LDA+DMFT: Linear Response Functions

Eva Pavarini

Institute for Advanced Simulation

Peter Grünberg Institut

Forschungszentrum Jülich

$$\mathbf{\Sigma}_k(\omega) = \varepsilon_k - a_1 - \cfrac{b_1^2}{\omega - a_2 - \cfrac{b_2^2}{\omega - a_3 - \cfrac{b_3^2}{\omega - a_4 - \cfrac{}{\omega - a_5}}}}$$

scheme of the lecture

- what is it all about?
- DMFT
  - Hubbard dimer
  - one-band Hubbard model
  - linear response functions
- LDA+DMFT
  - multi-band Hubbard model
  - model building
- conclusion

e.pavarini@fz-juelich.de

strong correlations: what are they?

cooperative effects that **cannot** be described in a single-particle picture

emergent phenomena

Philip Warren Anderson

more is different

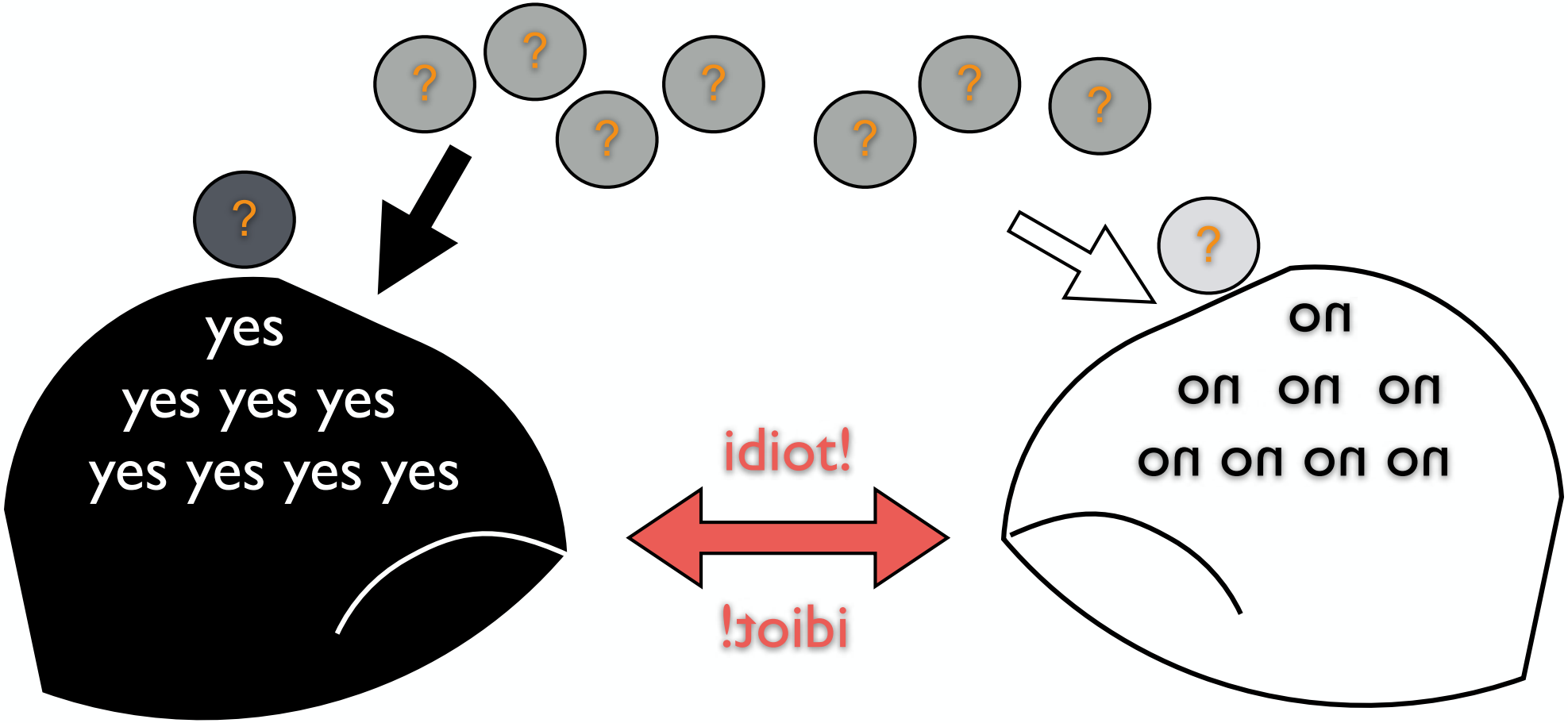
4 August 1972, Volume 177, Number 4047

SCIENCE

e.pavarini@fz-juelich.de

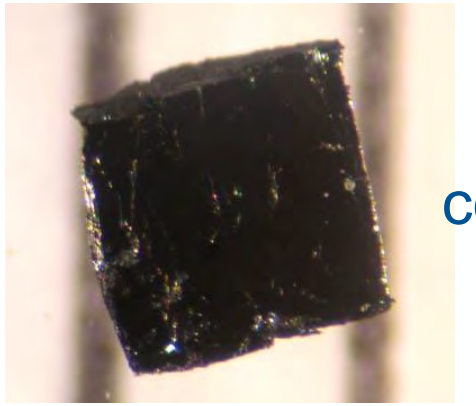
emergence in social media

formation of polarized opinion-bubbles



e.pavarini@fz-juelich.de

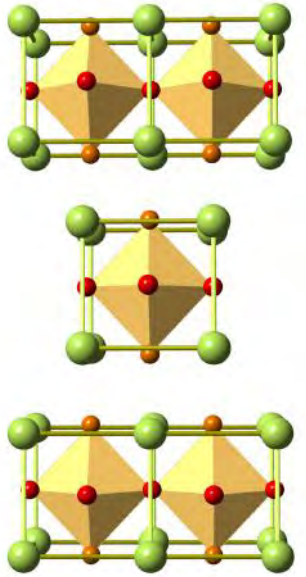
emergence in solid-state systems



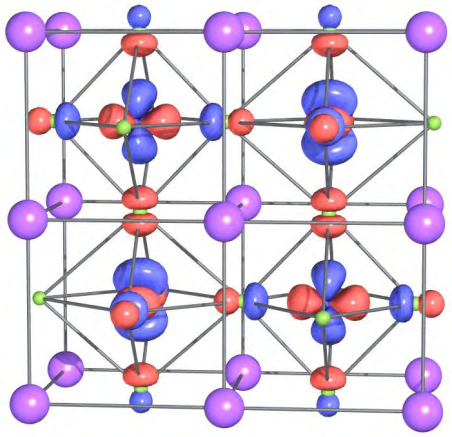
BSCCO-2223, photo from wikipedia

conventional superconductivity

non-conventional superconductivit

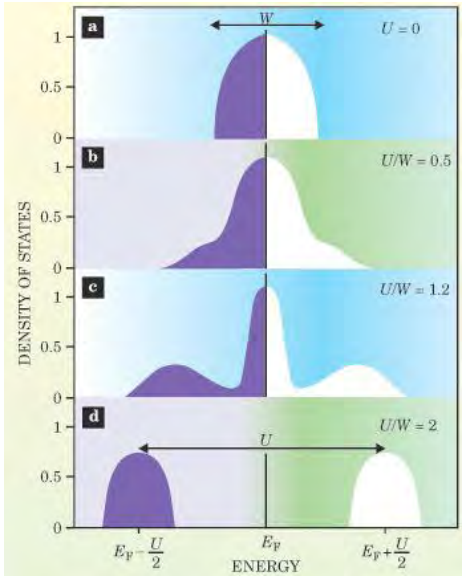


G. Zhang and E. Pavarini,
Rapid Research Letters **12**, 1800211 (2018)



orbital order

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



Mott transition

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

photo from wikipedia

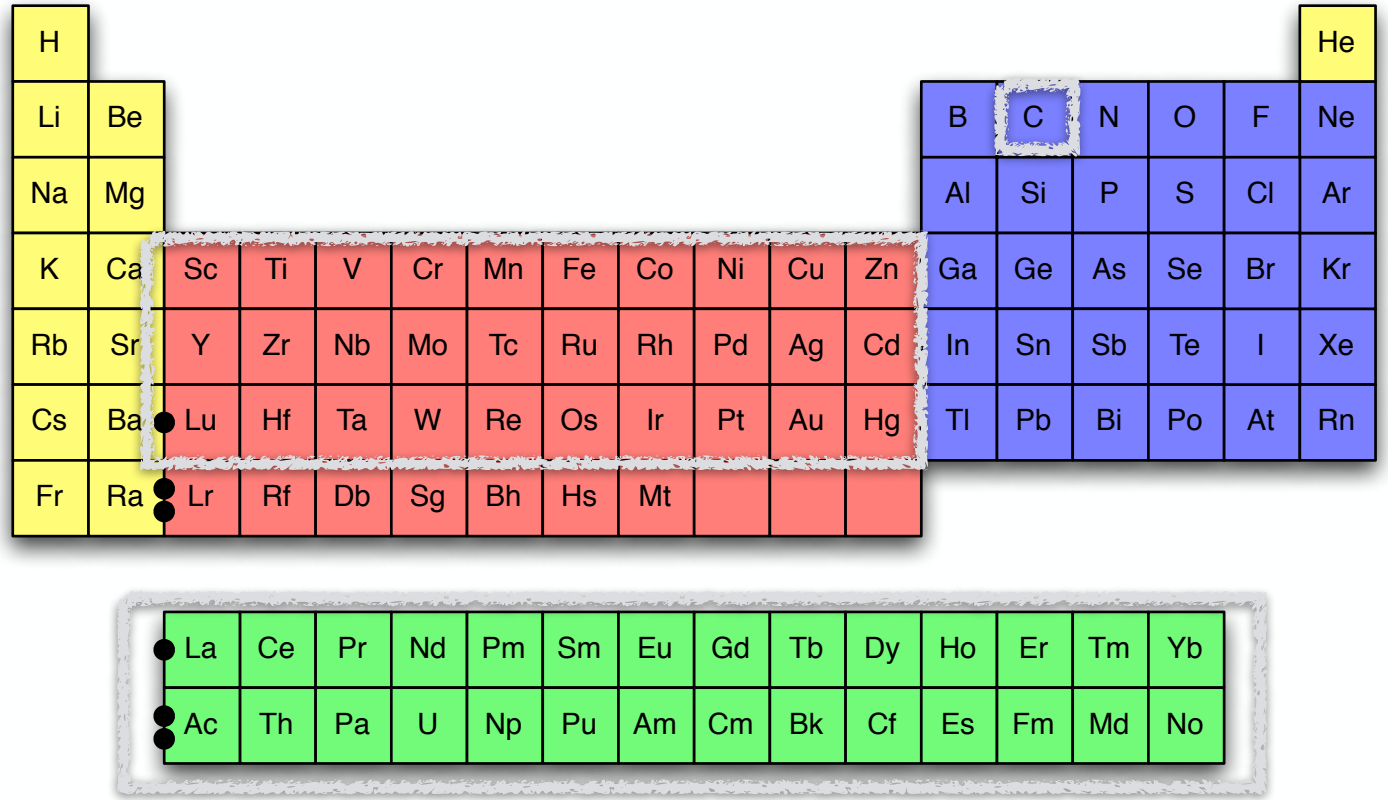
magnetic order

e.pavarini@fz-juelich.de

JÜLICH
FORSCHUNGSZENTRUM

strongly correlated systems

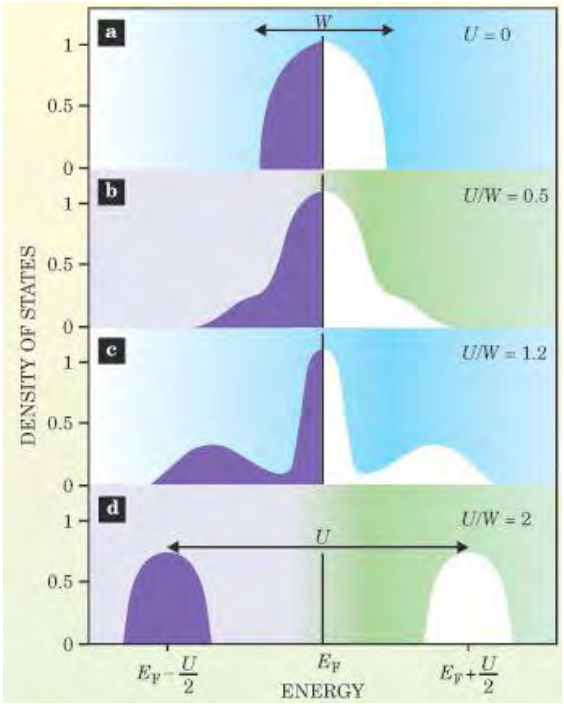
systems that retain atomic properties in the solid



