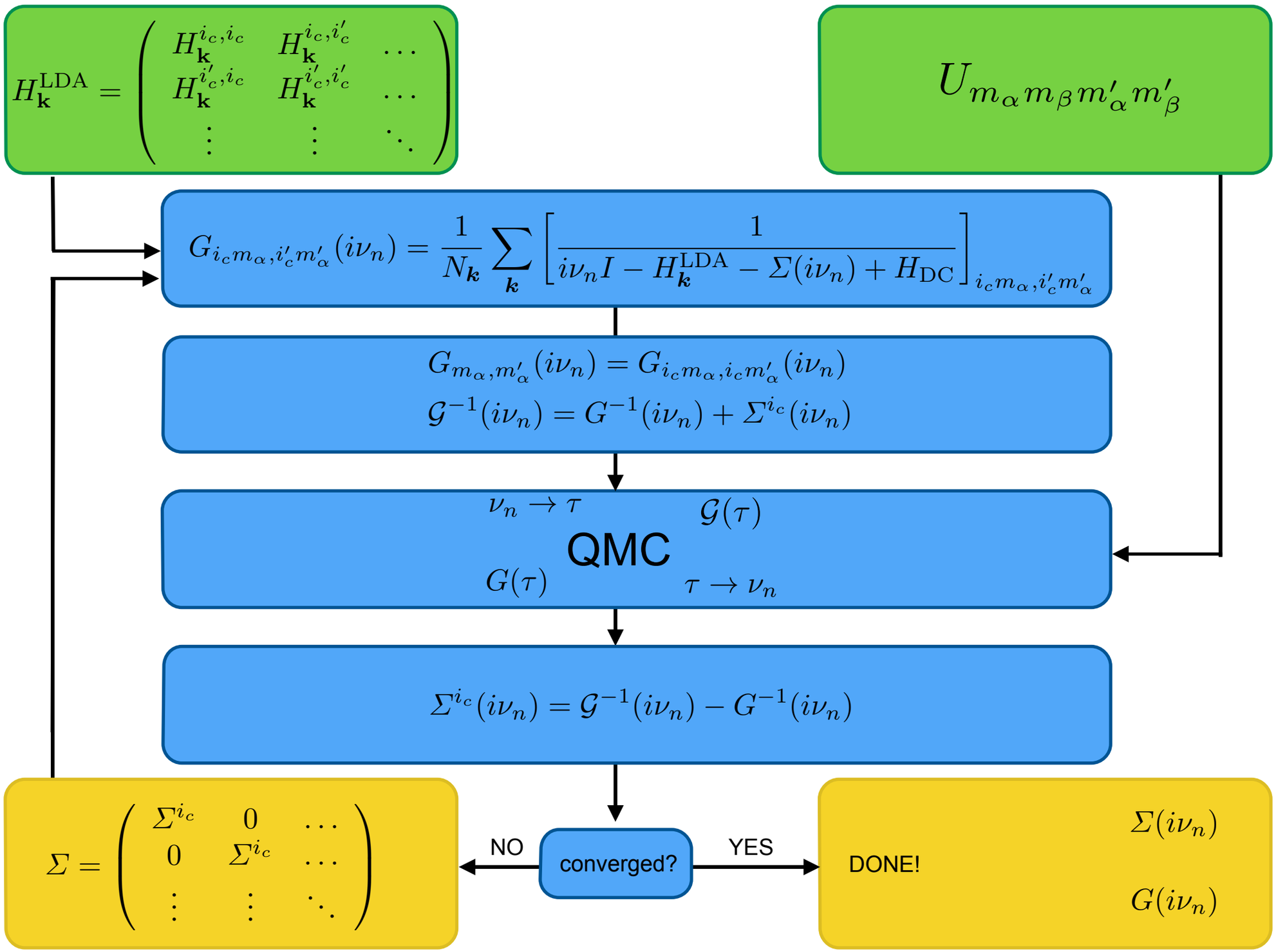
1. heavy electrons, light electrons



light electrons → DFT (LDA, GGA,…)

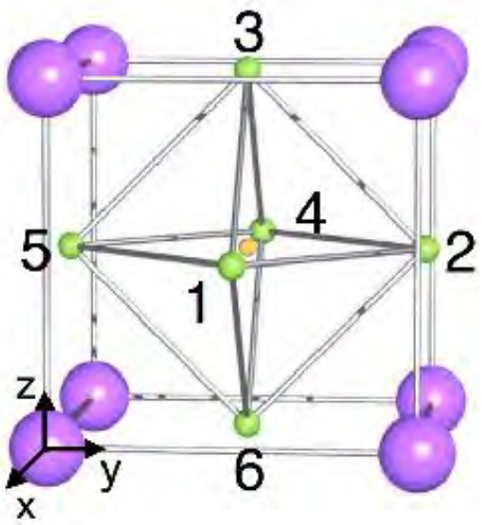
heavy electrons → ΔU correction, DMFT

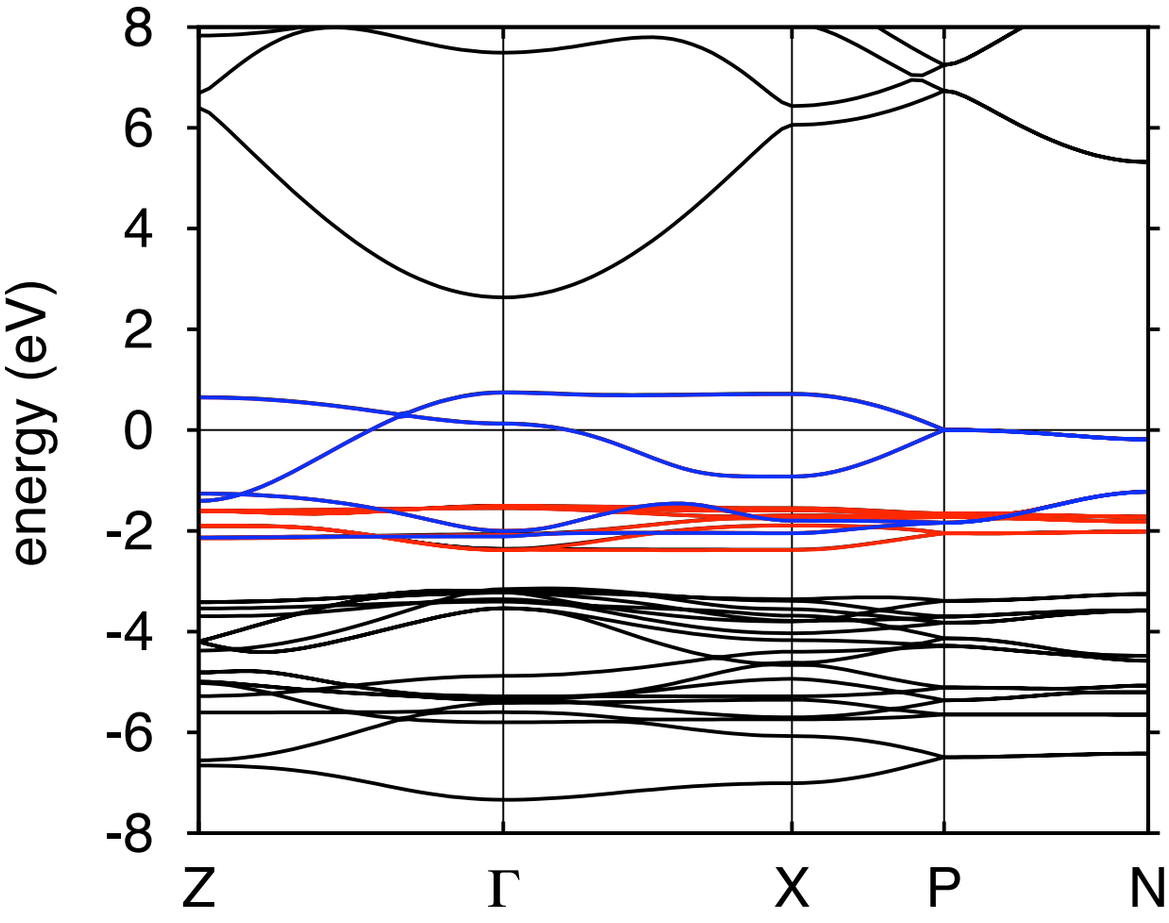
self-consistency loop



2. downfolding

$KCuF_3$





e_g

t_{2g}

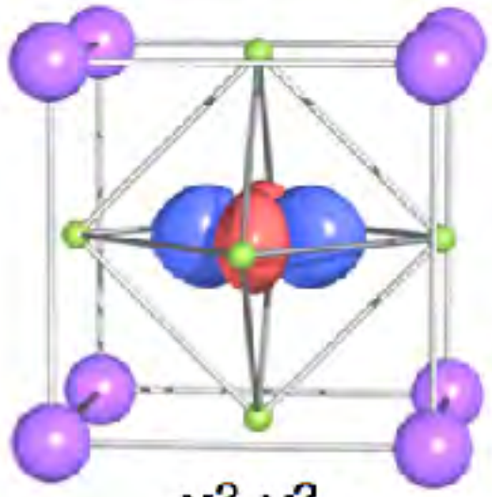
integrate out light electrons

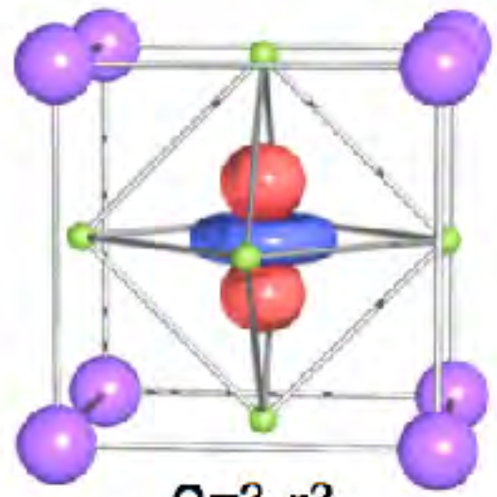
effects of downfolding

no downfolding

more parameters & H_{DC}

WF more localized



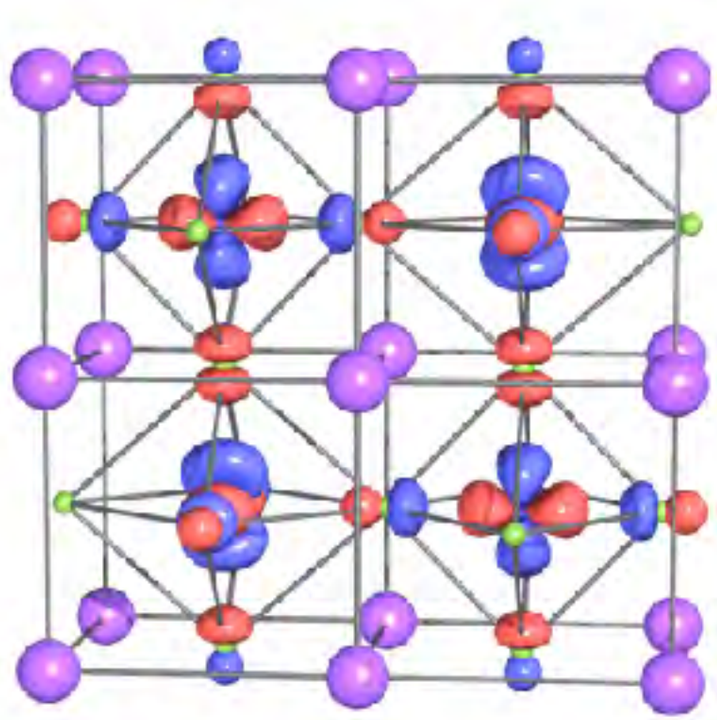


massive downfolding

e_g

less parameters & no H_{DC}

WF less localized



no DC correction

around mean-field approximation

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

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

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

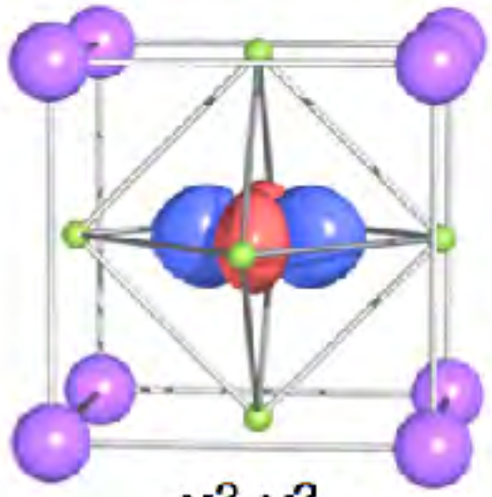
$$\hat{H}_{\mathrm{DC}} = \frac{n}{2} U \sum_i \left(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} - \frac{n}{2} \right) = \delta\mu \hat{N} - \mathrm{const}$$

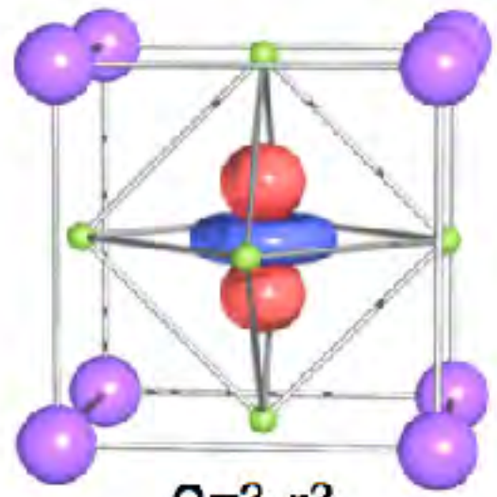
effects of downfolding

no downfolding

more parameters & H_{DC}

WF more localized



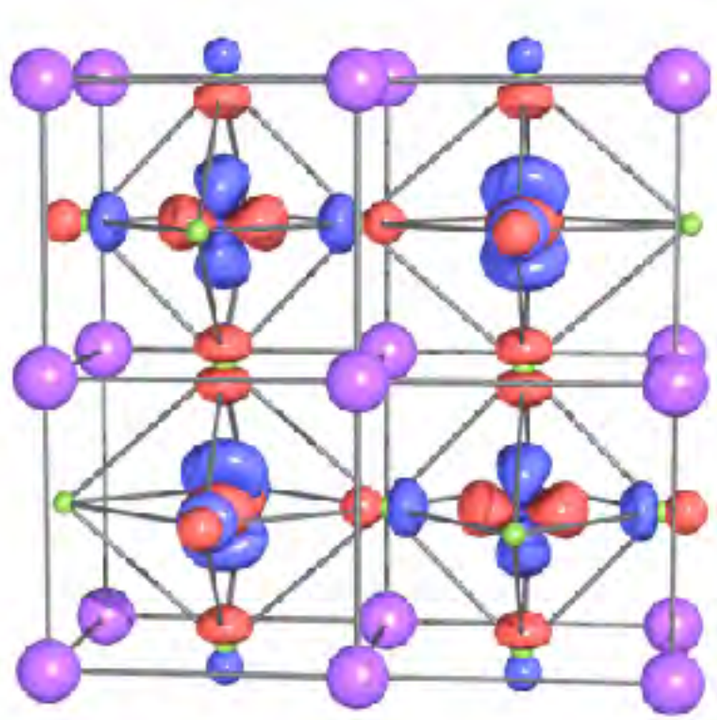


massive downfolding

e_g

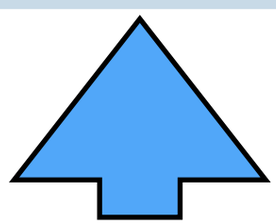
less parameters & no H_{DC}

WF less localized



how important is localization?

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



local or almost local

strong correlations arise from strong local Coulomb

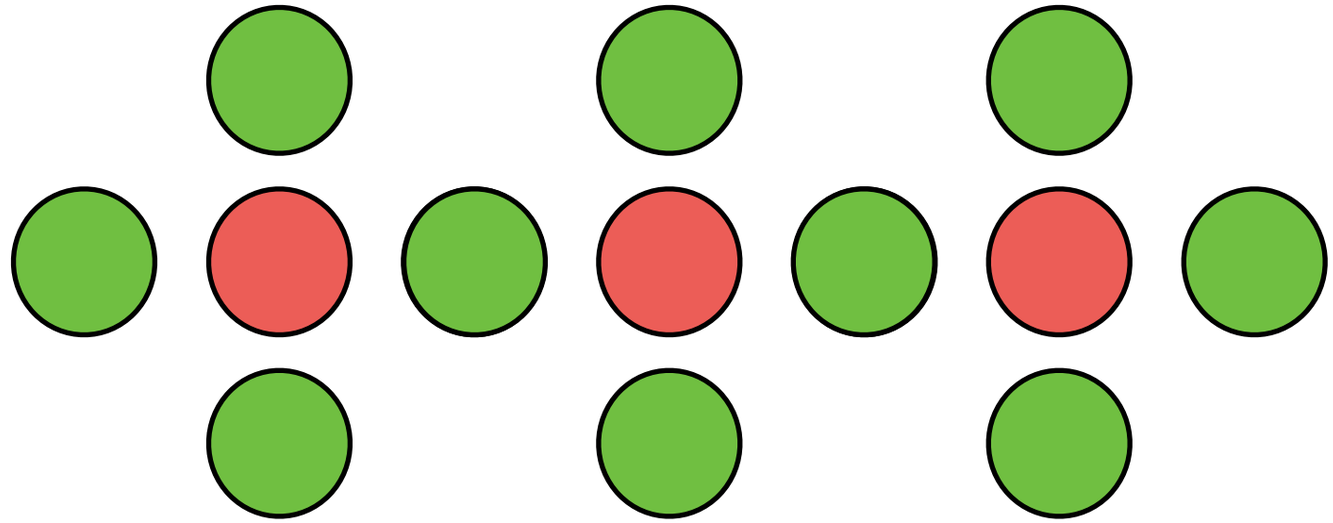
$$U^{iji'j'}_{np\ n'p'} = \int d\mathbf{r}_1 \int d\mathbf{r}_2\ \overline{\psi_{in\sigma}}(\mathbf{r}_1)\overline{\psi_{jp\sigma'}}(\mathbf{r}_2)\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\psi_{j'p'\sigma'}(\mathbf{r}_2)\psi_{i'n'\sigma}(\mathbf{r}_1).$$

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

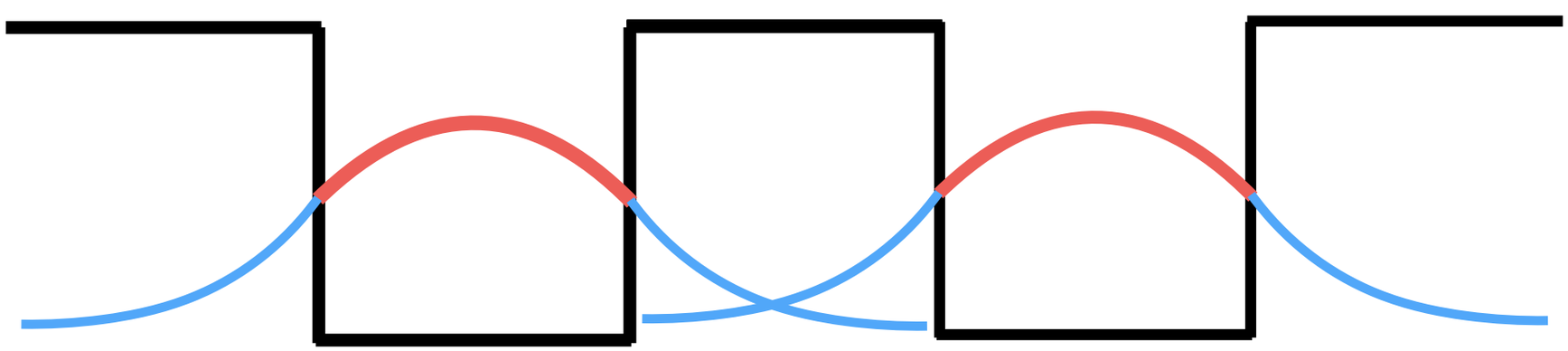
$$U^{iji'j'}_{mp\ m'p'} \propto \frac{\delta_{i,i'}\delta_{j,j'}}{|\boldsymbol{T}_i - \boldsymbol{T}_j|},$$

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?

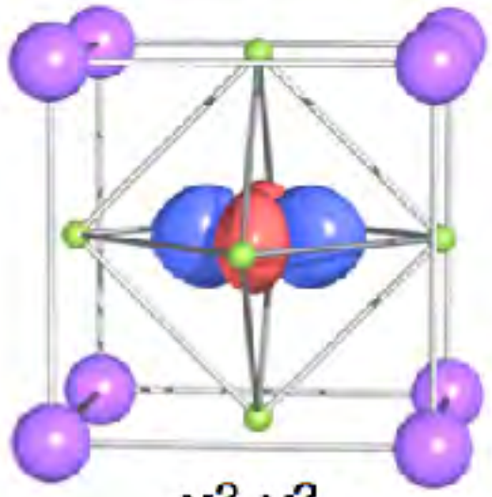


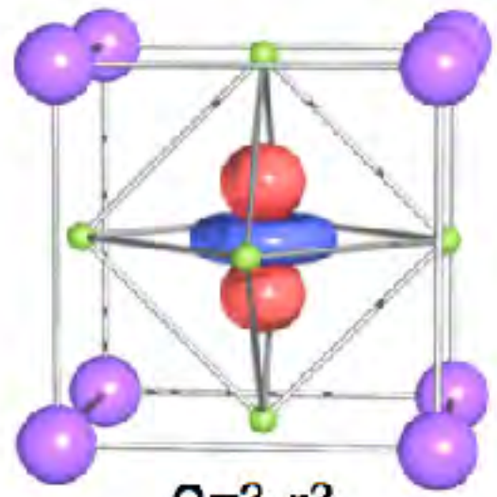
effects of downfolding

no downfolding

more parameters & H_{DC}

WF more localized



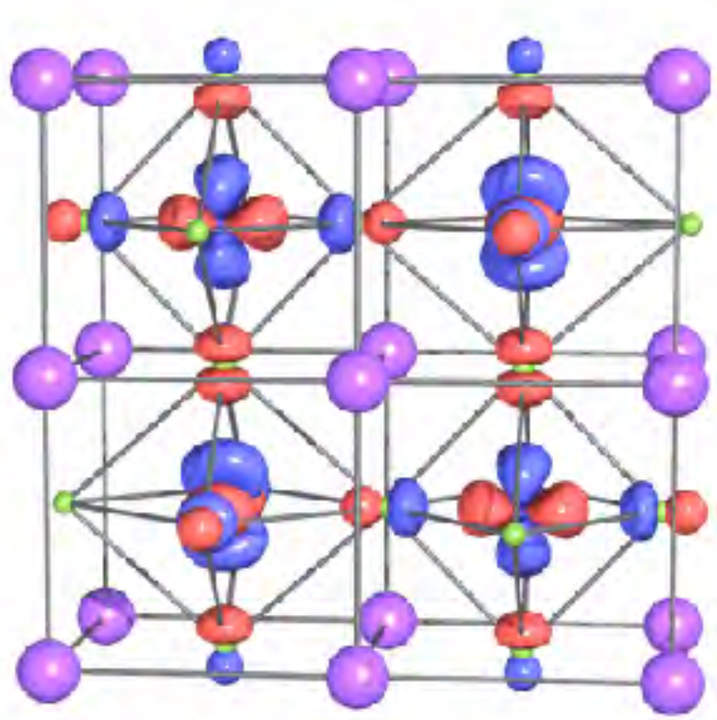


massive downfolding

e_g

less parameters & no H_{DC}

WF less localized



3. Screening

$$\hat{H}_e = \hat{H}^{\mathrm{LDA}} + \hat{H}^l_U - \hat{H}^l_{\mathrm{DC}}$$

$$\hat{H}^{\mathrm{LDA}} = \sum_{\boldsymbol{k}} \sum_{\sigma} \sum_{m_\alpha m'_\alpha} \left[H^{\mathrm{LDA}}_{\boldsymbol{k}}\right]_{m_\alpha, m'_\alpha} c^\dagger_{\boldsymbol{k} m_\alpha \sigma} c_{\boldsymbol{k} m'_\alpha \sigma},$$

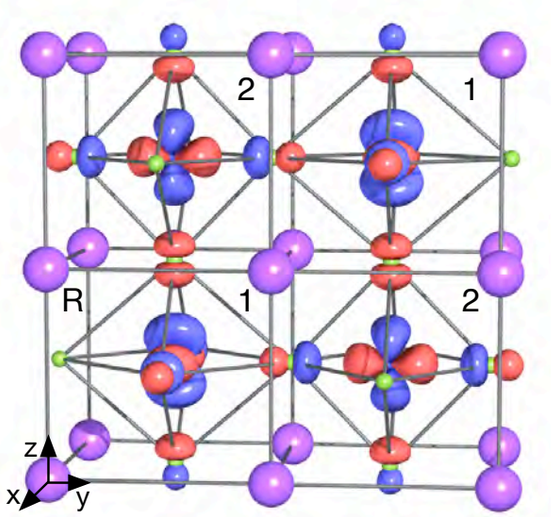
$$\hat{H}^l_U = \frac{1}{2} \sum_i \sum_{\sigma\sigma'} \sum_{m_\alpha m'_\alpha} \sum_{m_\beta m'_\beta} U_{m_\alpha m_\beta m'_\alpha m'_\beta} c^\dagger_{i m_\alpha \sigma} c^\dagger_{i m_\beta \sigma'} c_{i m'_\beta \sigma'} c_{i m'_\alpha \sigma}.$$

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

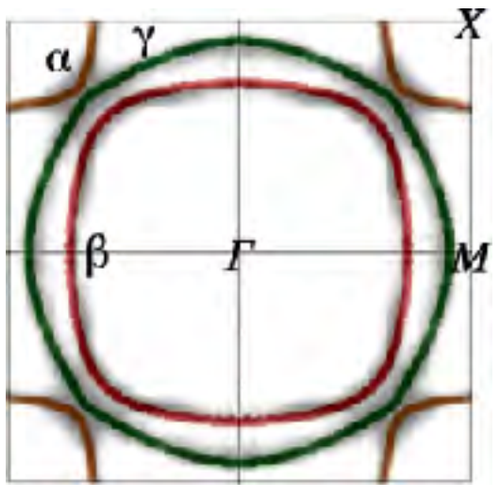
screening: **approximate** schemes such as cRPA, cLDA

what can we do?