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

e.pavarini@fz-juelich.de

the Mott metal-insulator transition



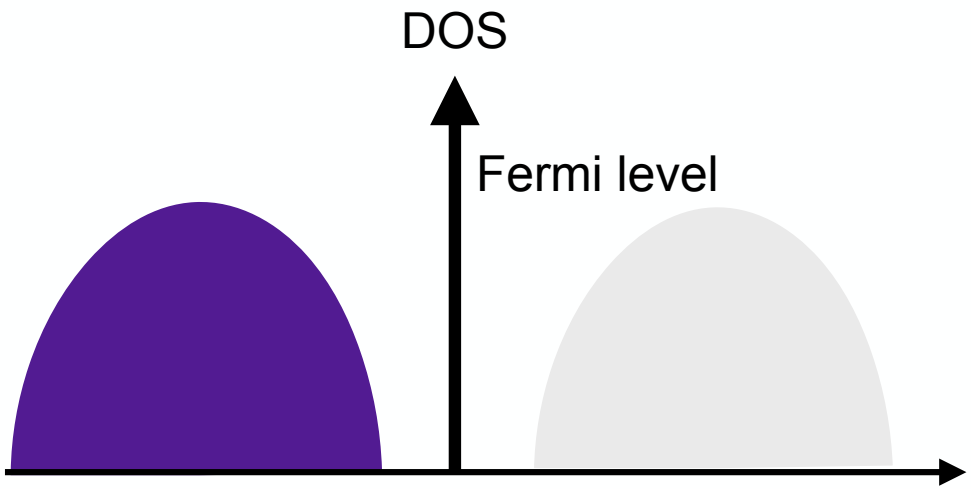
Mott transition

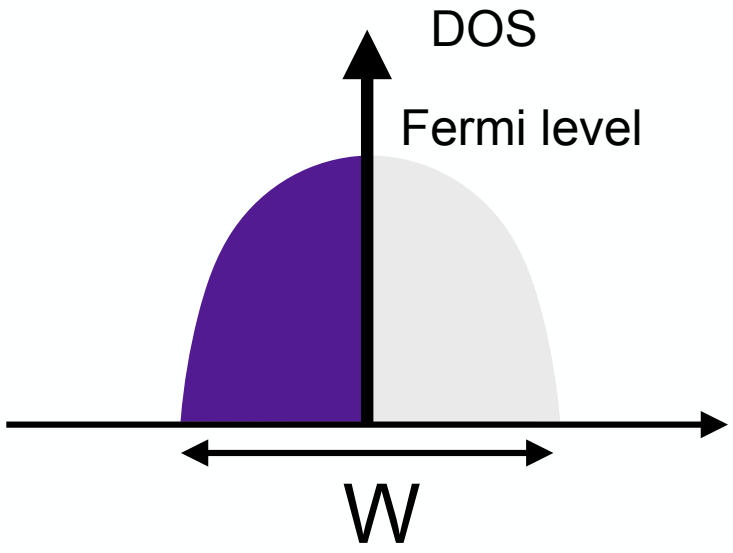
G. Kotliar and D. Vollhardt, Physics Today **57,** 53 (2004)

e.pavarini@fz-juelich.de

band metals vs band insulators

single-electron picture: states filled up to Fermi level





diamond

gold

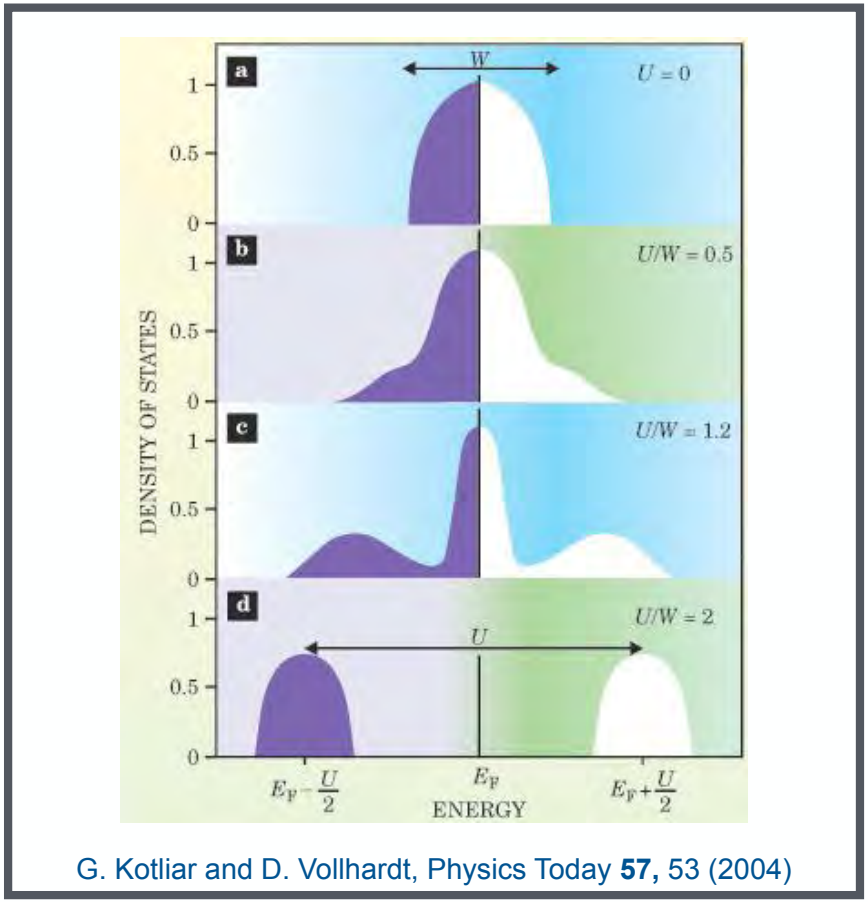
photos from Wikipedia

e.pavarini@fz-juelich.de

the **Mott** metal-insulator transition

metal in the single-electron picture, *insulator* in reality

origin: on-site Coulomb repulsion *U*
comparable with/larger than bandwidth W



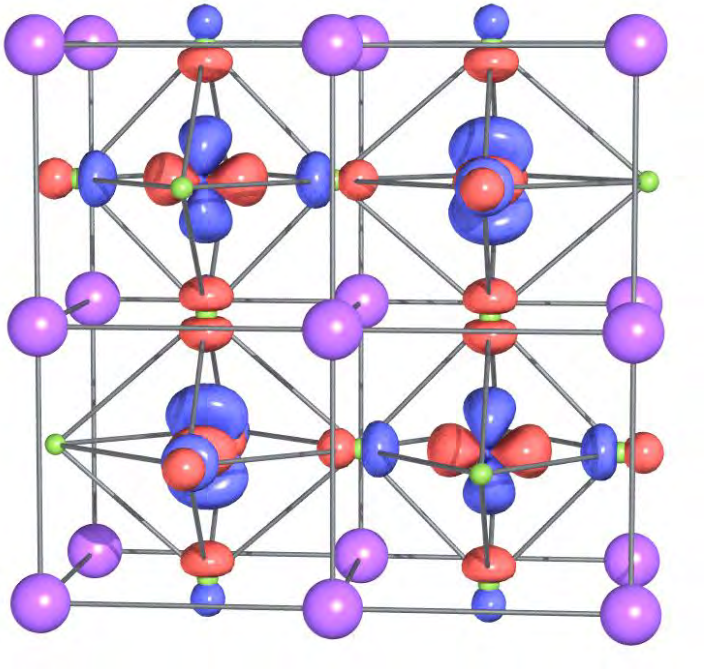
G. Kotliar and D. Vollhardt, Physics Today **57,** 53 (2004)

U/W

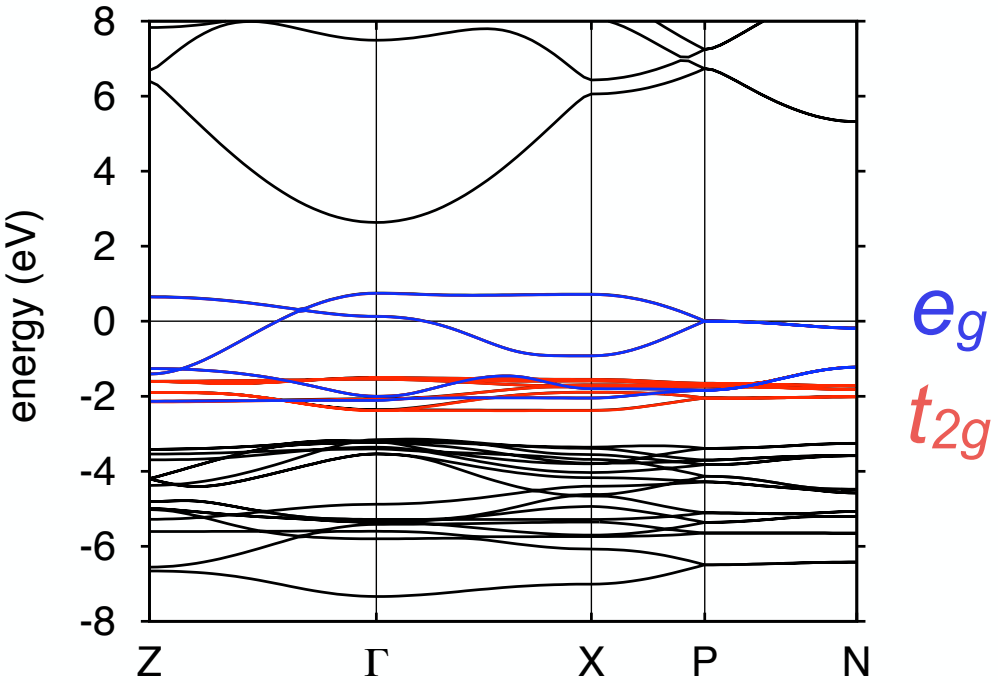
half filling

e.pavarini@fz-juelich.de

$KCuF_3$



one-electron picture



e.pavarini@fz-juelich.de

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

Mott systems: it is not just a matter of the gap

enhanced masses

quasiparticles with short lifetimes

local moment behavior

orbital, spin and charge ordering

anomalous superconductivity

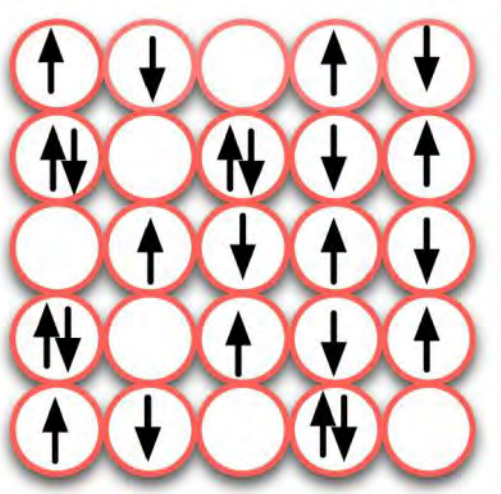
e.pavarini@fz-juelich.de

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

Hubbard model

atomic hoppings atomic

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

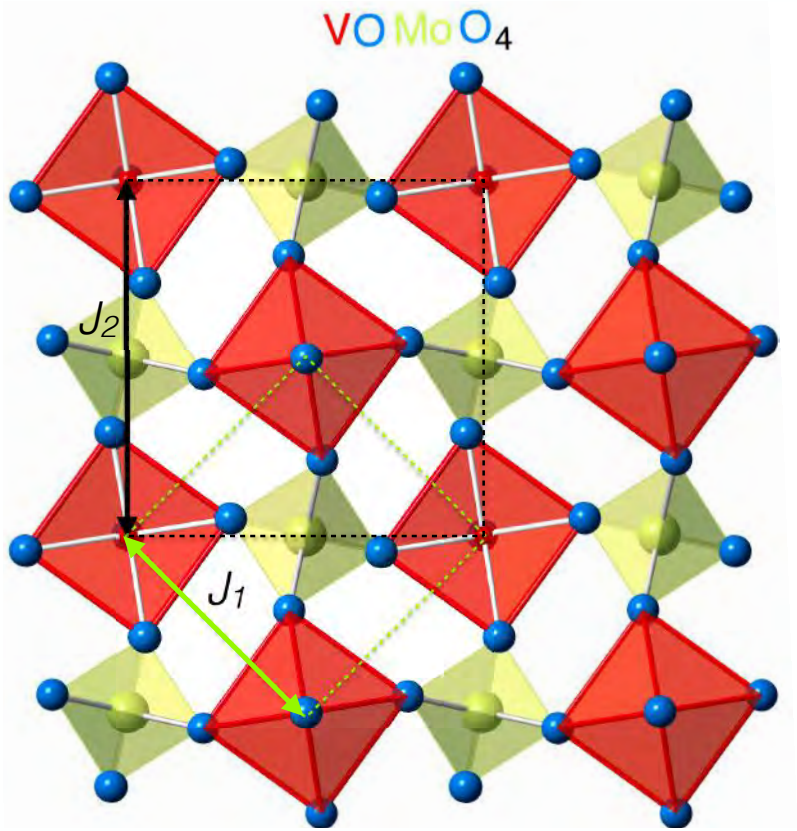


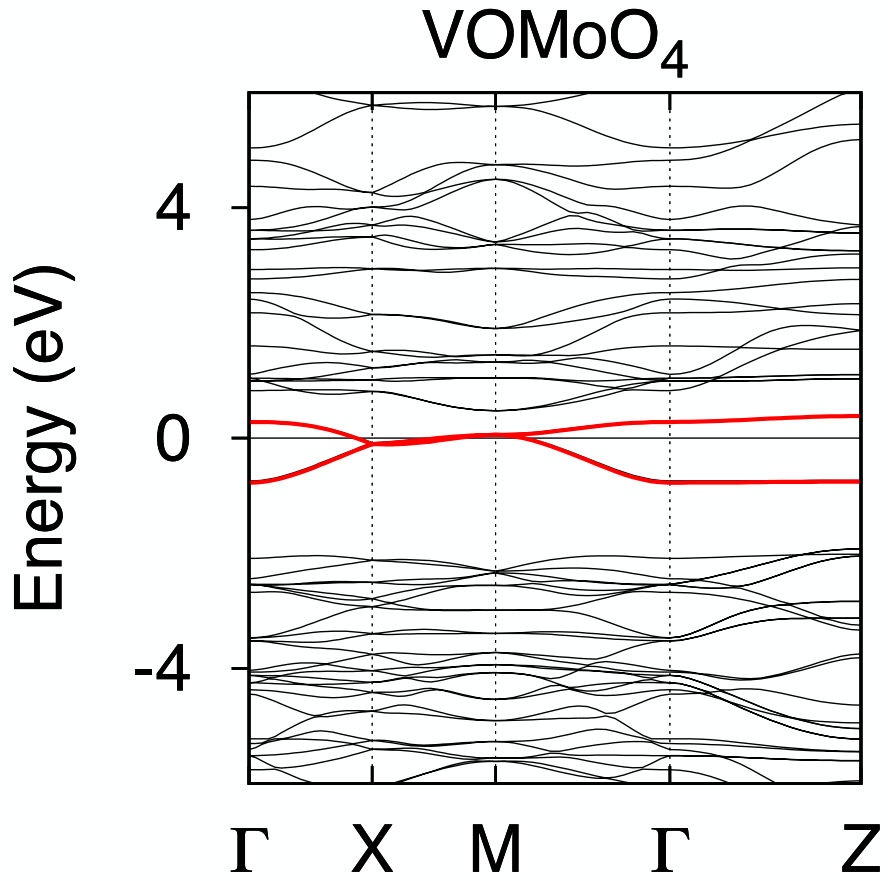
at half filling:

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

e.pavarini@fz-juelich.de

$VOMoO_4$





e.pavarini@fz-juelich.de

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

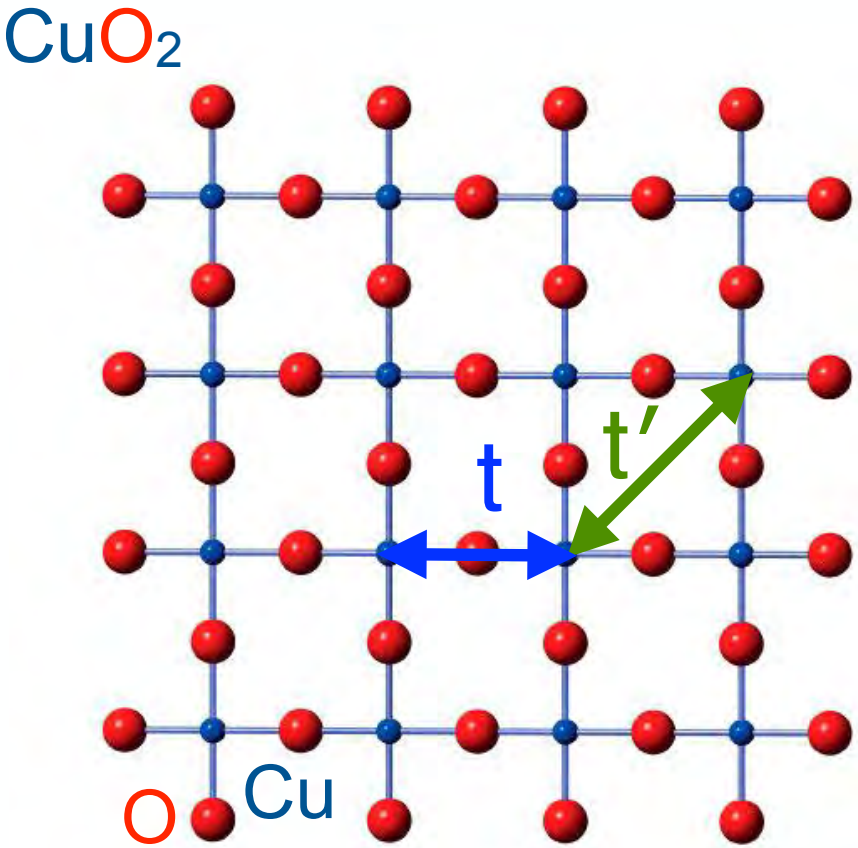
high-T_c superconducting cuprates

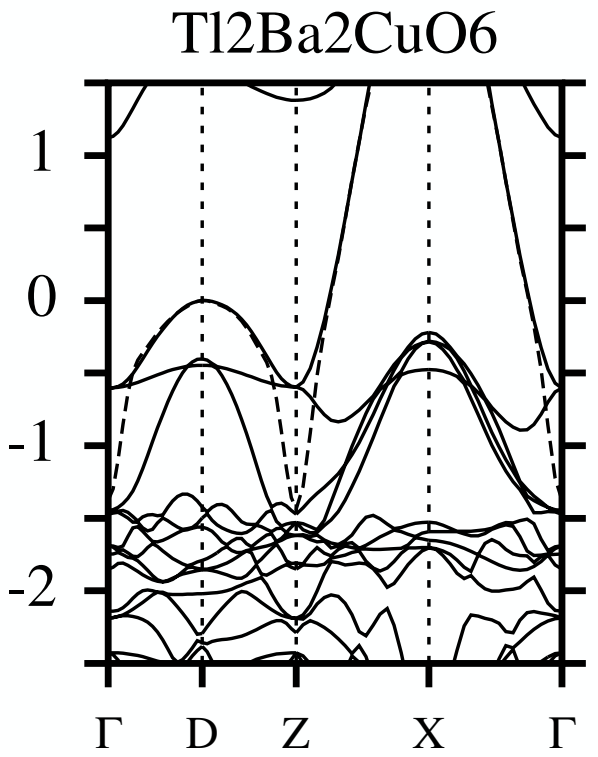
VOLUME 87, NUMBER 4 PHYSICAL REVIEW LETTERS 23 JULY 2001

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

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

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





e.pavarini@fz-juelich.de

JÜLICH FORSCHUNGSZENTRUM

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.

1963

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 main motivation was the need for a way to tackle the behaviour of correlated (rather than non-interacting) electrons in solids. Initially, the model was introduced to provide an explanation for the itinerant ferromagnetism of transition metals, such as iron and nickel, but the past 50 years have seen its relevance go far beyond that original context.

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 had Gutzwiller, Kanamori and Hubbard already extracted different physics from the model, it turned out to be a 'mathematically hard' problem: an exact solution has so far only been obtained for the one-dimensional case. Today, with ever-increasing computer power, numerical simulations of the model are mainstream — particularly when trying to get a grip on the role of the

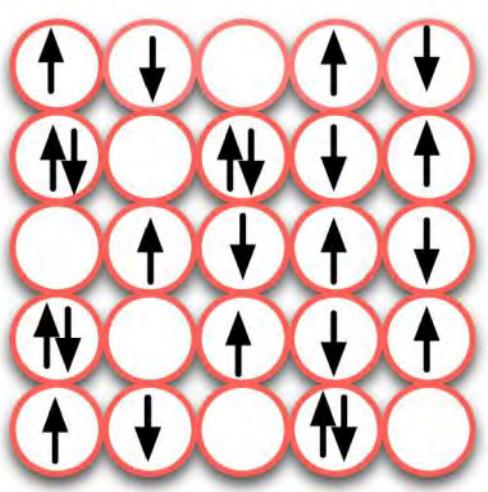
when the field of cold-atom optical trapping had advanced so far that experimental realizations of the Hubbard model could be achieved. A landmark experiment demonstrated how a lattice of bosonic atoms displays a transition from a superfluid to a Mott insulator[5], a result accounted for by the Bose–Hubbard 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 itself — and, more generally, how theoretical and experimental physics can entangle and spark further progress.

The simplicity of the Hubbard model, when written down, is deceptive.

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?

e.pavarini@fz-juelich.de

static mean-field approaches

Hartree-Fock approximation

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

simplest version: expectation value site independent

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

m: magnetization

$m \neq 0$ ferromagnetic solution

e.pavarini@fz-juelich.de

to open a gap* we must lower the symmetry

* within the one-electron picture

REPLACE THIS

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

WITH THIS

$$\hat{H} = \sum_i \sum_\sigma \tilde{\varepsilon}_{di\sigma} c^\dagger_{i\sigma} c_{i\sigma} - \sum_{ii'} \tilde{t}_{ii'\sigma} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma}$$

LET US FIRST DO THIS KEEPING THE ORIGINAL SYMMETRY

e.pavarini@fz-juelich.de

static mean-field approaches

Hartree-Fock approximation

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

ferromagnetic Hartree-Fock

$$\hat{H}_{\mathrm{MF}} = \sum_{\boldsymbol{k}\sigma}\left[\varepsilon_{\boldsymbol{k}} + U\left(\frac{1}{2} - \sigma m\right)\right]\hat{n}_{\boldsymbol{k}\sigma} \qquad m = 0$$

e.pavarini@fz-juelich.de

to open a gap* we must lower the symmetry

* within the one-electron picture

REPLACE THIS

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

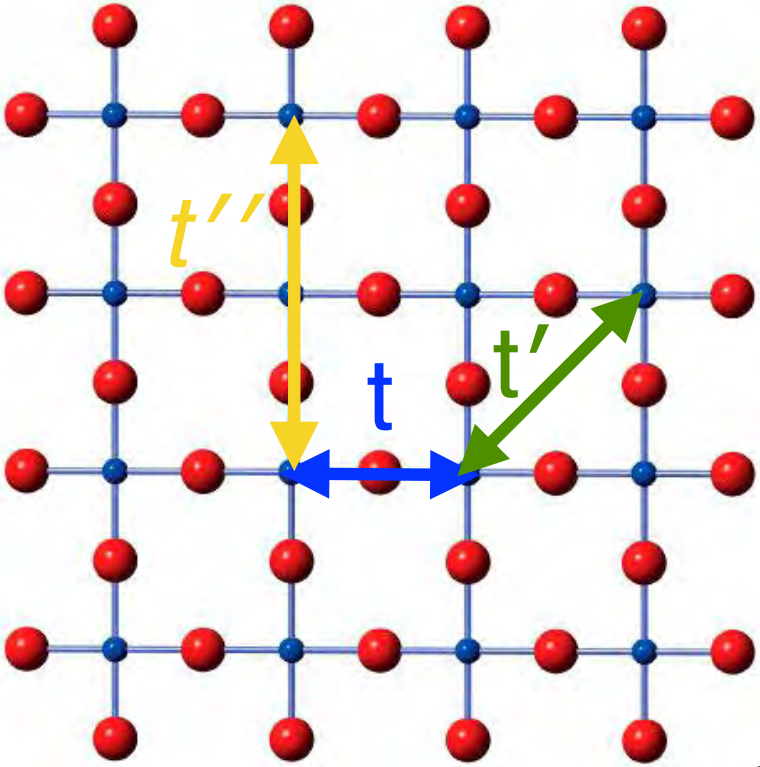
WITH THIS

$$\hat{H} = \sum_i \sum_\sigma \tilde{\varepsilon}_{di\sigma} c^\dagger_{i\sigma} c_{i\sigma} - \sum_{ii'} \tilde{t}_{ii'\sigma} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma}$$

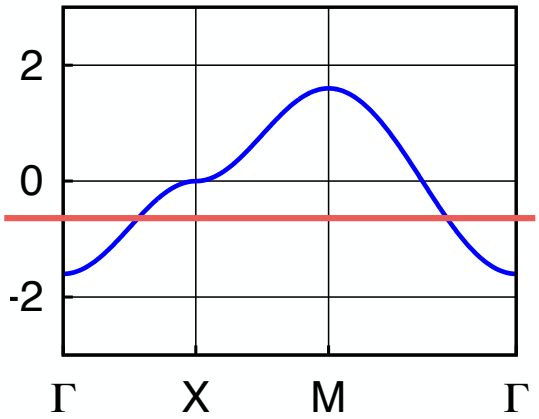
LET US FIRST DO THIS KEEPING THE ORIGINAL SYMMETRY

e.pavarini@fz-juelich.de

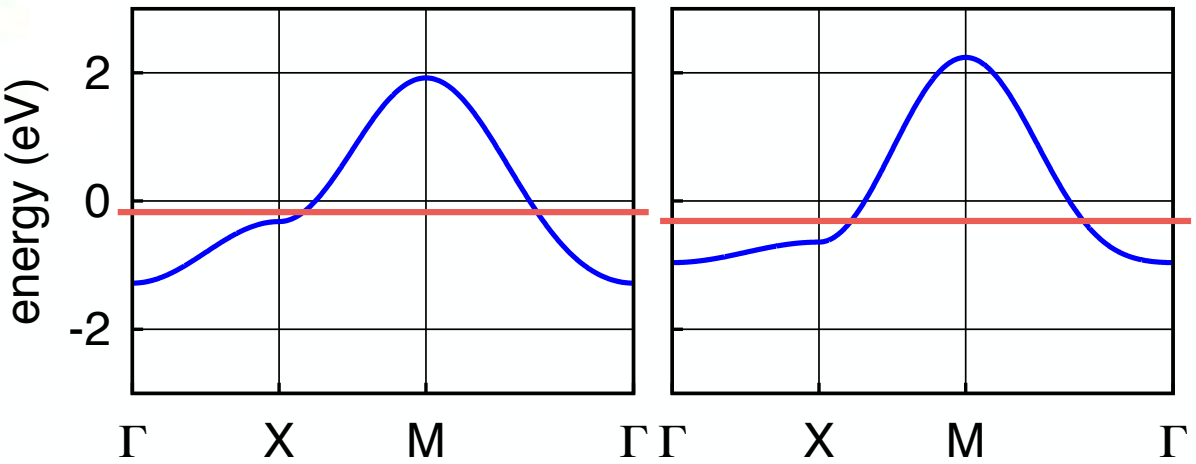
electron counting argument



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



t′/t= =0.2 t′/t= =0.4



``symmetry protected"

metallic state

half filling

to open a gap* we must lower the symmetry

* within the one-electron picture

REPLACE THIS

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

WITH THIS

$$\hat{H} = \sum_i \sum_\sigma \tilde{\varepsilon}_{di\sigma} c^\dagger_{i\sigma} c_{i\sigma} - \sum_{ii'\sigma} \tilde{t}_{ii'\sigma} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma}$$