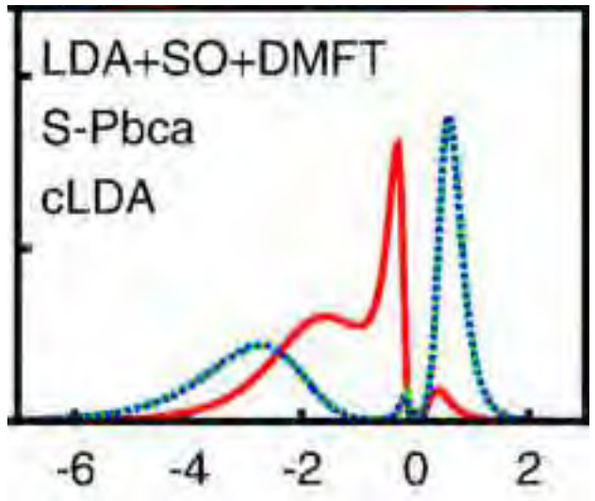
orbital order



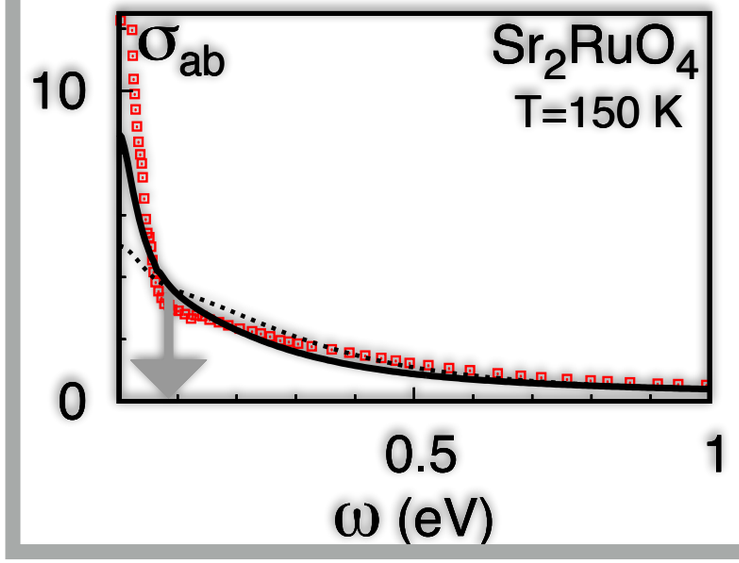
Fermi surface



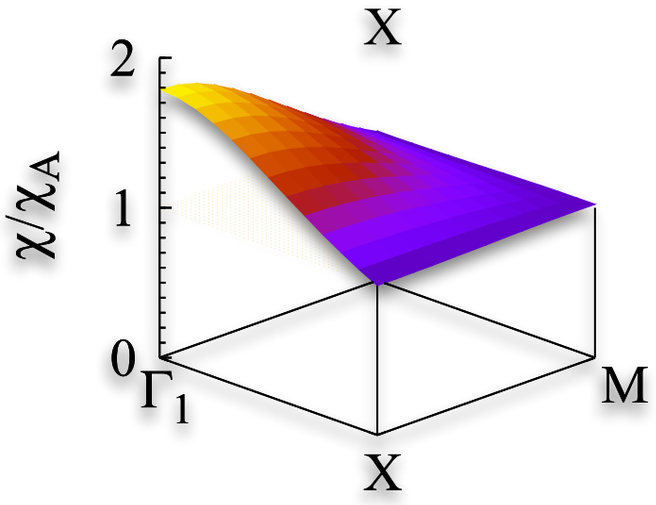
spin-orbit



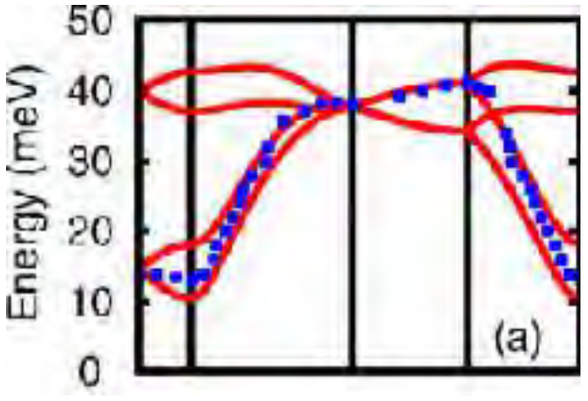
conductivity



response functions

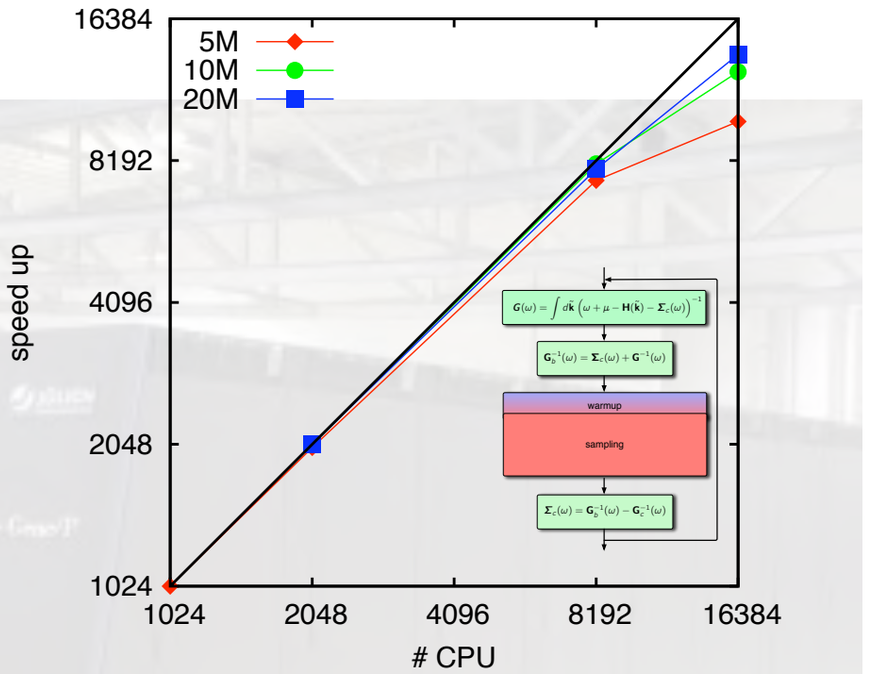


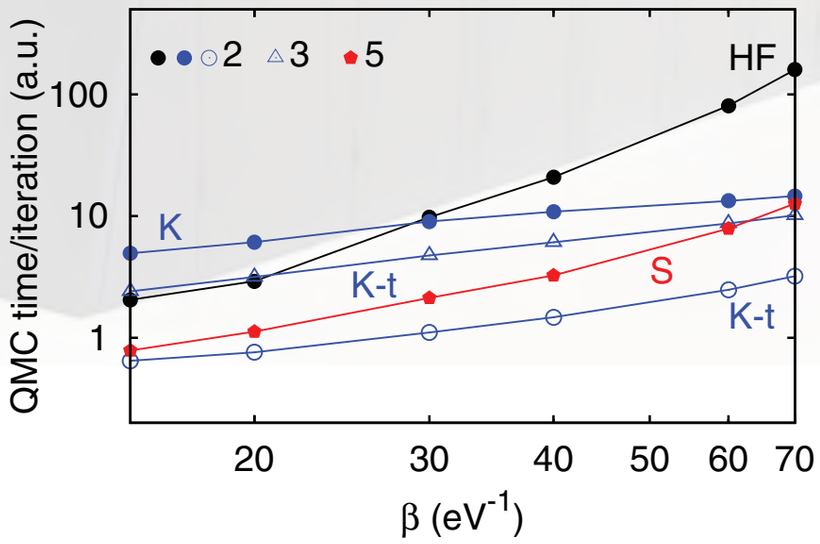
spin waves



our codes

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





DMFT and cDMFT

quantum impurity solvers:

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

JÜLICH
FORSCHUNGSZENTRUM

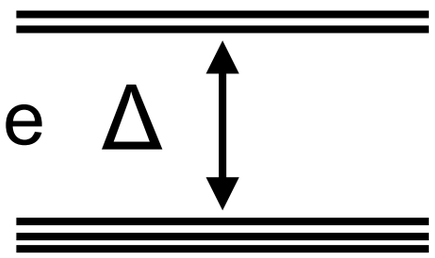
scheme of the lecture

- what is the final goal?
- minimal many-body models & DMFT
  - Hubbard dimer
  - one-band Hubbard model
  - multi-band Hubbard model
- building material-specific models
- what is special in multi-orbital models?

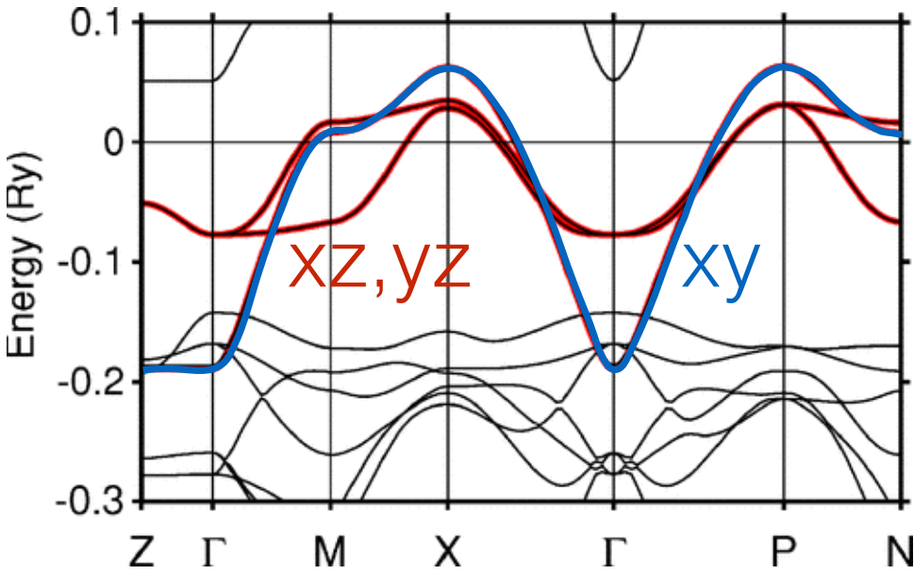
what is special in multi-orbital models?

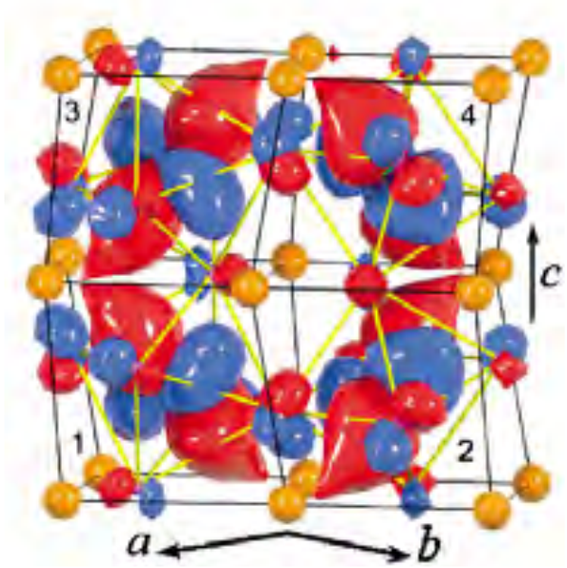
representative t_{2g} systems

perovskites with very large Δ



$YTiO_3$: orbitally-ordered insulator $t_{2g}^1 e_g^0$





Sr_2RuO_4: correlated metal $t_{2g}^4 e_g^0$

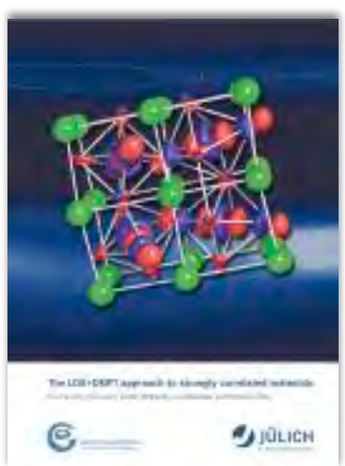
multi-orbital models for t_{2g} bands

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

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

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

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



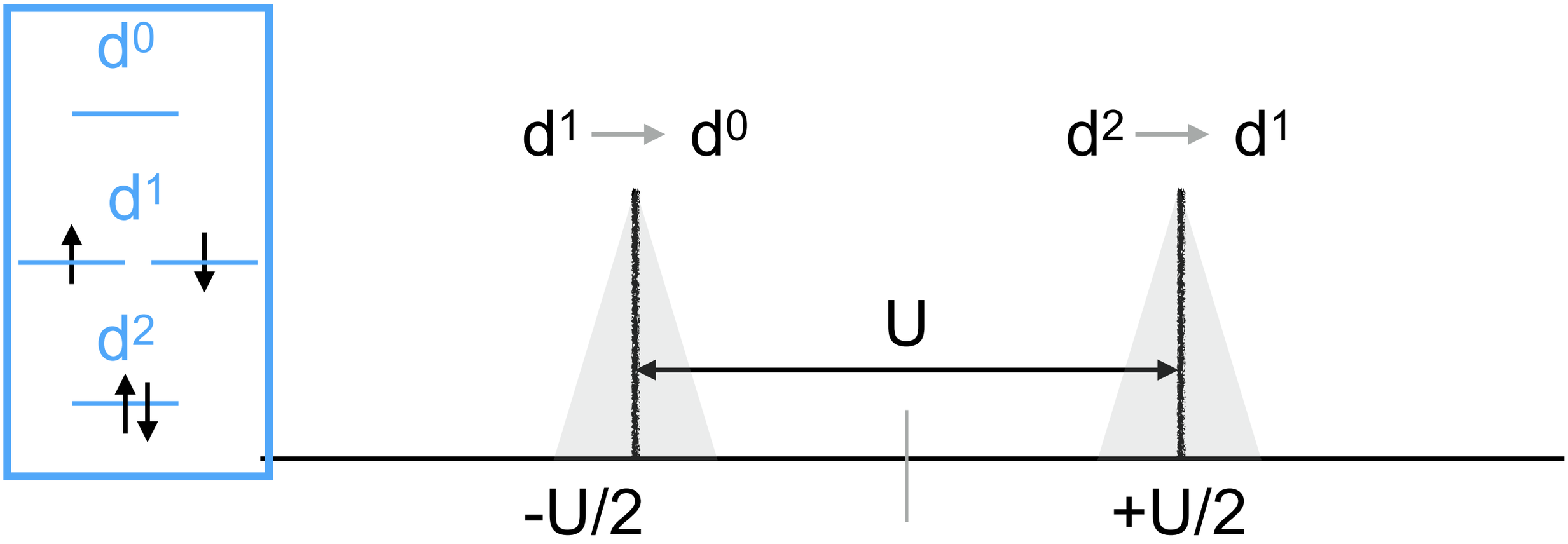
1. Hund’s rule coupling *J* & atomic multiplets
2. Orbital degeneracy, orbital order & crystal field
3. Spin-orbit coupling & non-spherical U