REDUCING THE SYMMETRY

e.pavarini@fz-juelich.de

static mean-field approaches

Hartree-Fock approximation

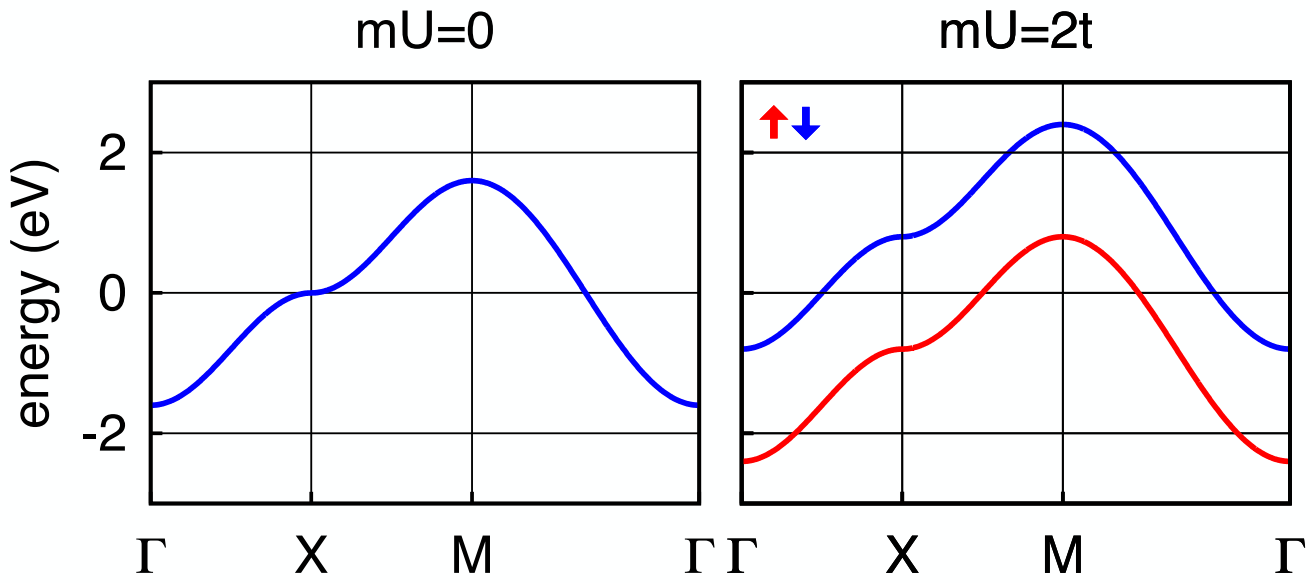
$$U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \longrightarrow U\left(\bar{n}_{i\uparrow}\hat{n}_{i\downarrow} + \hat{n}_{i\uparrow}\bar{n}_{i\downarrow} - \bar{n}_{i\uparrow}\bar{n}_{i\downarrow}\right)$$

ferromagnetic Hartree-Fock

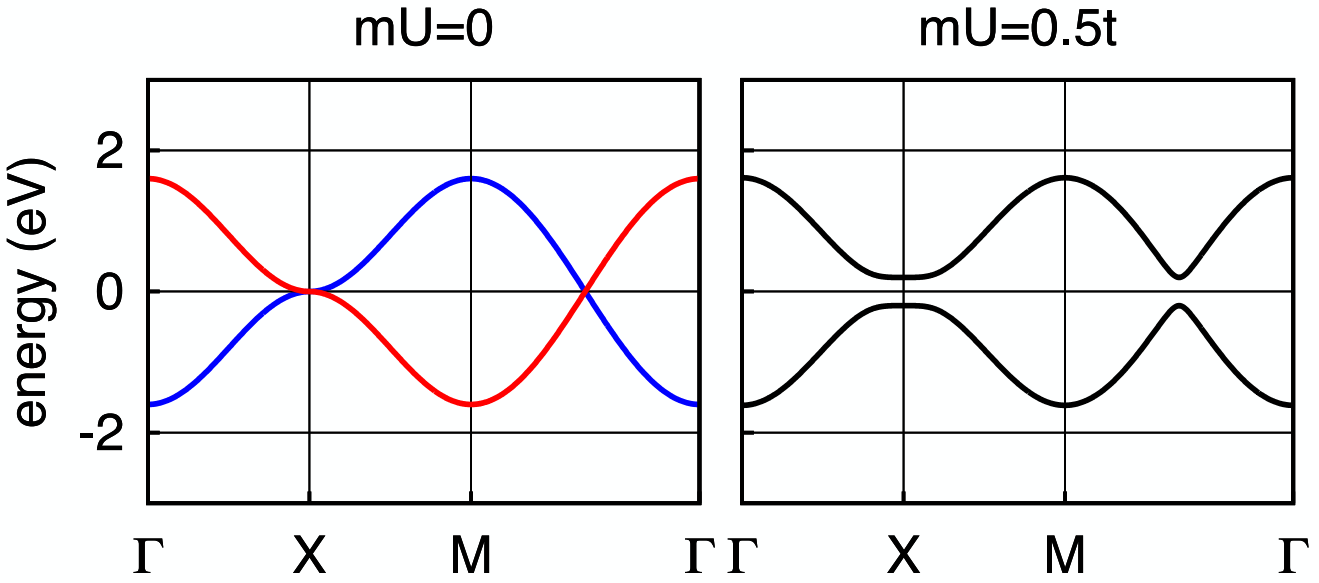
$$\hat{H}_{\mathrm{MF}} = \sum_{\boldsymbol{k}\sigma}\left[\varepsilon_{\boldsymbol{k}} + U\left(\frac{1}{2} - \sigma m\right)\right]\hat{n}_{\boldsymbol{k}\sigma} \qquad m \neq 0$$

e.pavarini@fz-juelich.de

to open a gap we lower the symmetry



FM



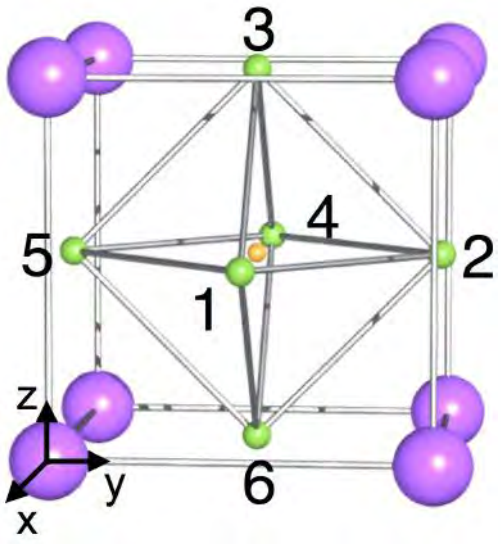
AFM

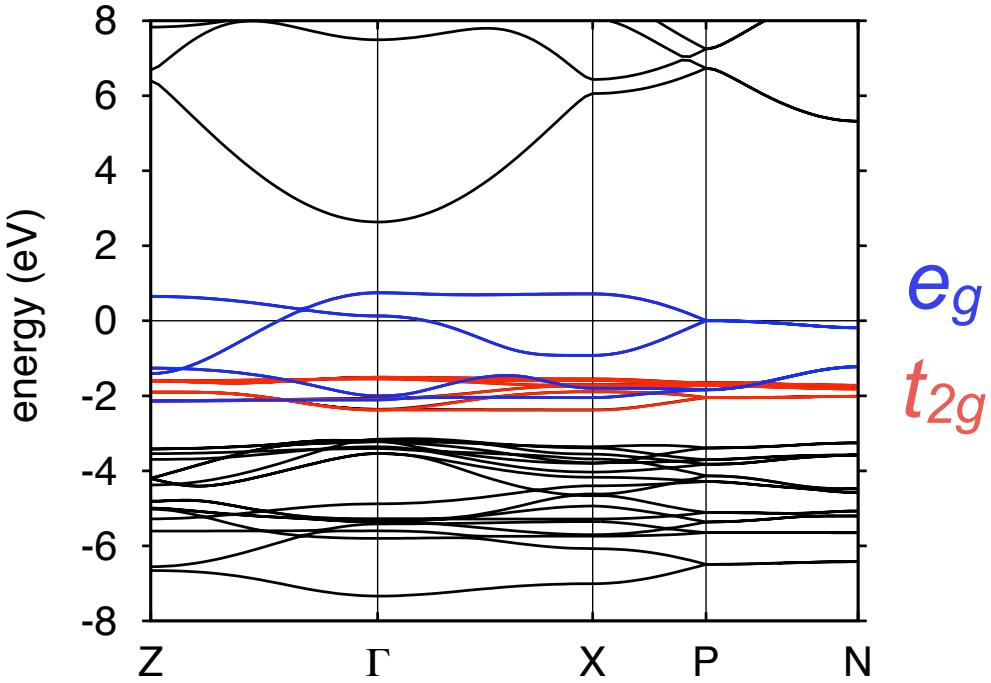
e.pavarini@fz-juelich.de

$KCuF_3$

one-electron picture: metal

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





e.pavarini@fz-juelich.de

methods to lower the symmetry

magnetic/orbital/charge order

spin-glass

....

Slater insulator

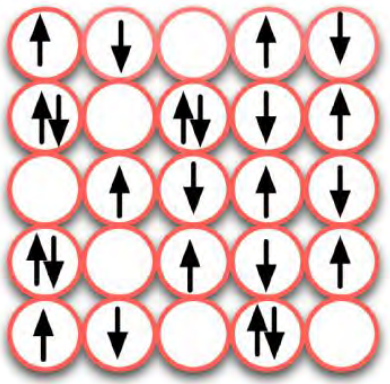
e.pavarini@fz-juelich.de

Mott insulators and systems sufficiently close to the Mott transition have different properties wrt Slater insulators

1989-1992: dynamical mean-field theory

Hubbard model

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

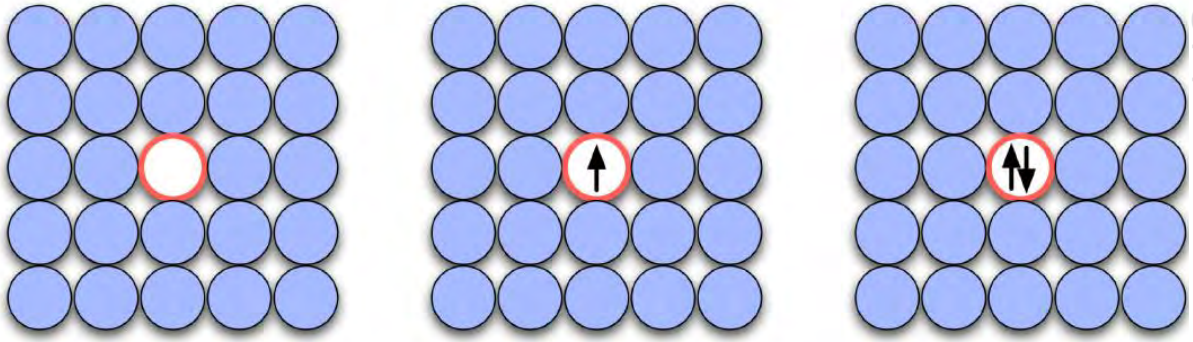


$G^{i,j}$

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).

e.pavarini@fz-juelich.de

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)

e.pavarini@fz-juelich.de

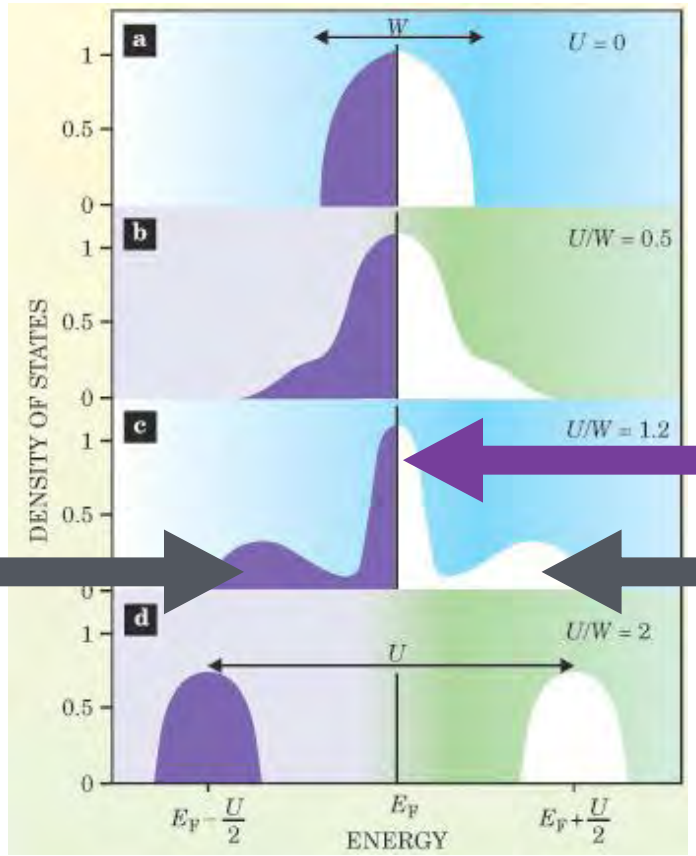
dynamical mean-field theory

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

U/W

W: band width

half filling



QP

LHB

UHB

$\Sigma(\omega)$

e.pavarini@fz-juelich.de

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

Bethe Lattice

how does it work?