1. Hund’s rule coupling *J* & multiplets

one band model, atomic limit d^1

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

$$G^{\sigma}_{ii}(i\nu_n) = \frac{1}{2}\left[\frac{1}{i\nu_n - (\underbrace{\varepsilon_d - \mu}_{E(N)-E(N-1)-\mu})} + \frac{1}{i\nu_n - (\underbrace{\varepsilon_d + U - \mu}_{E(N+1)-E(N)-\mu})} \right]$$



atomic limit and multiplets

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

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

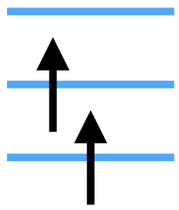
$$- J \sum_{i\ m \neq m'} \left(c^{\dagger}_{im\uparrow} c^{\dagger}_{im\downarrow} c_{im'\uparrow} c_{im'\downarrow} + c^{\dagger}_{im\uparrow} c_{im\downarrow} c^{\dagger}_{im'\downarrow} c_{im'\uparrow} \right)$$

t_{2g} atomic levels & Hund's rule

$\lvert N; S, m_S\rangle$			$E(N,S)$
$\lvert 0\rangle$			
$\lvert 1; \frac{1}{2}, \frac{\sigma}{2}\rangle$	$=$	$c^\dagger_{m\sigma}\lvert 0\rangle$	
$\lvert 2; 0, 0\rangle_a$	$=$	$\frac{1}{\sqrt{3}}\left[c^\dagger_{xz\uparrow}c^\dagger_{xz\downarrow} + c^\dagger_{yz\uparrow}c^\dagger_{yz\downarrow} + c^\dagger_{xy\uparrow}c^\dagger_{xy\downarrow}\right]\lvert 0\rangle$	$U+2J$
$\lvert 2; 0, 0\rangle_b$	$=$	$\frac{1}{\sqrt{6}}\left[c^\dagger_{xz\uparrow}c^\dagger_{xz\downarrow} + c^\dagger_{yz\uparrow}c^\dagger_{yz\downarrow} - 2c^\dagger_{xy\uparrow}c^\dagger_{xy\downarrow}\right]\lvert 0\rangle$	$U-J$
$\lvert 2; 0, 0\rangle_c$	$=$	$\frac{1}{\sqrt{2}}\left[c^\dagger_{xz\uparrow}c^\dagger_{xz\downarrow} - c^\dagger_{yz\uparrow}c^\dagger_{yz\downarrow}\right]\lvert 0\rangle$	$U-J$
$\lvert 2; 1, \sigma, m''\rangle$	$=$	$c^\dagger_{m\sigma}c^\dagger_{m'\sigma}\lvert 0\rangle$	$U-3J$
$\lvert 2; 1, 0, m''\rangle$	$=$	$\frac{1}{\sqrt{2}}\left[c^\dagger_{m\uparrow}c^\dagger_{m'\downarrow} + c^\dagger_{m\downarrow}c^\dagger_{m'\uparrow}\right]\lvert 0\rangle$	$U-3J$
$\lvert 2; 0, 0, m''\rangle$	$=$	$\frac{1}{\sqrt{2}}\left[c^\dagger_{m\uparrow}c^\dagger_{m'\downarrow} - c^\dagger_{m\downarrow}c^\dagger_{m'\uparrow}\right]\lvert 0\rangle$	$U-J$
$\lvert 3; \frac{3}{2}, \frac{3\sigma}{2}\rangle$	$=$	$c^\dagger_{xz\sigma}c^\dagger_{yz\sigma}c^\dagger_{xy\sigma}\lvert 0\rangle$	$3U-9J$
$\lvert 3; \frac{3}{2}, \frac{\sigma}{2}\rangle$	$=$	$\frac{1}{\sqrt{3}}\left[c^\dagger_{xz\sigma}c^\dagger_{yz\sigma}c^\dagger_{xy-\sigma} + c^\dagger_{xz\sigma}c^\dagger_{yz-\sigma}c^\dagger_{xy\sigma} + c^\dagger_{xz-\sigma}c^\dagger_{yz\sigma}c^\dagger_{xy\sigma}\right]\lvert 0\rangle$	$3U-9J$

d^0 1 state

d^1 6 states



d^2 S=1

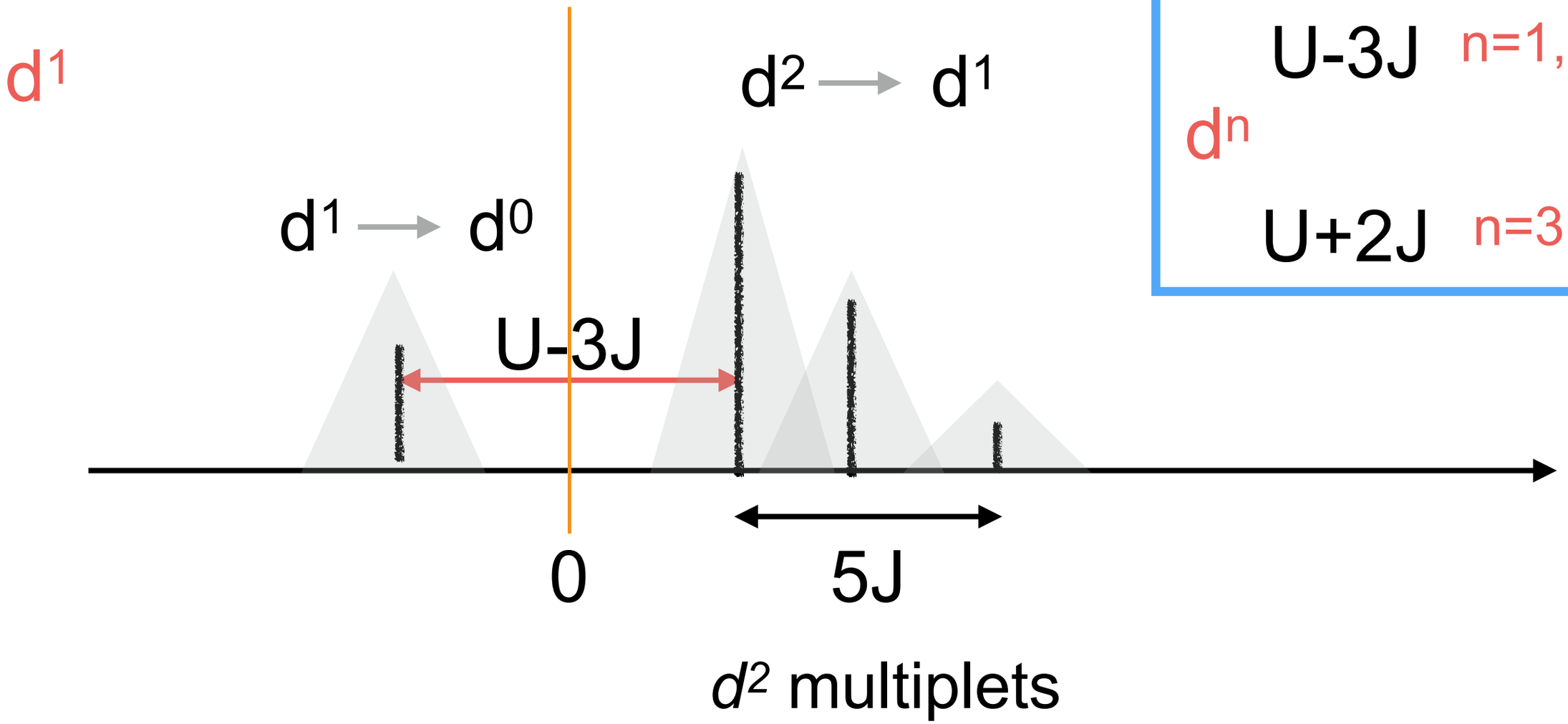
15 states

no crystal -field, t_{2g} Green function

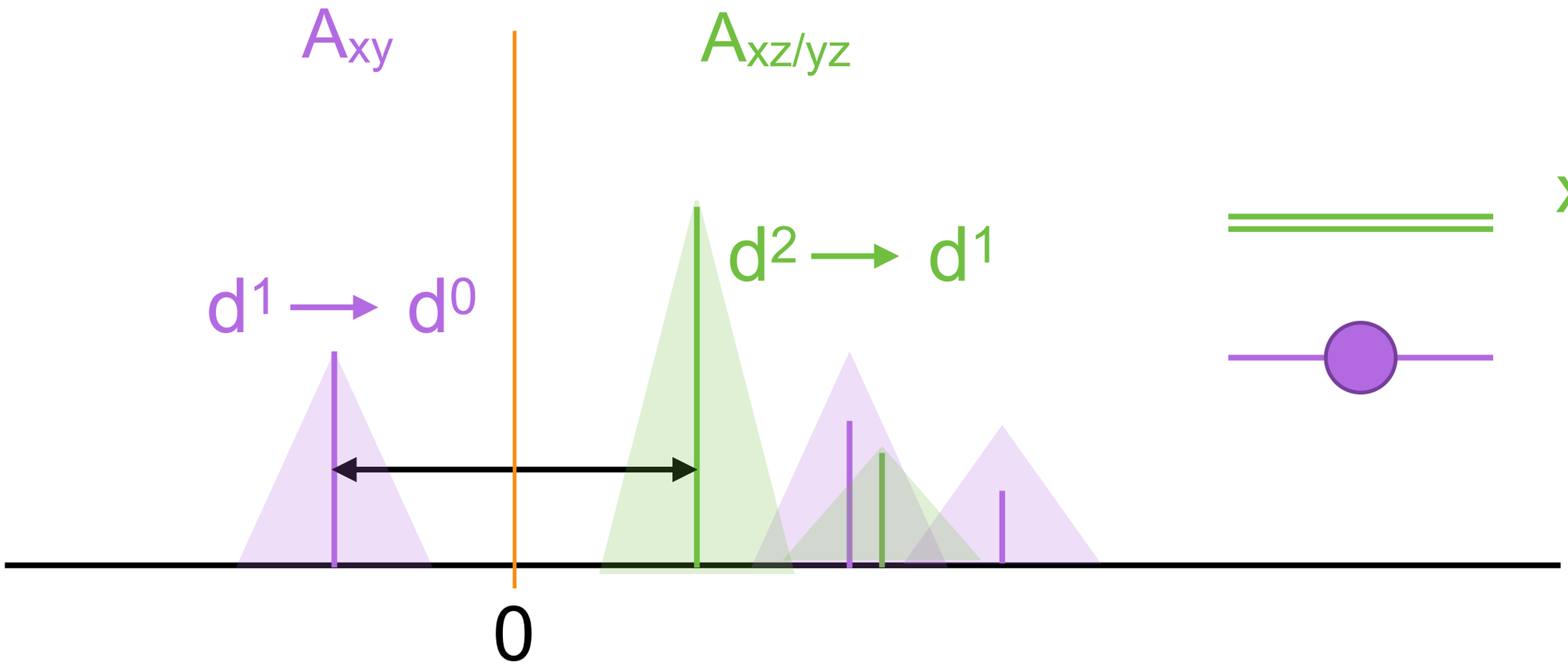
m=xy,xz,yz

$$G^{\sigma}_{m}(i\nu_n) = \frac{1}{6}\left[\frac{1}{i\nu_n + (\varepsilon_{t_{2g}} - \mu)} + \frac{3}{i\nu_n - (\varepsilon_{t_{2g}} + U - 3J - \mu)}\right.$$

$$\left. + \frac{5/3}{i\nu_n - (\varepsilon_{t_{2g}} + U - J - \mu)} + \frac{1/3}{i\nu_n - (\varepsilon_{t_{2g}} + U + 2J - \mu)}\right]$$