e.pavarini@fz-juelich.de

DMFT for the Hubbard dimer

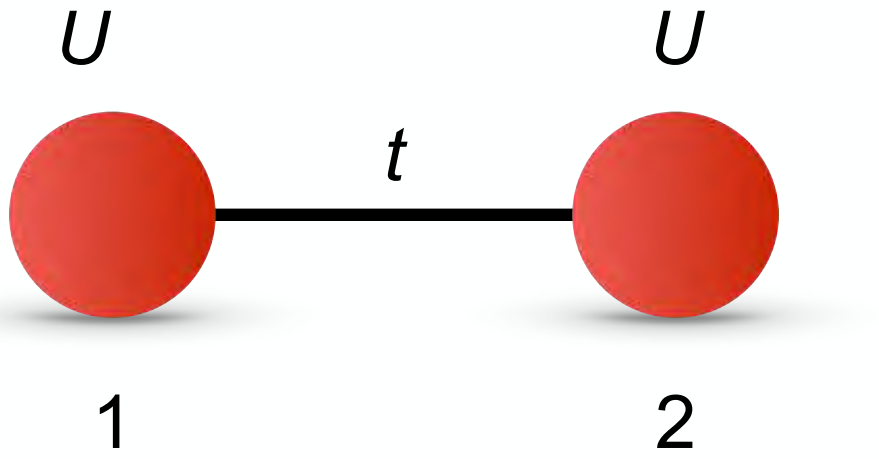
this is a **toy** model: coordination number is one

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

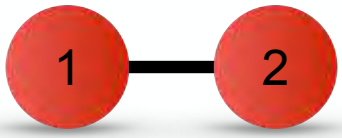
e.pavarini@fz-juelich.de

the Hubbard dimer

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



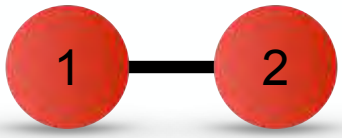
e.pavarini@fz-juelich.de



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	$4\varepsilon_d+2U$

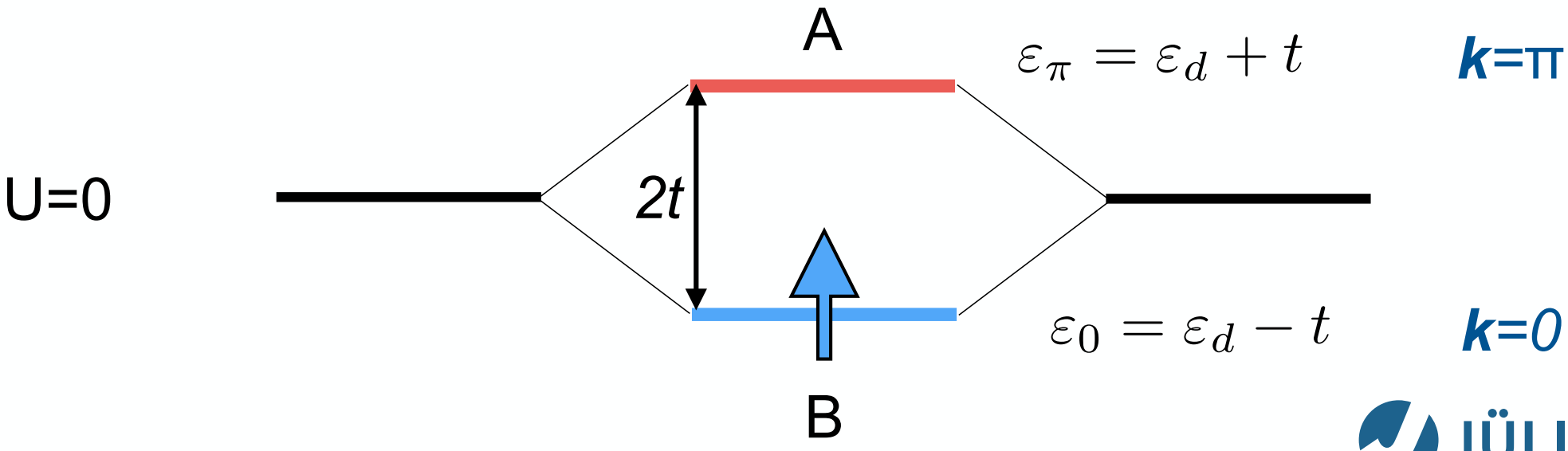
e.pavarini@fz-juelich.de

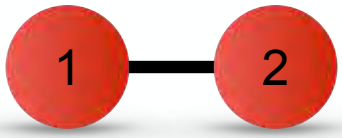


finite *t*: exact diagonalization

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



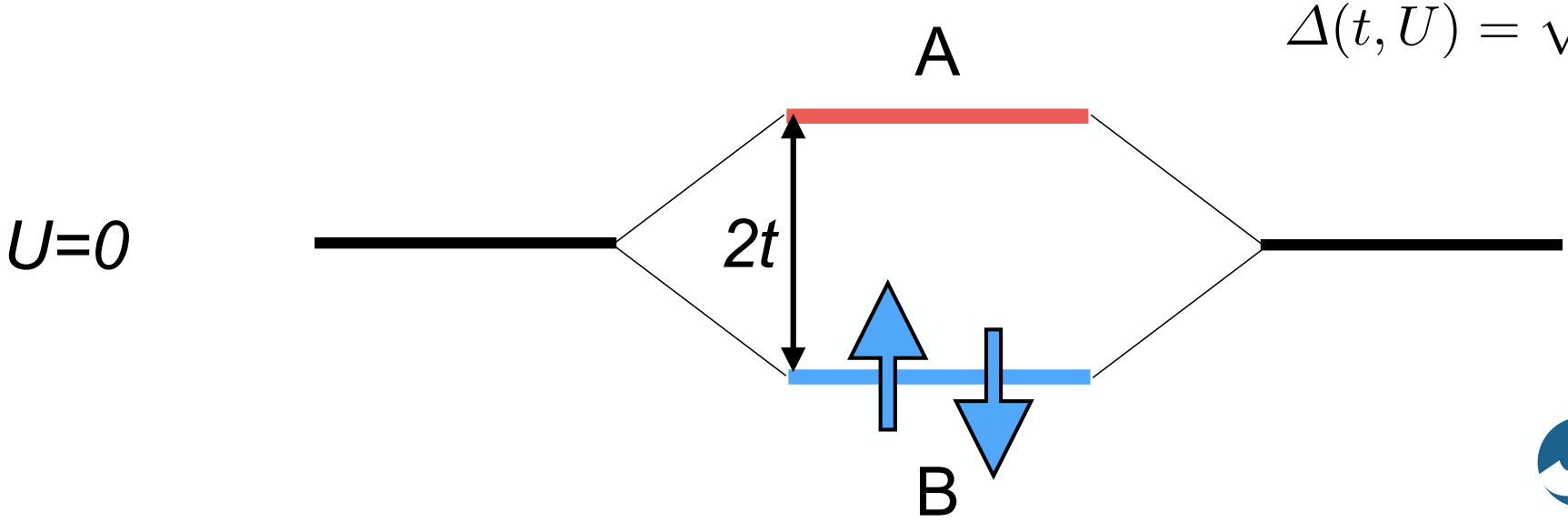


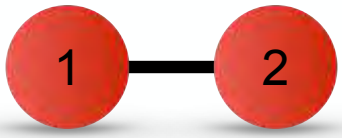
finite *t*: exact diagonalization N=2

half filling (N=2)

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

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



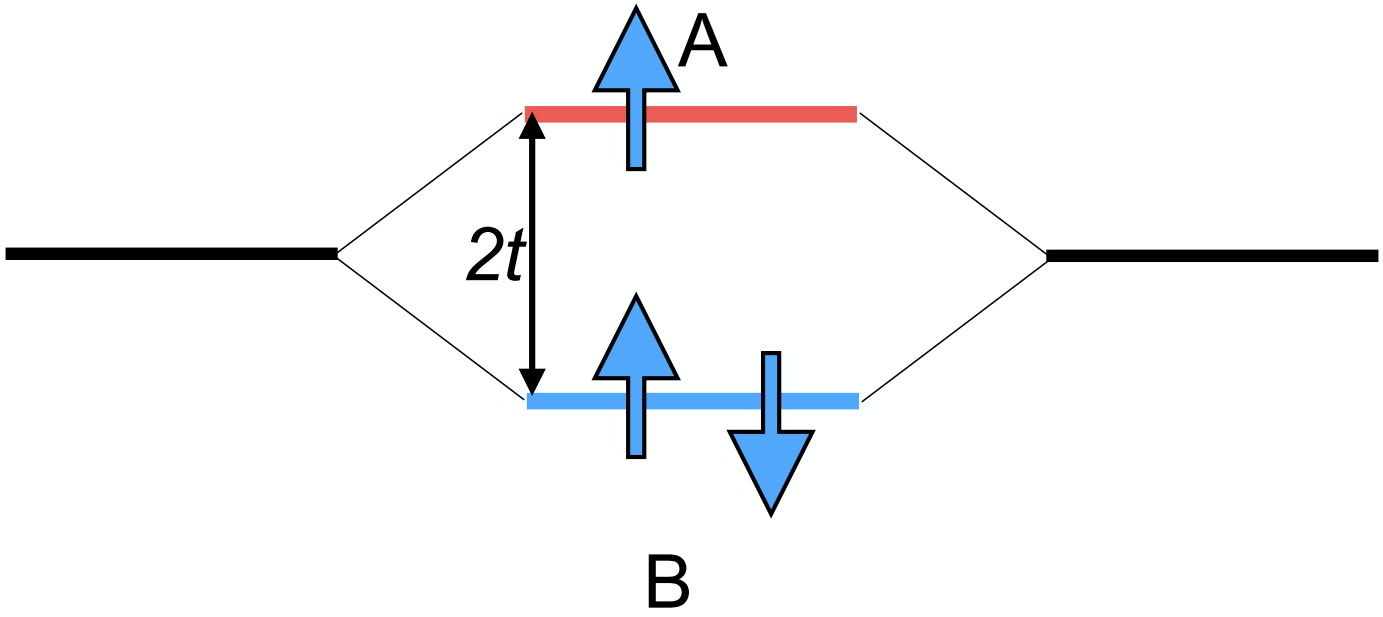


finite *t*: exact diagonalization

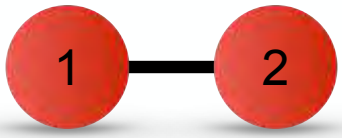
N=3

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

U=0



e.pavarini@fz-juelich.de



the local Green function, N=2

Lehmann representation

$d^1 \rightarrow d^0$

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

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

E(2)-E(1)

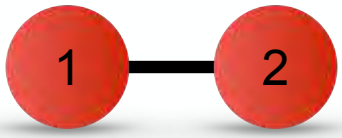
$$|\langle 3|c^\dagger_\sigma|2\rangle|^2$$

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

E(3)-E(2)

$d^2 \rightarrow d^1$

e.pavarini@fz-juelich.de



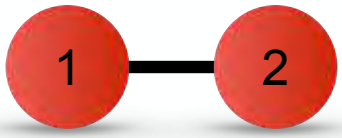
the local Green function, N=2

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

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

$k = 0$ $\qquad$ $k = \pi$

change basis $\qquad c_{k\sigma} = \frac{1}{\sqrt{2}} \left(c_{1\uparrow} \pm c_{2\uparrow} \right)$