tetragonal crystal field splitting



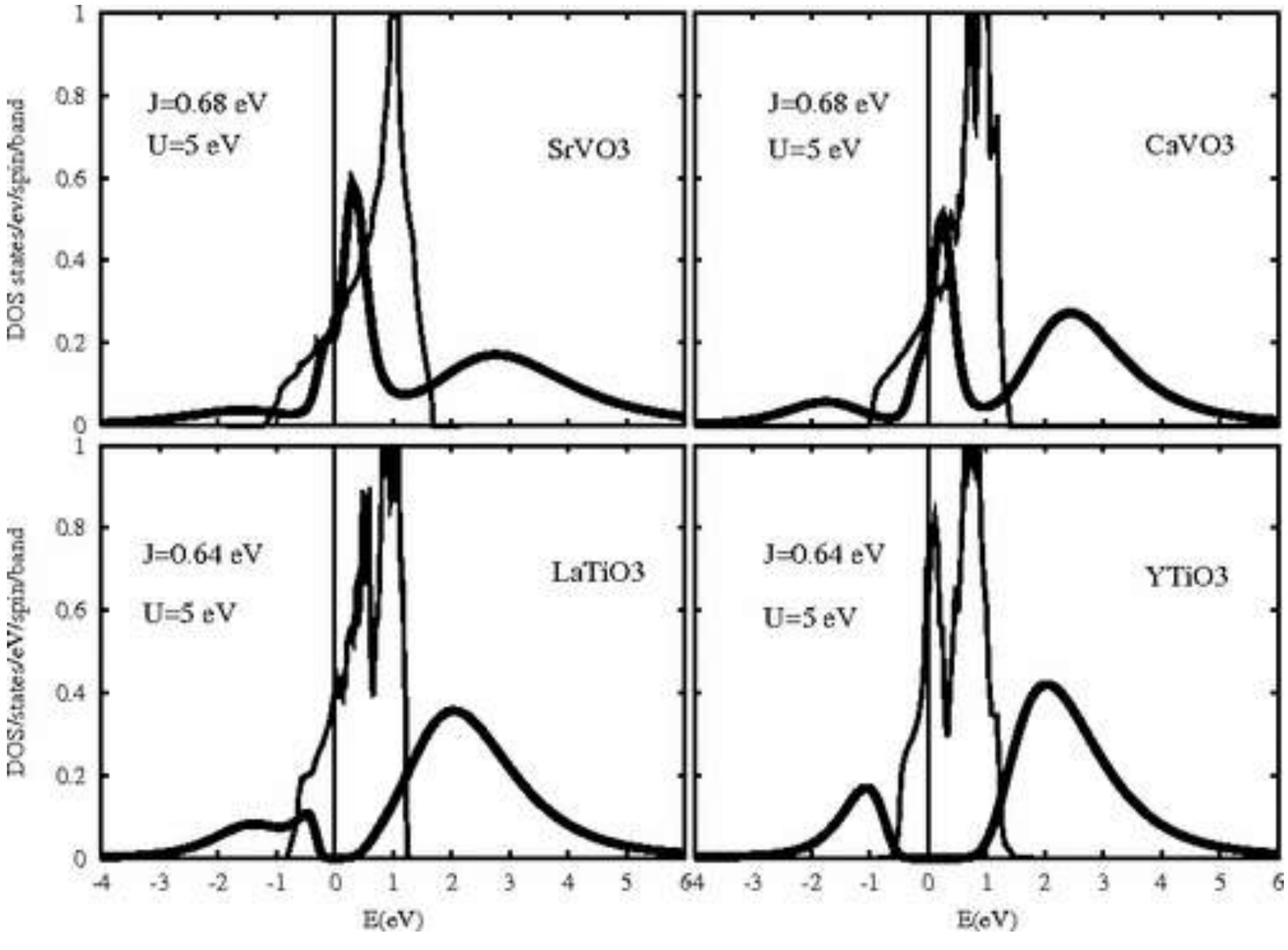
$$E_g(1) \sim U - 3J + \varepsilon_{\mathrm{CF}}.$$

spectral functions

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

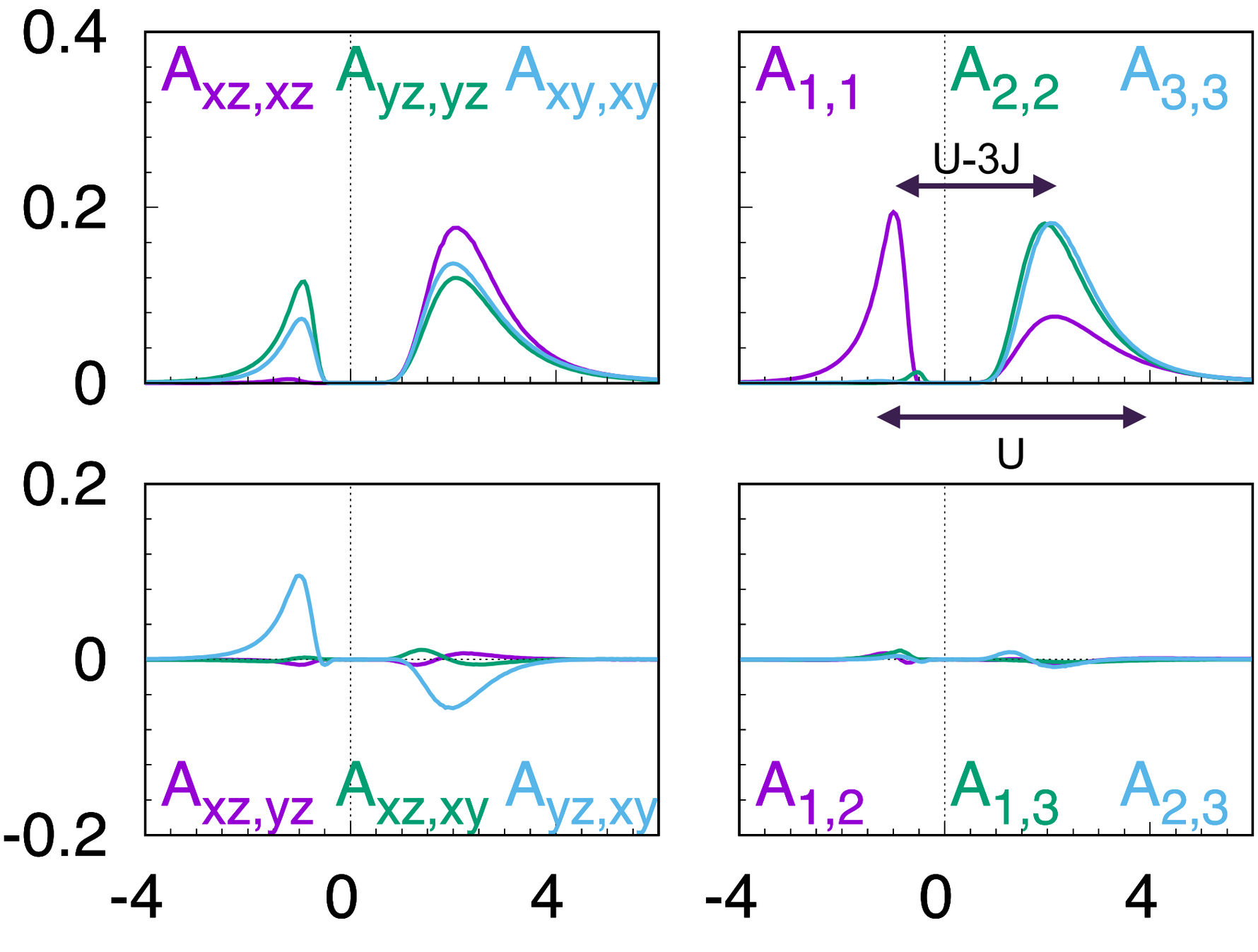
Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites

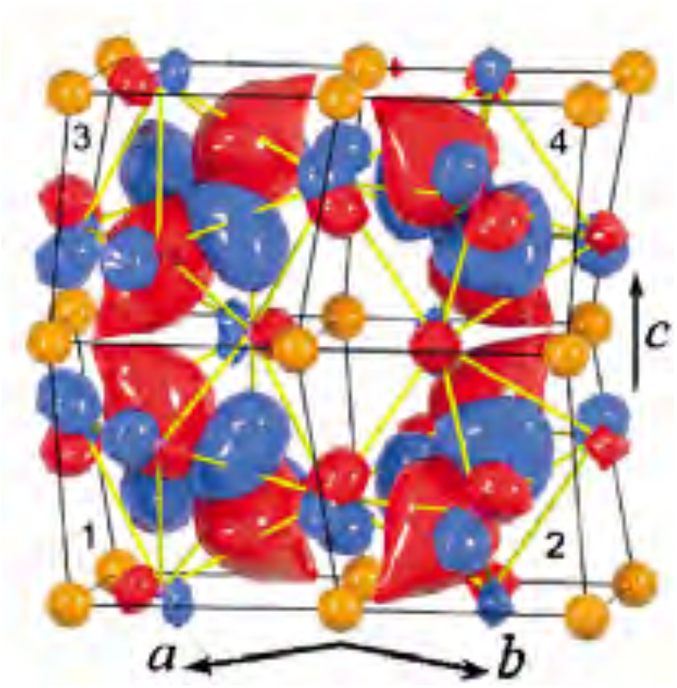
E. Pavarini,[1] S. Biermann,[2] A. Poteryaev,[3] A. I. Lichtenstein,[3] A. Georges,[2] and O. K. Andersen[4]