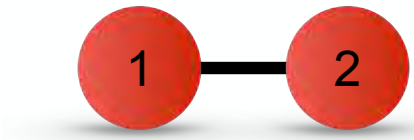
the local Green function

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

number k points

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

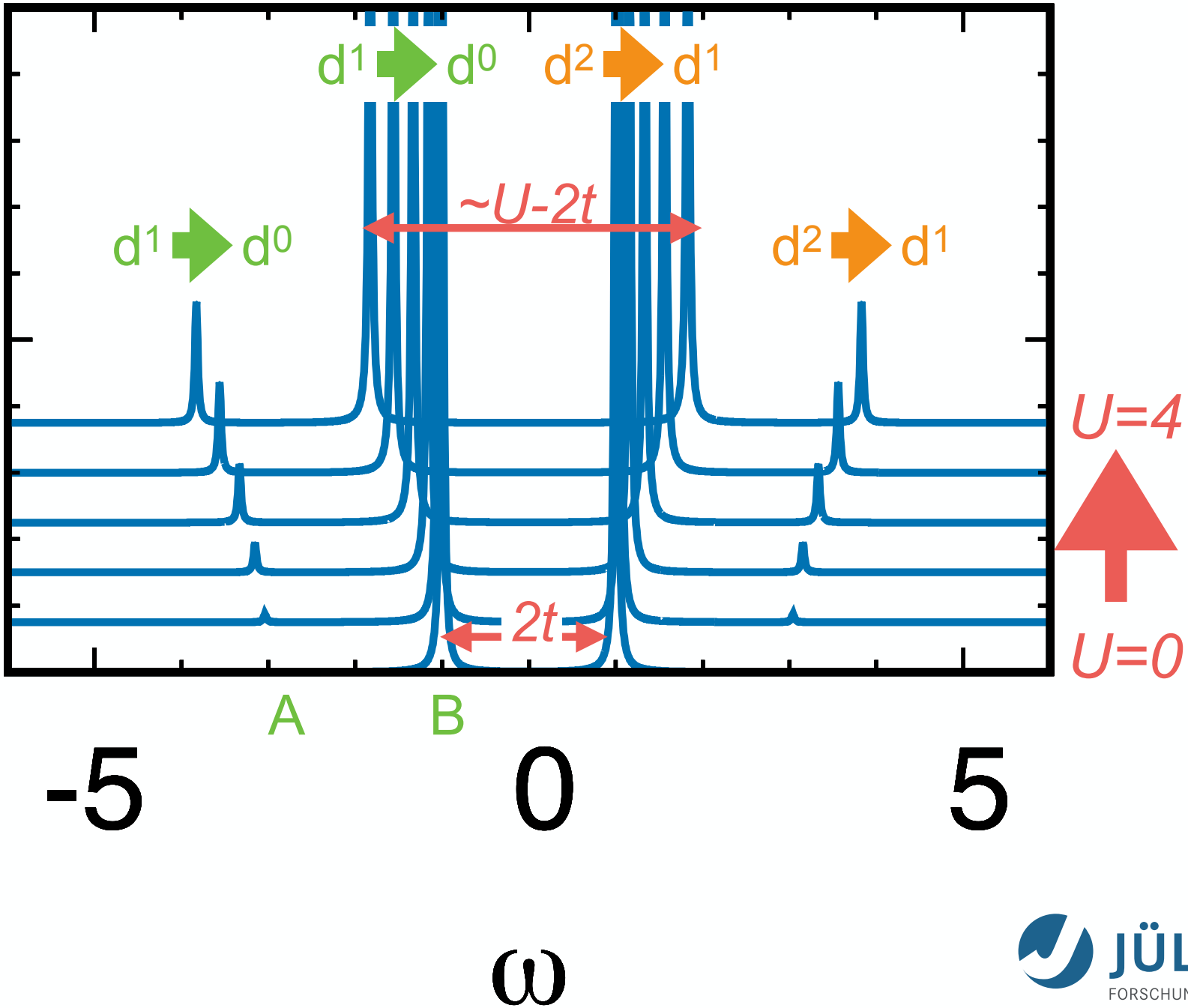
e.pavarini@fz-juelich.de



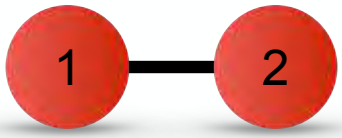
the local spectral function

W=2t

t=1



e.pavarini@fz-juelich.de



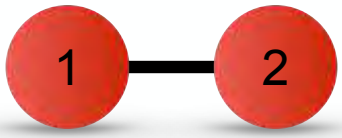
the local Green function

U=0 vs finite *U*

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

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

e.pavarini@fz-juelich.de



the local Green function

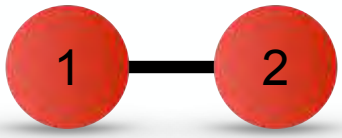
local self-energy

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

non-local self-energy

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

e.pavarini@fz-juelich.de



the local Green function

hybridization function

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

modified **hybridization function**

NON-LOCAL

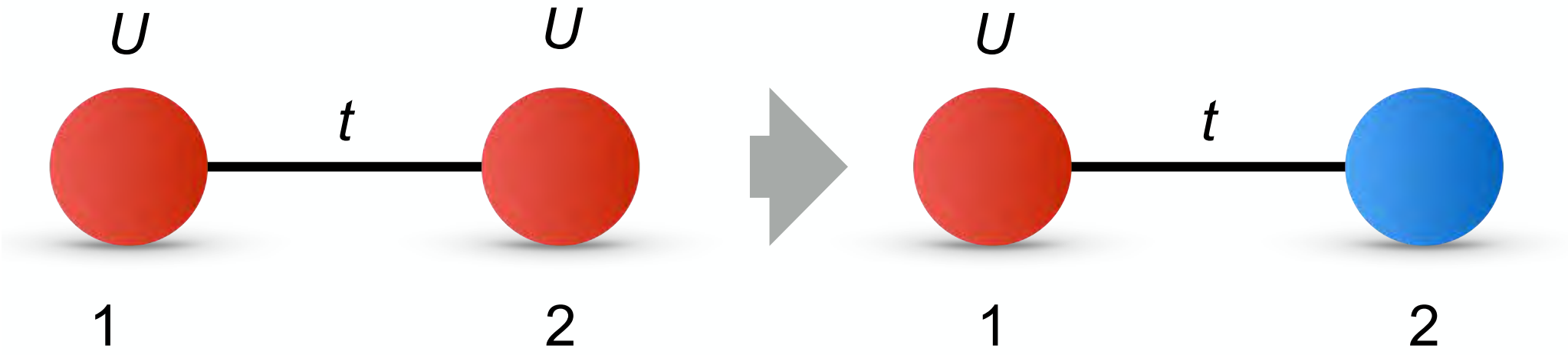
$$F^\sigma(i\nu_n) = \frac{(t + \Delta\Sigma_l(i\nu_n))^2}{i\nu_n - (\varepsilon_d - \mu + \Sigma_l^\sigma(i\nu_n))}.$$

LOCAL

e.pavarini@fz-juelich.de

map to a quantum impurity model ?

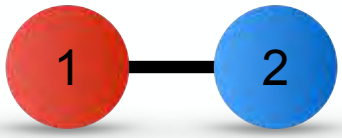
the Anderson molecule



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

~ same local Green function ?

e.pavarini@fz-juelich.de



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

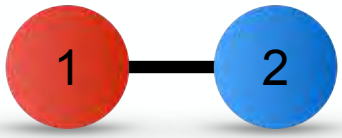
$$\hat{H}_2^A(\varepsilon_d, U, t; \varepsilon_s) = \begin{pmatrix} \varepsilon_d+\varepsilon_s & 0 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_d+\varepsilon_s & 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_d+\varepsilon_s & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_d+\varepsilon_s & -\sqrt{2}t & -\sqrt{2}t \\ 0 & 0 & 0 &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

Anderson

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

same occupations of Hubbard dimer

e.pavarini@fz-juelich.de



solution: Hubbard vs Anderson

Anderson molecule

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

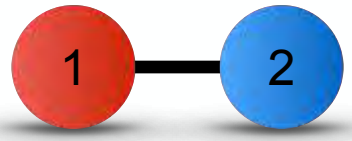
Hubbard dimer

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

LOCAL

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

e.pavarini@fz-juelich.de



solution: Hubbard vs Anderson

hybridization function

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

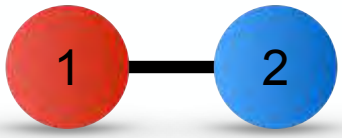
modified **hybridization function**

NON-LOCAL

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

LOCAL

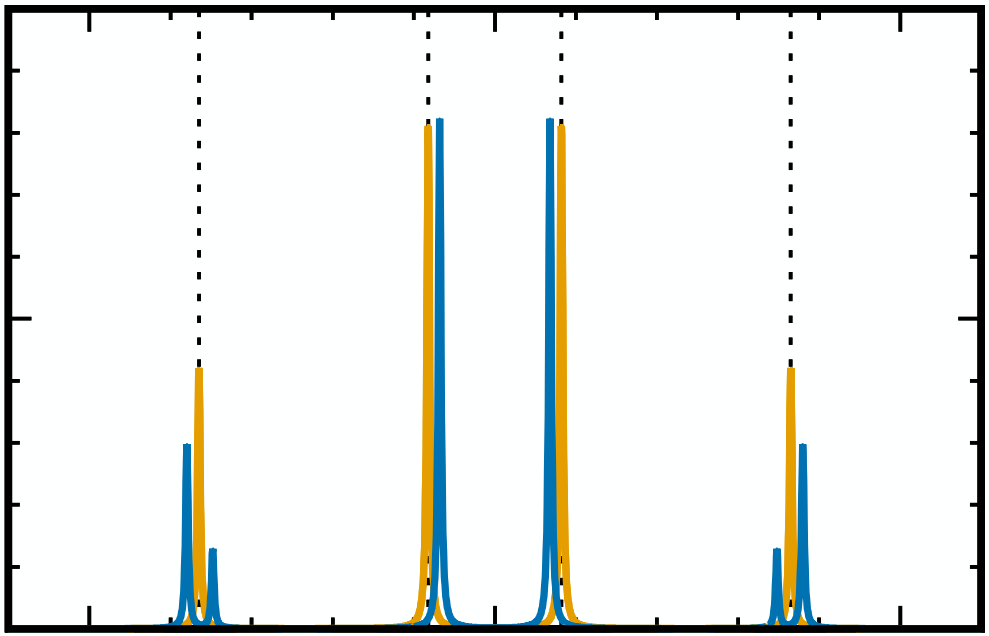
e.pavarini@fz-juelich.de



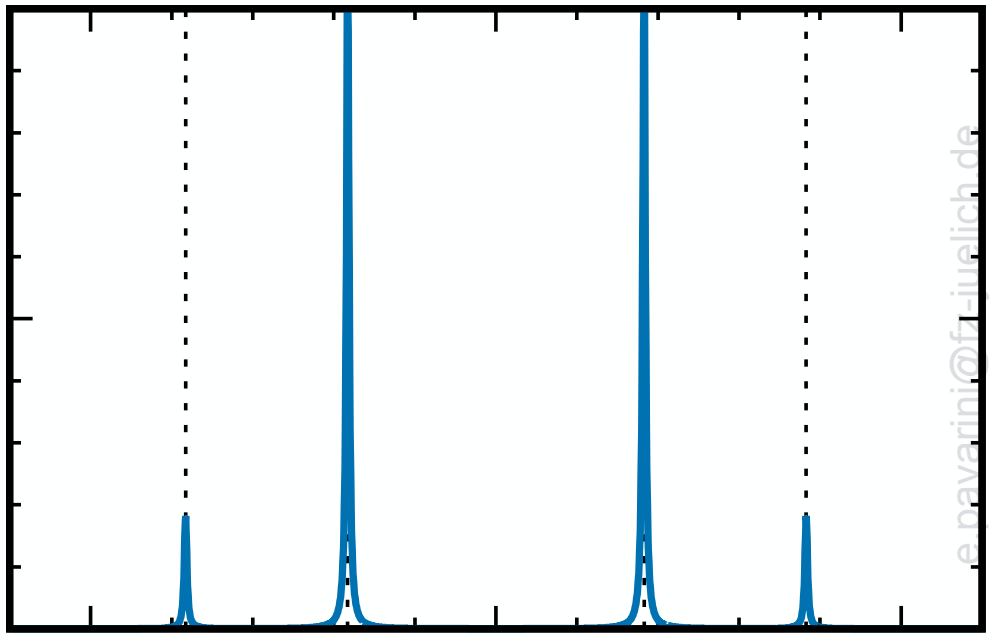
Green function *U=4t*

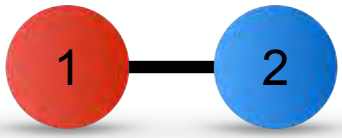
Anderson vs **Hubbard**

only **local** self-energy



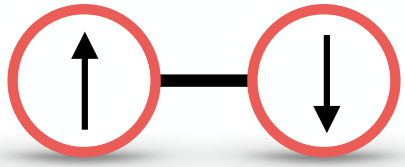
exact





DMFT for the dimer

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

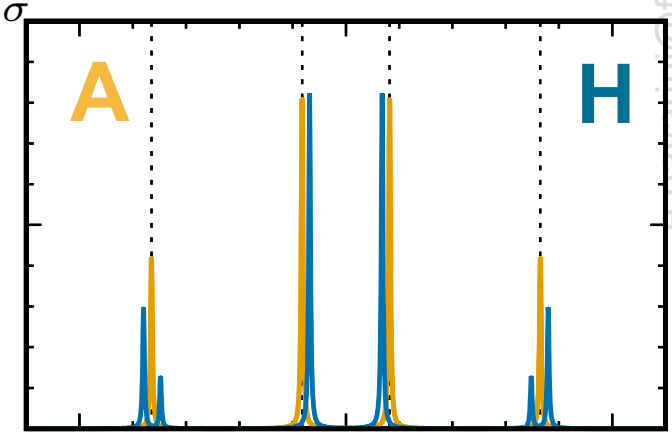


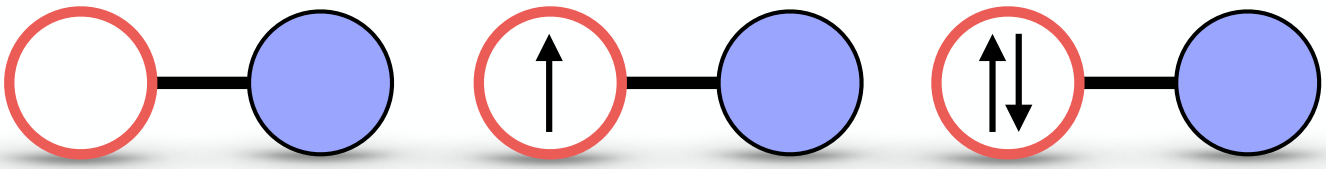
map to quantum impurity model (QIM) in local self-energy approximation