a real d^1 case: $YTiO_3$

DMFT spectral-function matrix





2. orbital degeneracy *d can* reduce the gap in the large U limit

d degenerate orbitals

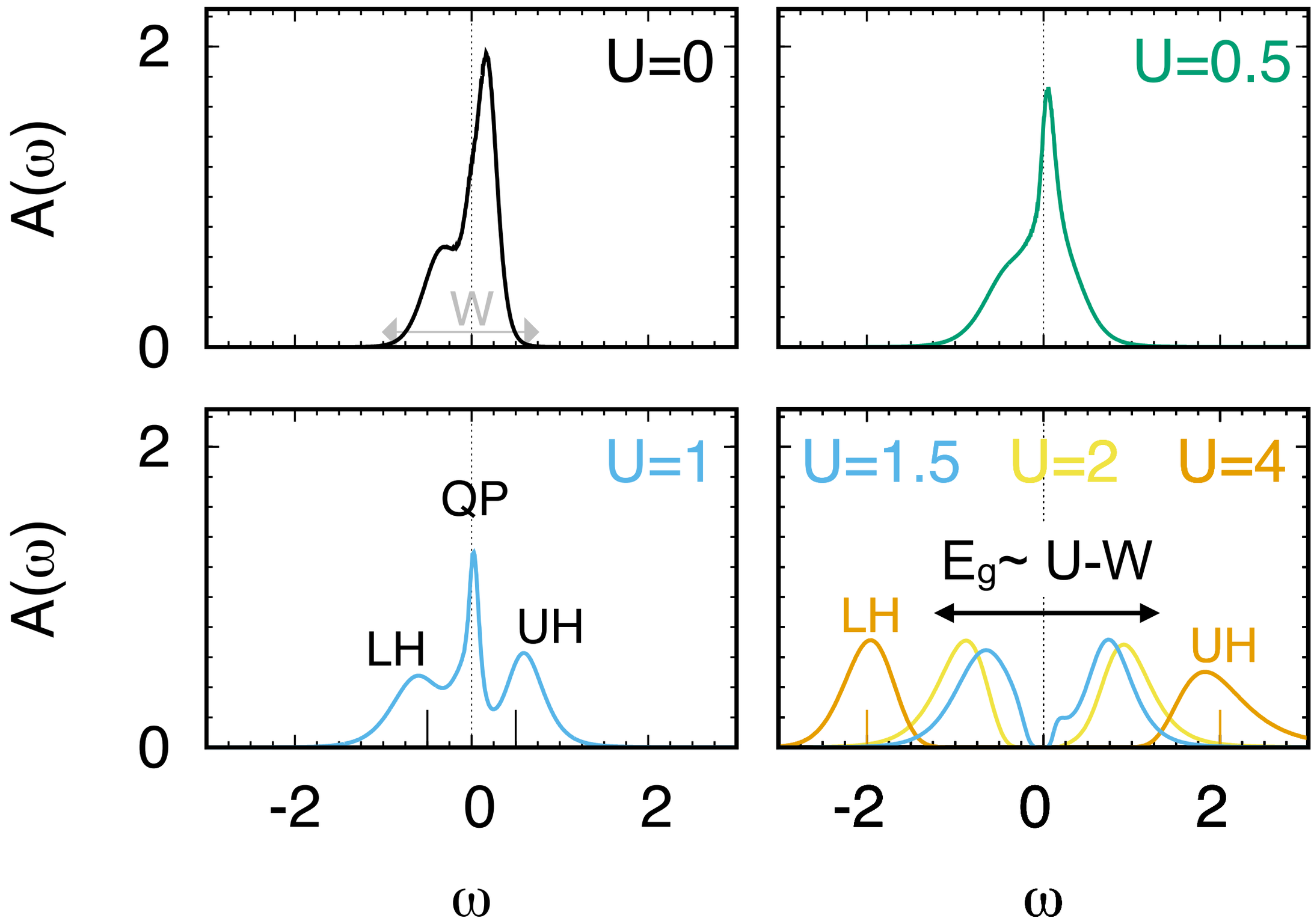
example: t_{2g},cubic symmetry

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

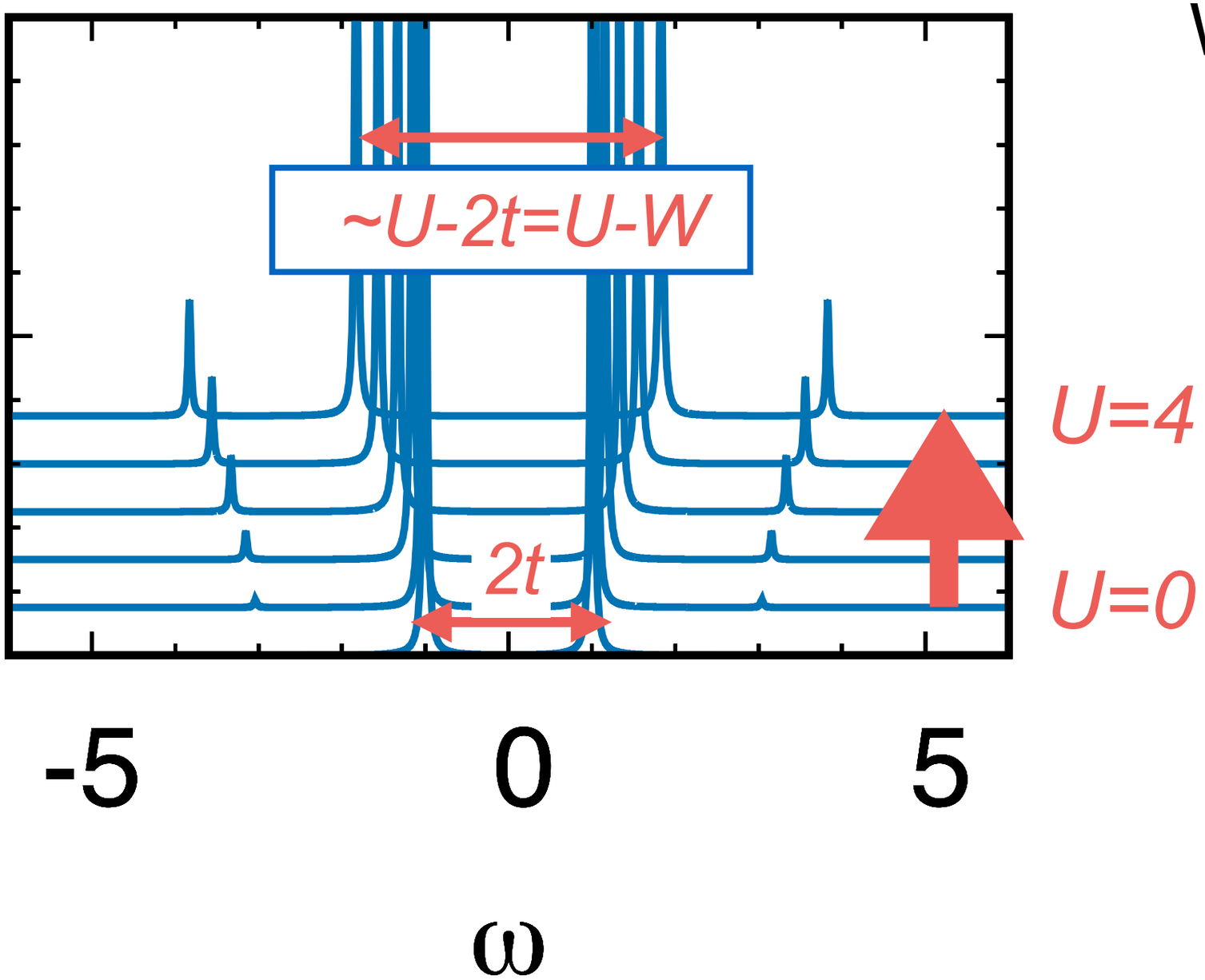
$$+ U \sum_{i\ m} \hat{n}_{im\uparrow} \hat{n}_{im\downarrow} + \frac{1}{2} \sum_{\substack{i\sigma\sigma' \\ m \neq m'}} \left(U - 2J - J\delta_{\sigma,\sigma'} \right) \hat{n}_{im\sigma} \hat{n}_{im'\sigma'}$$

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

one-band case



the spectral function of the Hubbard dimer



the gap in the large U limit (J=0)

$$E_g(N) = E(N+1) + E(N-1) - 2E(N)$$

$E_A(N+1)$

$$E(N+1) \sim \boxed{nU + E(N)} - \sqrt{k_+}\, W/2$$

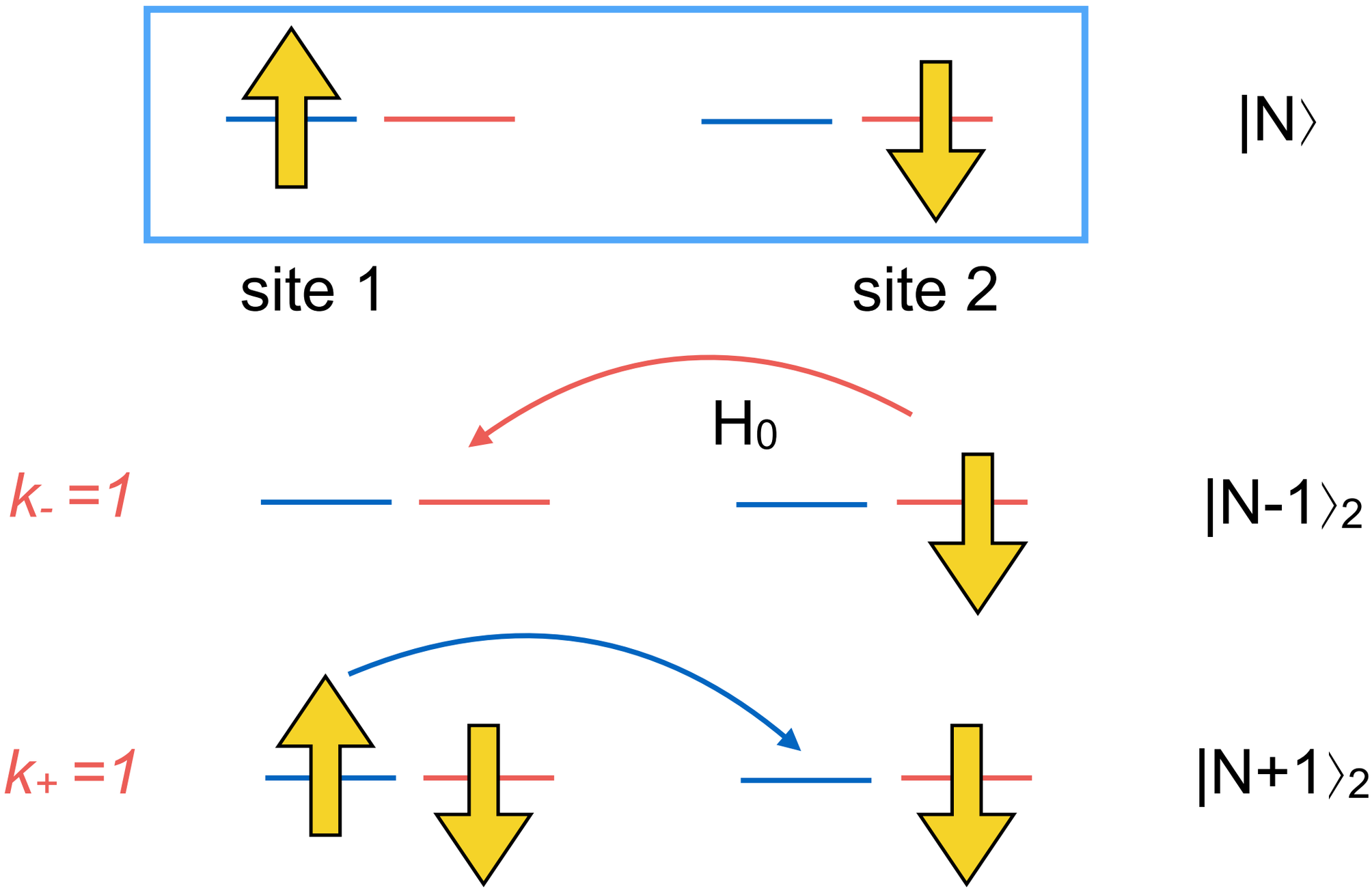
$$E(N-1) \sim \boxed{(n-1)U + E(N)} - \sqrt{k_-}\, W/2$$

$E_A(N-1)$

$$E_g(N) \sim U - \frac{\sqrt{k}_- + \sqrt{k}_+}{2} W.$$

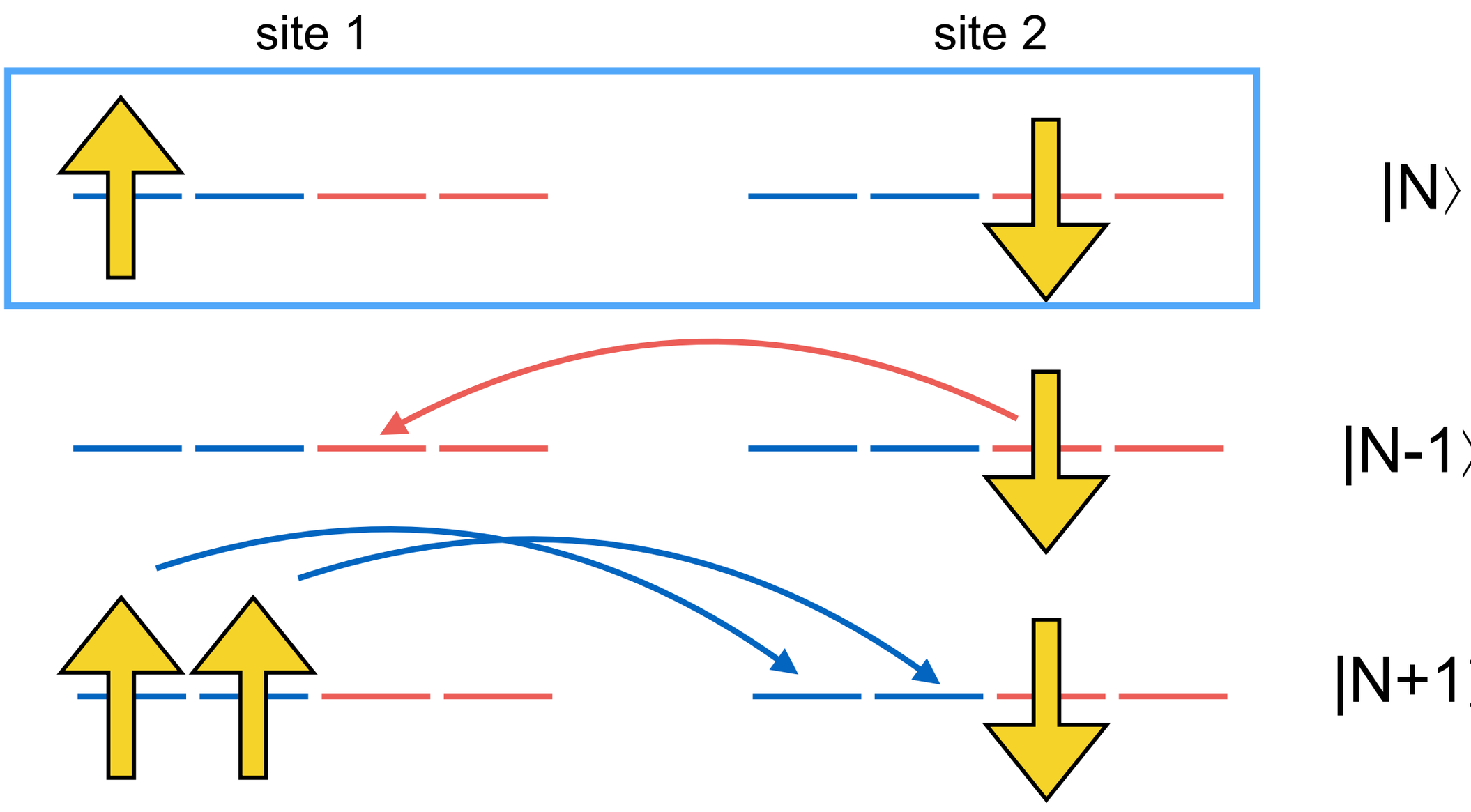
Erik Koch, Olle Gunnarsson, and Richard M. Martin, Phys. Rev. B **60**, 15714 (1999)

Hubbard dimer, large U



$$E_g(N) \sim U - \frac{\sqrt{k}_- + \sqrt{k}_+}{2} W = U - W$$

orbital degenerate case



$$E_g(N) \sim U - \frac{\sqrt{k}_- + \sqrt{k}_+}{2} W.$$

a crystal field helps Mott transition

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

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

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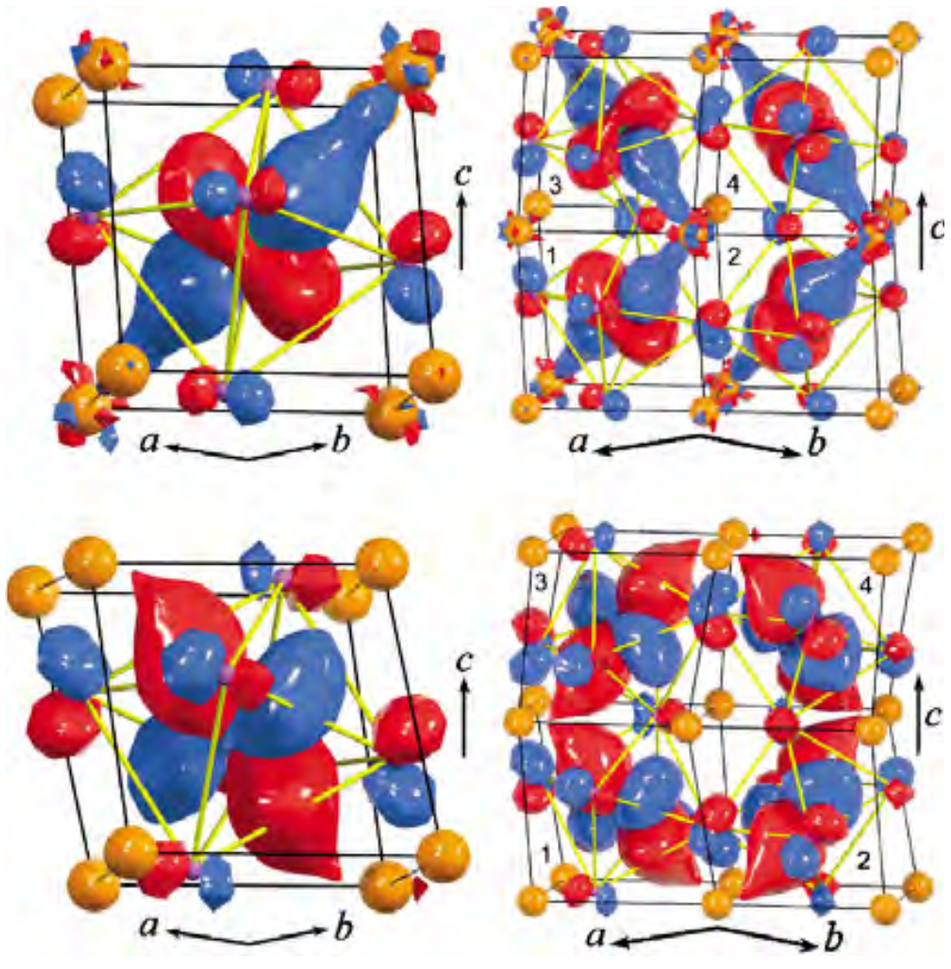
t_{2g}^1

Δ=200-300 meV

LDA+DMFT 770 K



a small crystal field plays a key role

3. spin-orbit interaction

multi-orbital models for t_{2g} (or e_g) bands

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

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

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

atomic spin-orbit interaction

$$\hat{H}_{\mathrm{SO}} = \sum_{\mu} \lambda_{\mu} \sum_{mm'} \sum_{\sigma\sigma'} \epsilon^{\mu}_{m\sigma,m'\sigma'} \, c^{\dagger}_{m\sigma} c_{m'\sigma'}$$

$$\lambda_{\mu} = \lambda$$

$$\lambda \sim g\mu_B^2 \left\langle \frac{1}{r} \frac{d}{dr} v_R(r) \right\rangle .$$

couples e_g and t_{2g}!

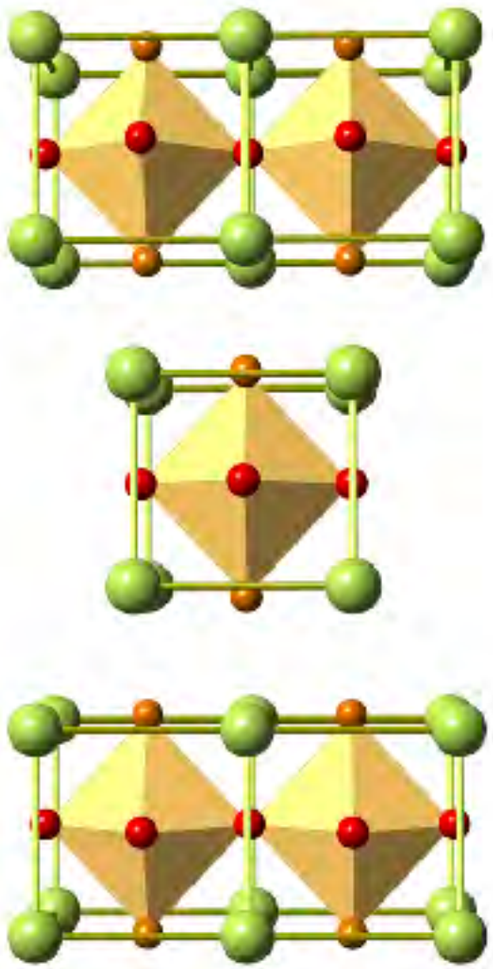
$$\epsilon^{\mu}_{m\sigma,m'\sigma'} = \langle m\sigma | l_{\mu} s_{\mu} | m'\sigma' \rangle$$

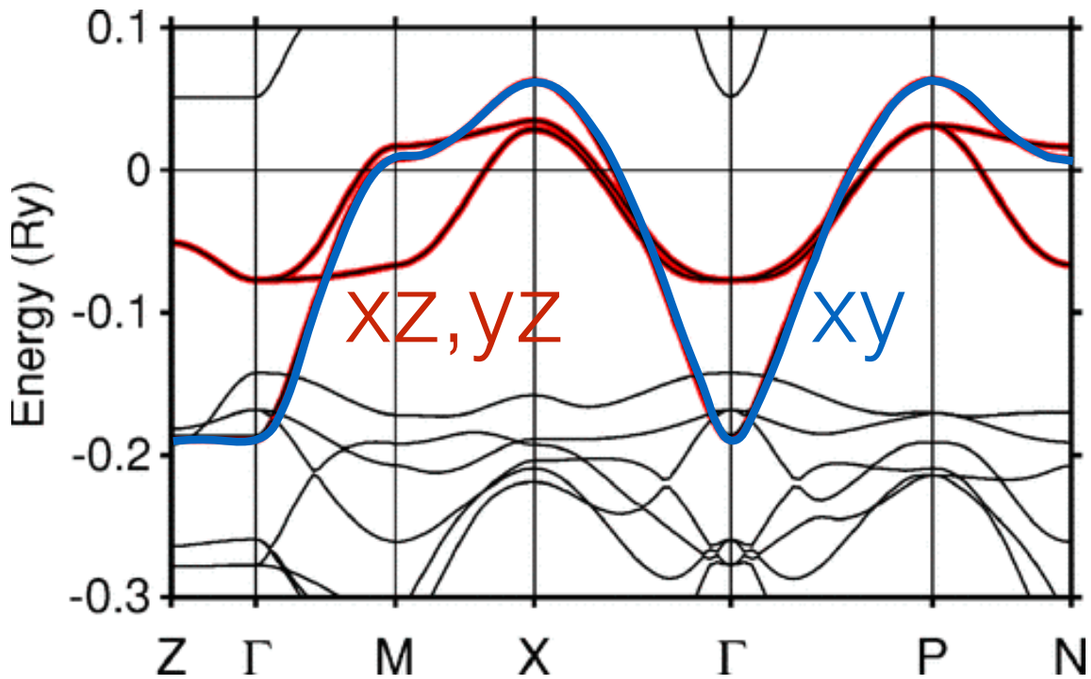
here: limit case

λ small compared to Hund's rule couplings J_1 and J_2

λ small compared to cubic crystal-field splitting

example: Sr_2RuO_4



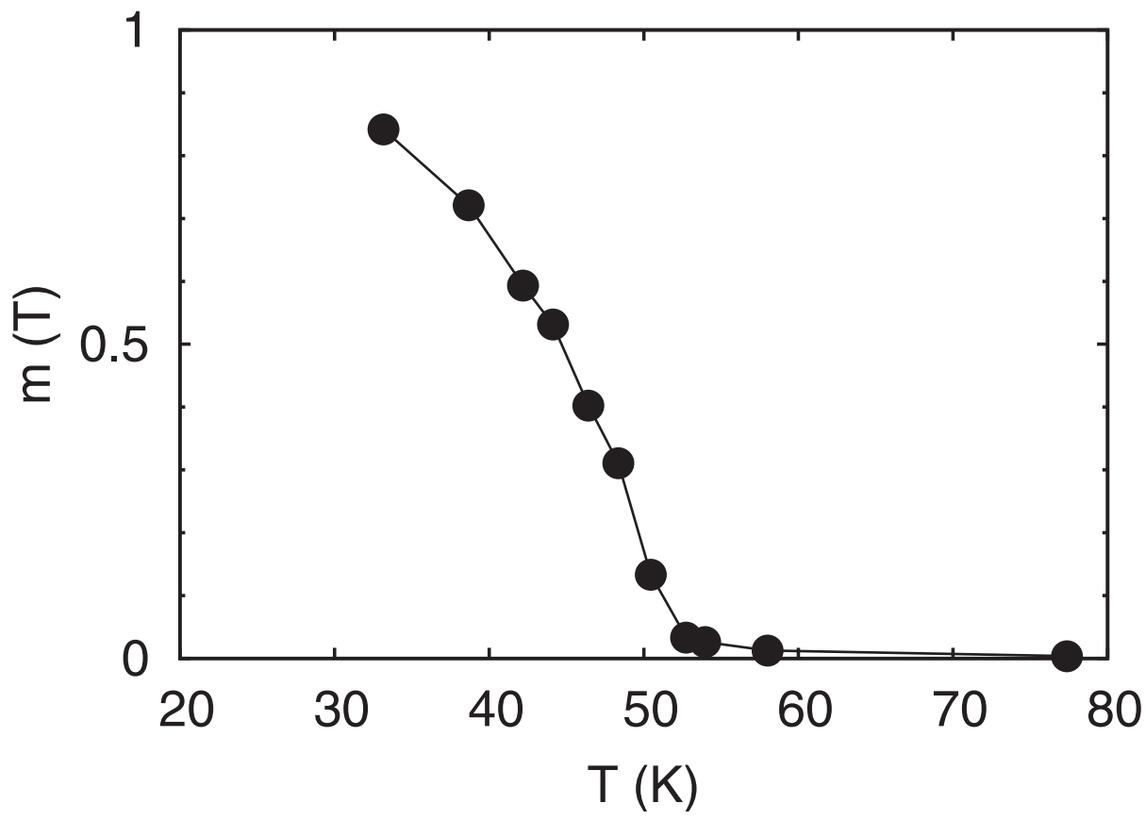


G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)

what is the problem?

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)

in the t_{2g} basis, use symmetries!

cubic & tetragonal symmetry

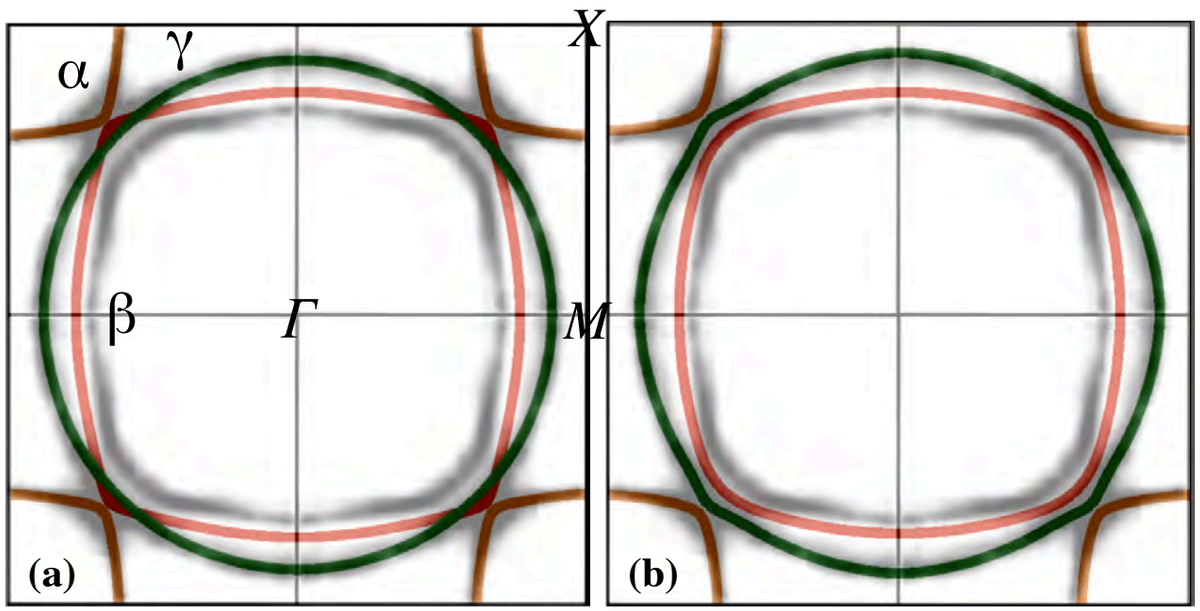
$$\left(\begin{array}{ccc|ccc}
G^{i\uparrow\uparrow}_{xy}(\tau) & 0 & 0 & 0 & G^{i\uparrow\downarrow}_{y}(\tau) & -iG^{i\uparrow\downarrow}_{x}(\tau) \\
0 & G^{i\uparrow\uparrow}_{yz}(\tau) & iG^{i\uparrow\uparrow}_{z}(\tau) & -G^{i\uparrow\downarrow}_{y}(\tau) & 0 & 0 \\
0 & -iG^{i\uparrow\uparrow}_{z}(\tau) & G^{i\uparrow\uparrow}_{xz}(\tau) & iG^{i\uparrow\downarrow}_{x}(\tau) & 0 & 0 \\
\hline
0 & -G^{i\downarrow\uparrow}_{y}(\tau) & -iG^{i\downarrow\uparrow}_{x}(\tau) & G^{i\downarrow\downarrow}_{xy}(\tau) & 0 & 0 \\
G^{i\downarrow\uparrow}_{y}(\tau) & 0 & 0 & 0 & G^{i\downarrow\downarrow}_{yz}(\tau) & -iG^{i\downarrow\downarrow}_{z}(\tau) \\
iG^{i\downarrow\uparrow}_{x}(\tau) & 0 & 0 & 0 & iG^{i\uparrow\uparrow}_{z}(\tau) & G^{i\downarrow\downarrow}_{xz}(\tau)
\end{array}\right)$$