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

QIM solver

self-consistency loop





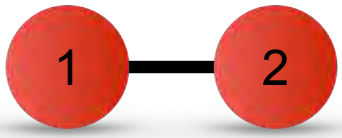
$$\Sigma(\mathbf{k},\omega) \longrightarrow \Sigma_d(\omega)$$

non-local self-energy terms

vs non-local interaction

$$U_{ijij}$$

e.pavarini@fz-juelich.de

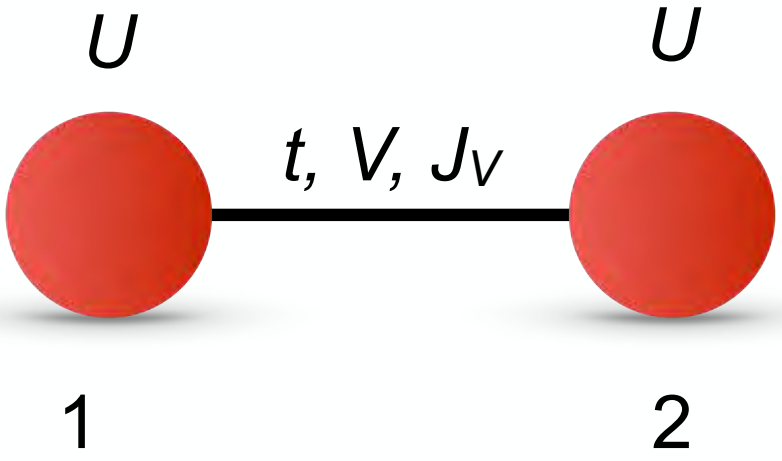


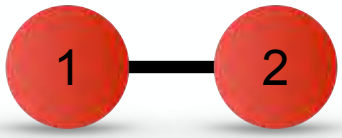
non-local Coulomb terms

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

Hubbard

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

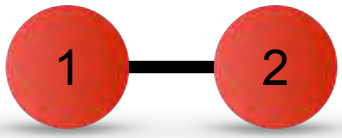
N=2 half filling

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 $U' = U - V$.

e.pavarini@fz-juelich.de



non-local Coulomb terms

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

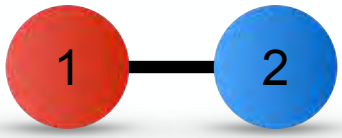
strong-correlation effects typically appear when the local electron-electron repulsion dominates over non-local terms

if Coulomb interaction independent on site distance, we can map to (some) effective weakly correlated model

e.pavarini@fz-juelich.de

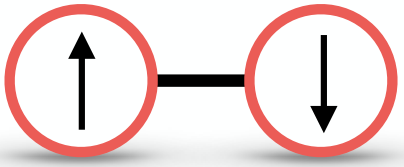
quantum-impurity solvers

e.pavarini@fz-juelich.de



DMFT for the dimer

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

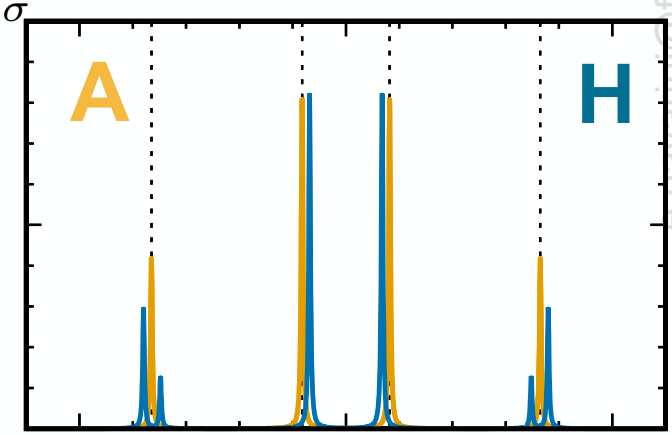


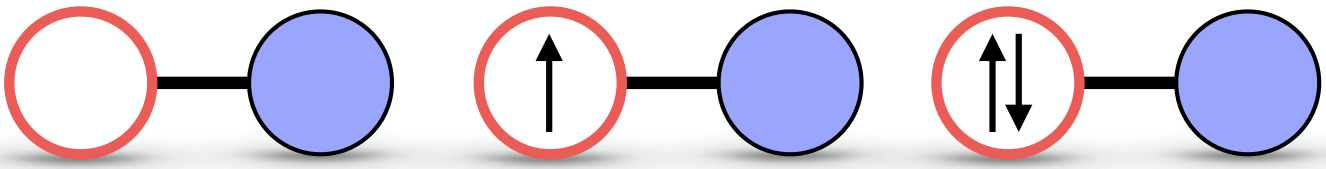
map to quantum impurity model (QIM) in local self-energy approximation

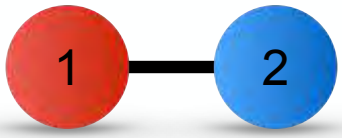
$$\hat{H}^{\mathrm{A}} = \varepsilon_s \sum_{\sigma} \hat{n}_{s\sigma} - t \sum_{\sigma} \left(c^{\dagger}_{d\sigma} c_{s\sigma} + c^{\dagger}_{s\sigma} c_{d\sigma} \right) + \varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$

QIM solver

self-consistency loop







quantum-impurity solver

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

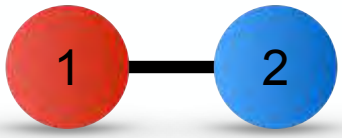
hybridization-expansion CT-QMC

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

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

only even orders survive (*m=2k*)

e.pavarini@fz-juelich.de



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 $\quad t^k_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})$

see lecture notes

e.pavarini@fz-juelich.de

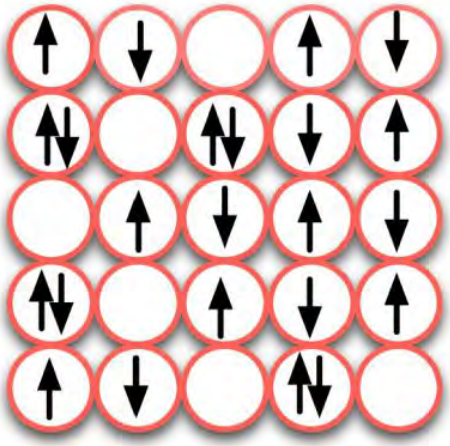
some exact limits at half filling

DMFT for the one-band Hubbard model

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

e.pavarini@fz-juelich.de

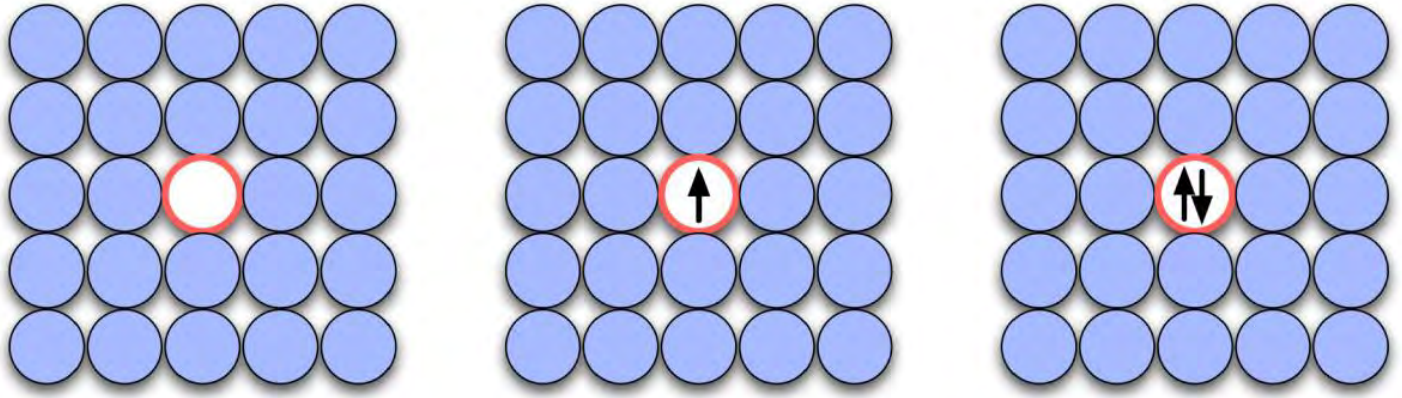
dynamical mean-field theory



$G^{i,j}$

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)

e.pavarini@fz-juelich.de

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)

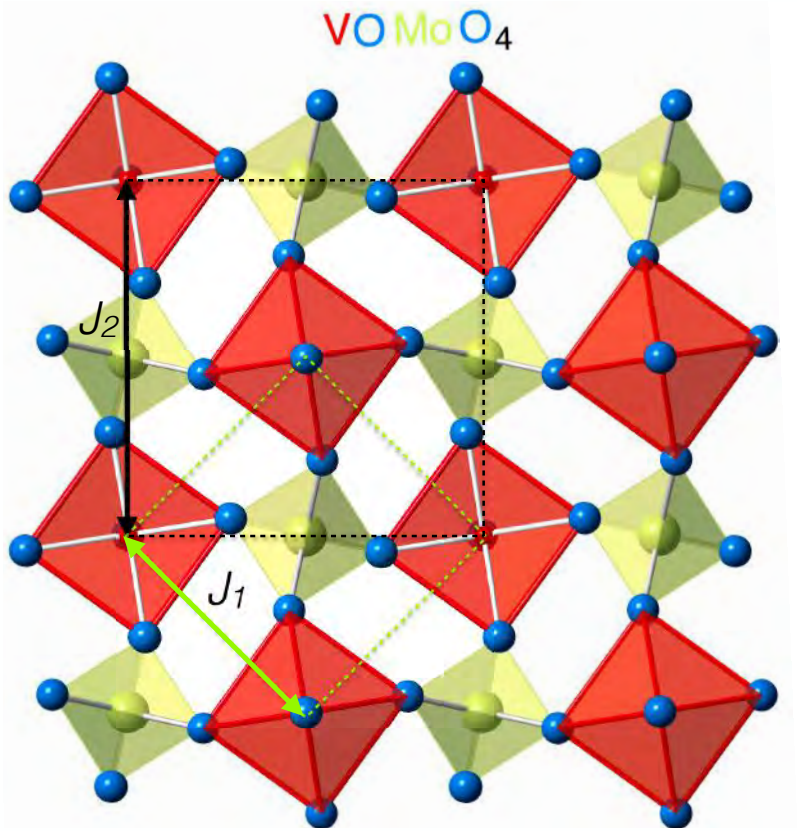
$$\hat{H}^A = \underbrace{\sum_{\boldsymbol{k}\sigma} \varepsilon^s_{\boldsymbol{k}} \hat{n}_{\boldsymbol{k}\sigma}}_{\hat{H}_{\text{bath}}} + \underbrace{\sum_{\boldsymbol{k}\sigma} \left(V^s_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{d\sigma} + \text{h.c.} \right)}_{\hat{H}_{\text{hyb}}}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