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

E. Sarvestani, G. Zhang, E. Gorelov, and E. Pavarini, Phys. Rev. B **97**, 085141 (2018)

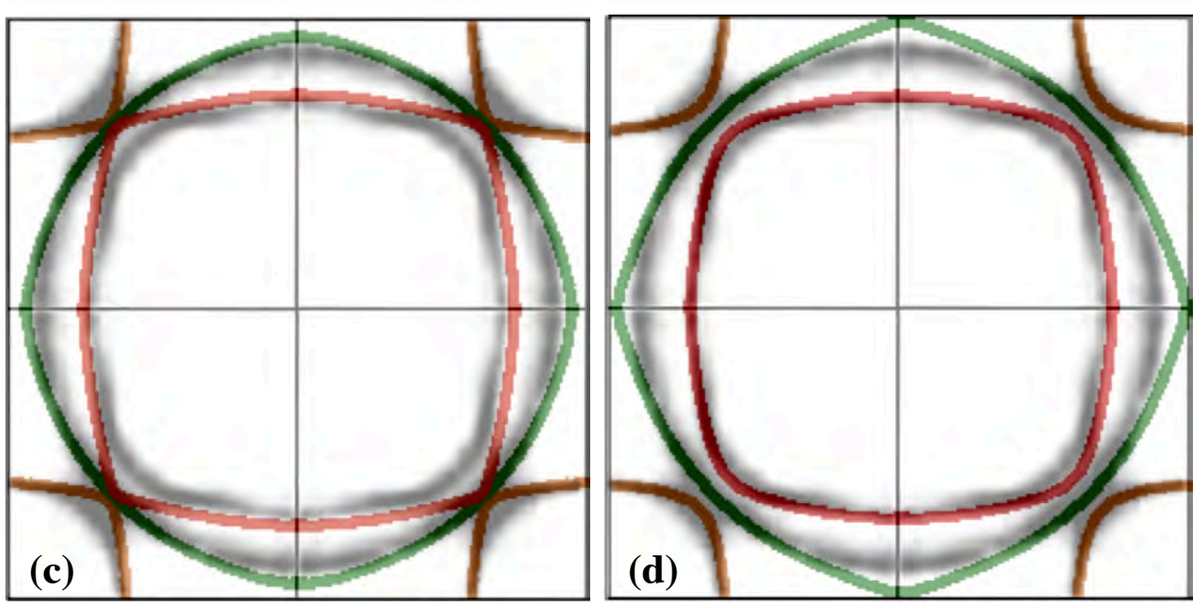
the Fermi surface

LDA



LDA+SO

LDA+DMFT



LDA+SO+DMFT

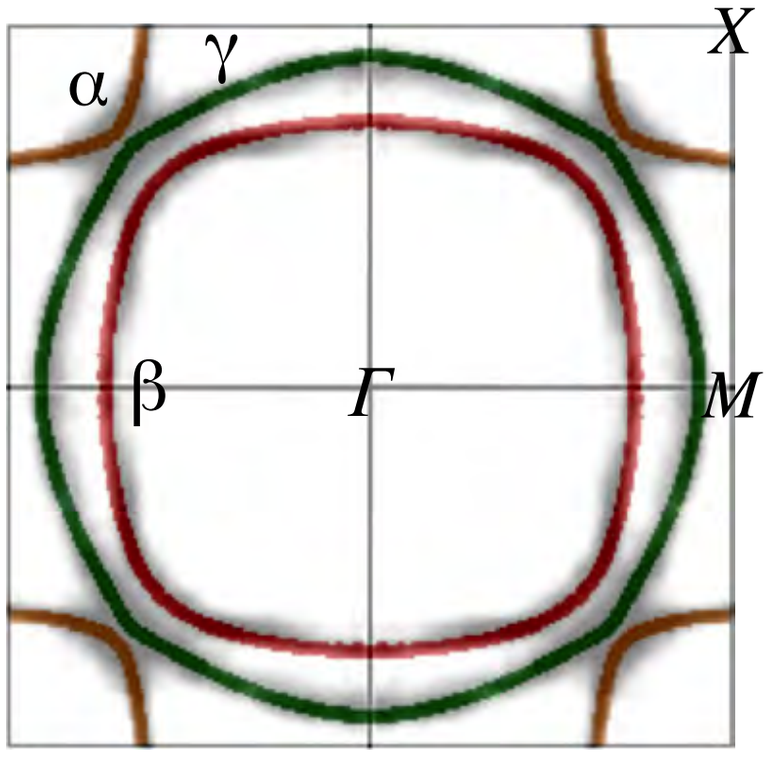
$\varepsilon_{CF} \Rightarrow \varepsilon_{CF} + \Delta\varepsilon_{CF}$ $\quad\quad$ $\lambda \Rightarrow \lambda + \Delta\lambda$

something still missing!

Is the Coulomb interaction spherical?

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

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

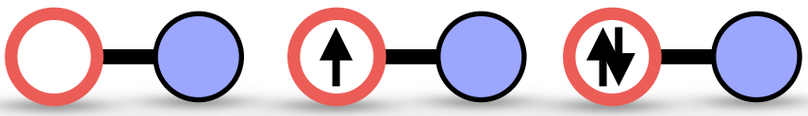


G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)

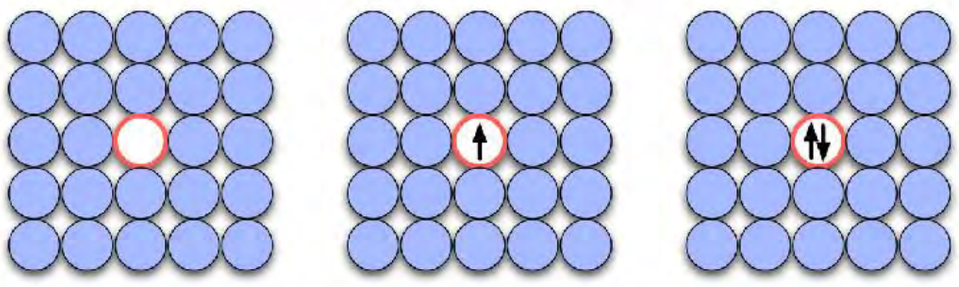
LDA+DMFT: conclusions

DMFT

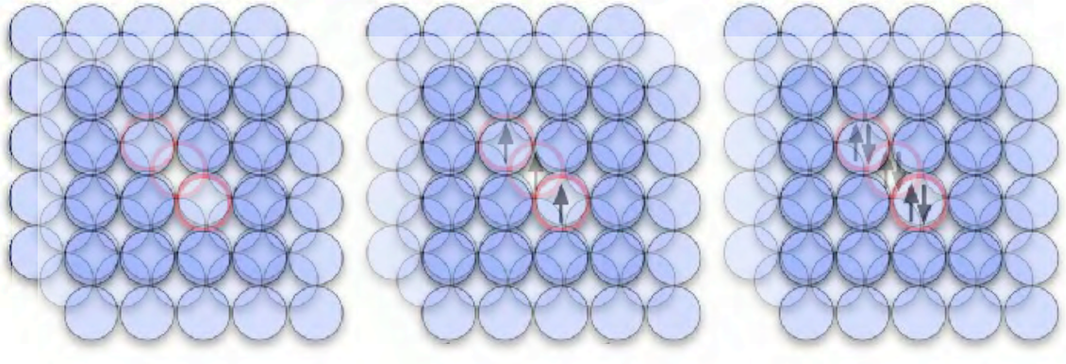
dimer



one band

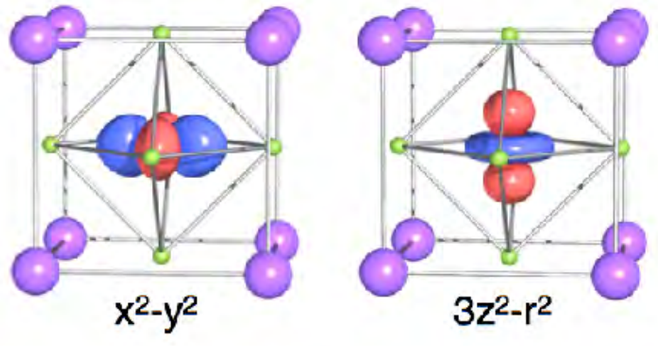


multiband



model building

basis, downfolding, localization

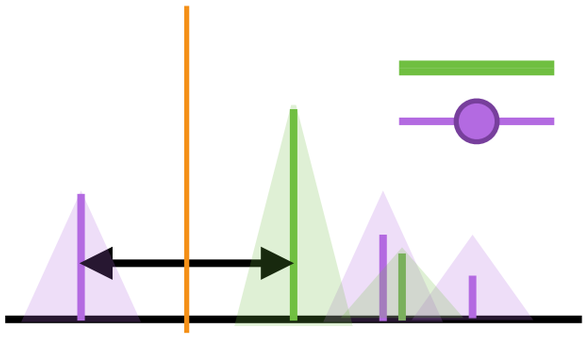


double counting & screening

LDA+DMFT: conclusions

effects & interactions

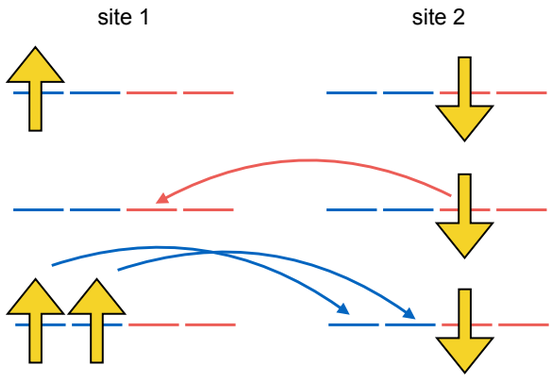
multiplets

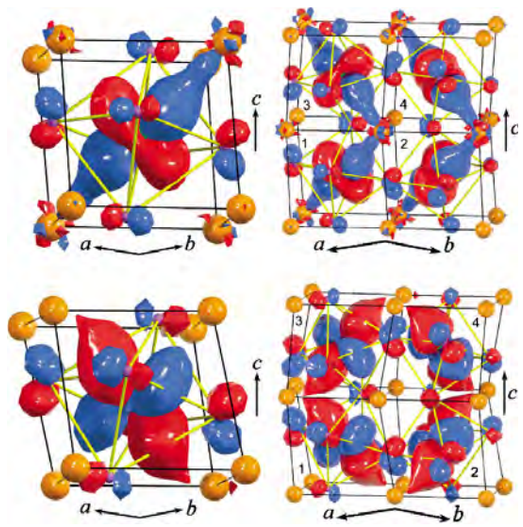


spin-orbit interaction

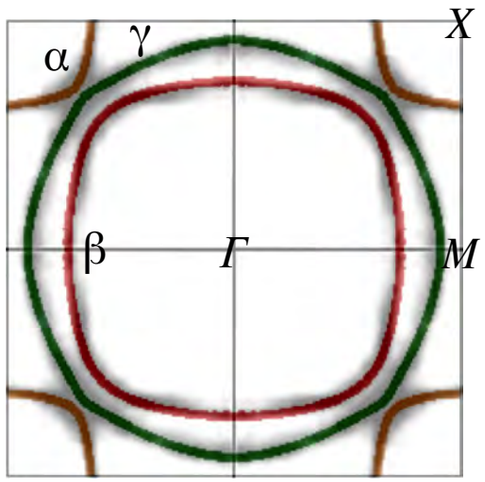
$$G^{\sigma,\sigma'}_{im,im'}(\tau) = \left(\begin{array}{ccc|ccc} G^{i\uparrow\uparrow}_{xy}(\tau) & 0 & 0 & 0 & G^{i\uparrow\downarrow}_{y}(\tau) & -iG^{i\uparrow\downarrow}_{x}(\tau) \\ 0 & G^{i\uparrow\uparrow}_{yz}(\tau) & iG^{i\uparrow\uparrow}_{z}(\tau) & -G^{i\uparrow\downarrow}_{y}(\tau) & 0 & 0 \\ 0 & -iG^{i\uparrow\uparrow}_{z}(\tau) & G^{i\uparrow\uparrow}_{xz}(\tau) & iG^{i\uparrow\downarrow}_{x}(\tau) & 0 & 0 \\ \hline 0 & -G^{i\downarrow\uparrow}_{y}(\tau) & -iG^{i\downarrow\uparrow}_{x}(\tau) & G^{i\downarrow\downarrow}_{xy}(\tau) & 0 & 0 \\ G^{i\downarrow\uparrow}_{y}(\tau) & 0 & 0 & 0 & G^{i\downarrow\downarrow}_{yz}(\tau) & -iG^{i\downarrow\downarrow}_{z}(\tau) \\ iG^{i\downarrow\uparrow}_{x}(\tau) & 0 & 0 & 0 & iG^{i\uparrow\uparrow}_{z}(\tau) & G^{i\downarrow\downarrow}_{xz}(\tau) \end{array}\right)$$

orbital degeneracy & crystal field





non-spherical U



thank you!