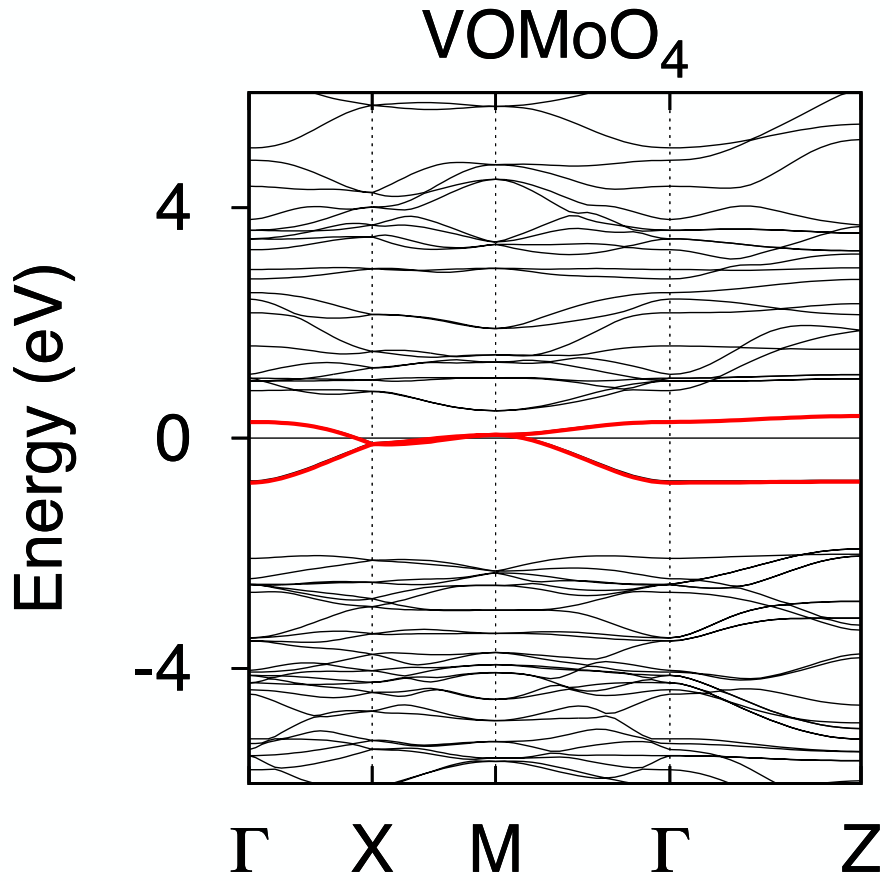
QIM solver: **QMC**, ED, NRG, DMRG,…

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

e.pavarini@fz-juelich.de

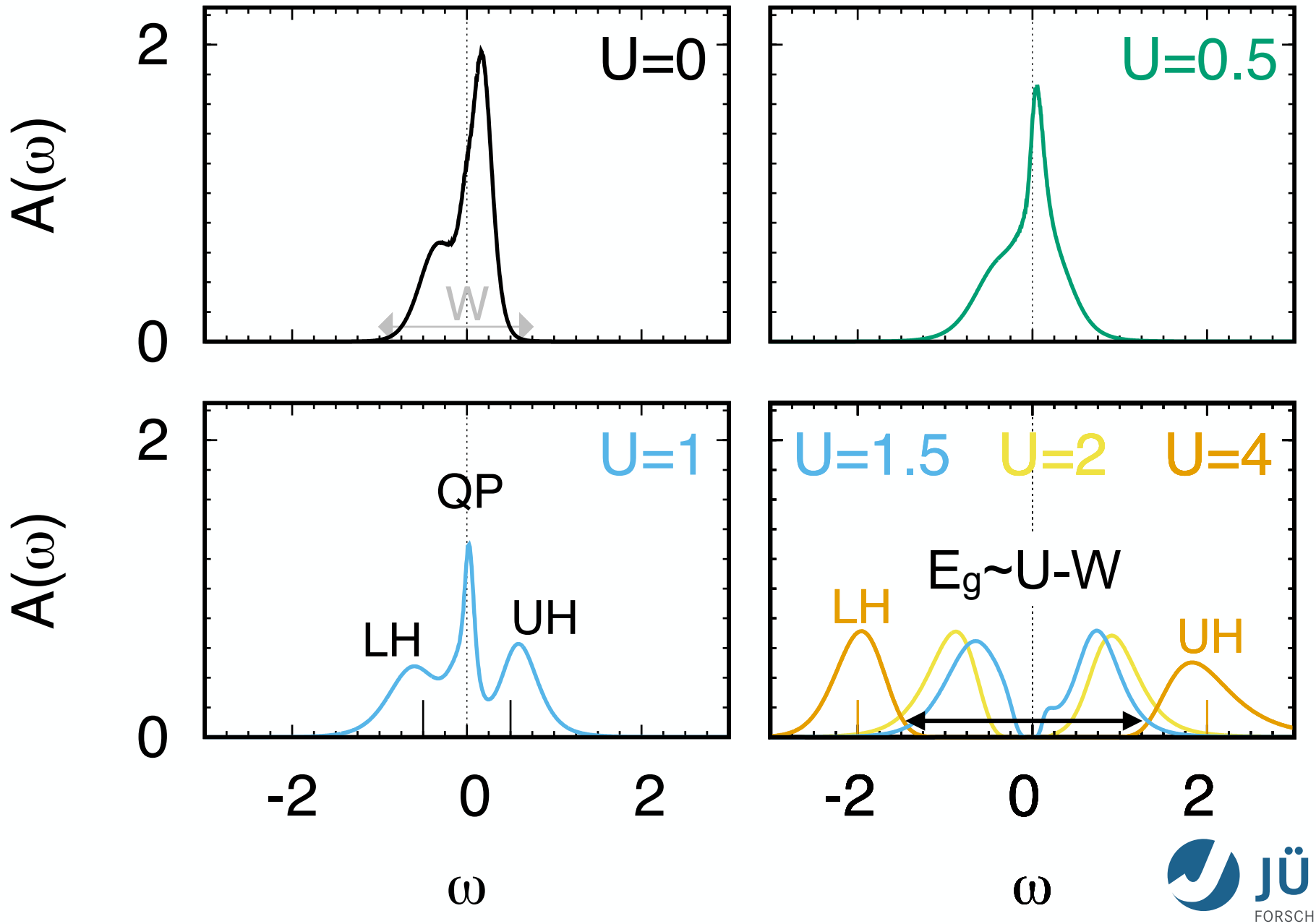
a real-system case: $VOMoO_4$





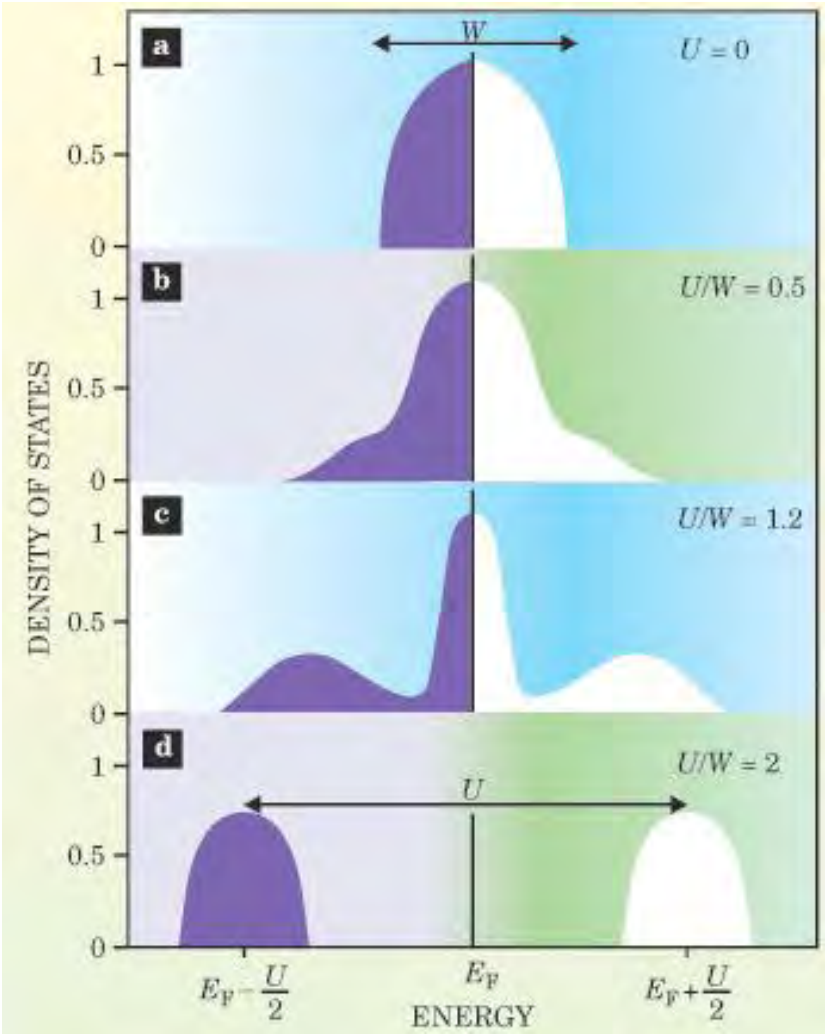
Amin Kiani and Eva Pavarini, Phys. Rev. B **94**, 075112 (2016)

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)

e.pavarini@fz-juelich.de

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

Hartree-Fock Hamiltonian and bands

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

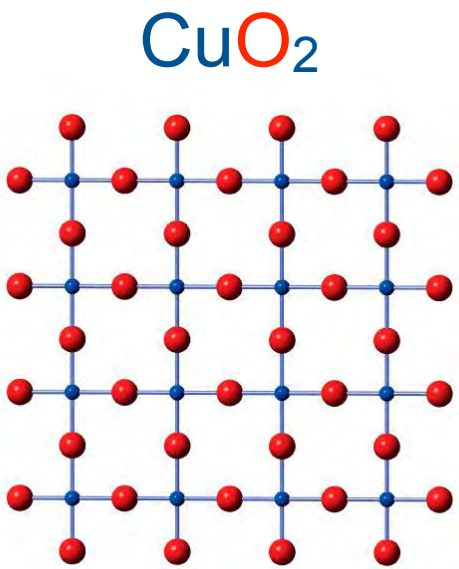
ferromagnetic Hartree-Fock

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

self-energy

e.pavarini@fz-juelich.de

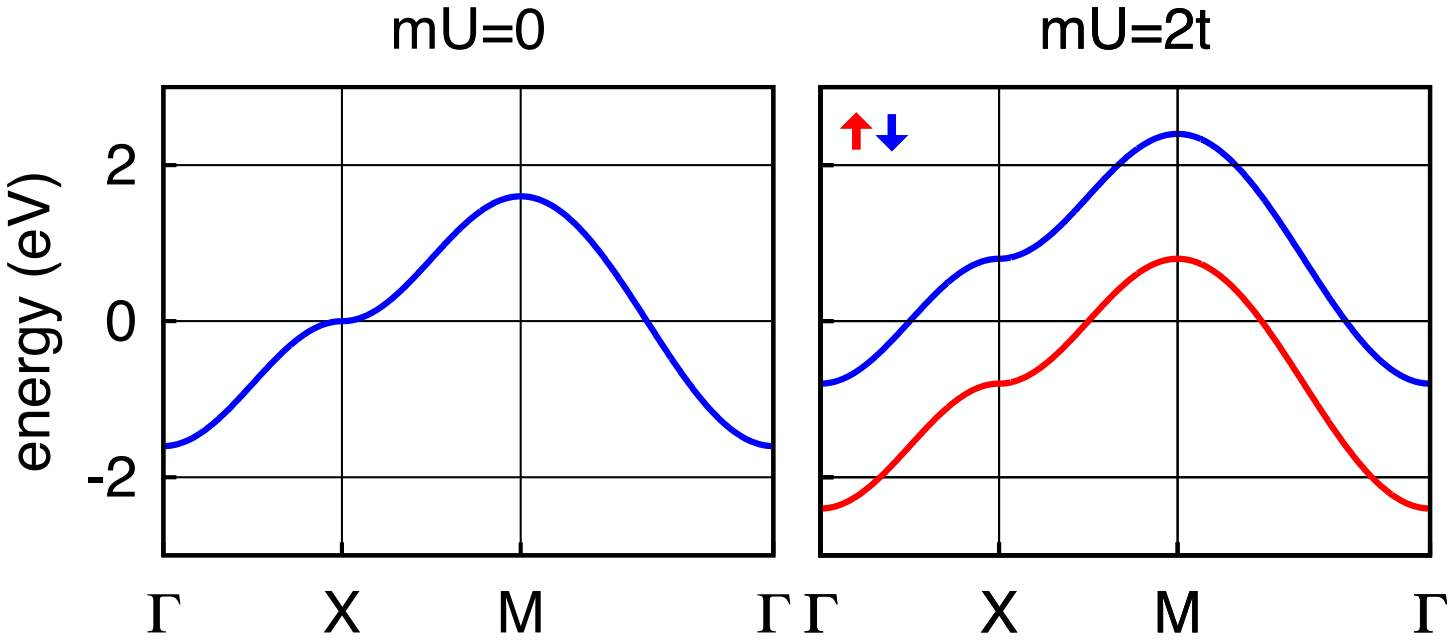
ferromagnetic Hartree-Fock



2d-tight binding model

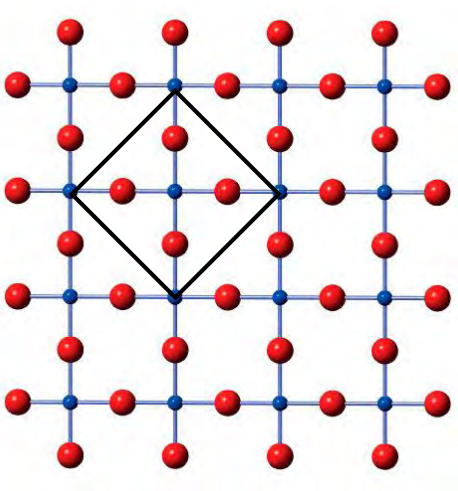
$$\varepsilon_{\boldsymbol{k}} = -2t[\cos k_x + \cos k_y]$$

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

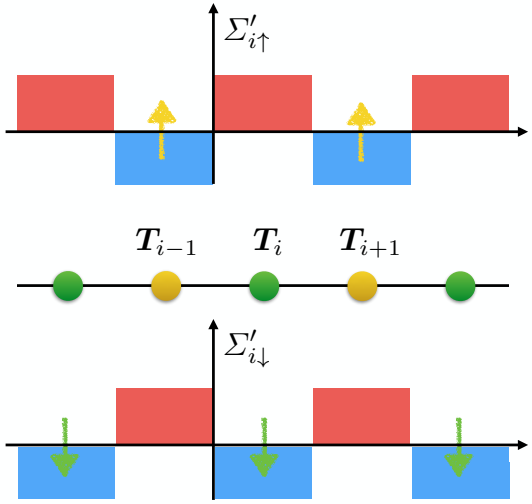


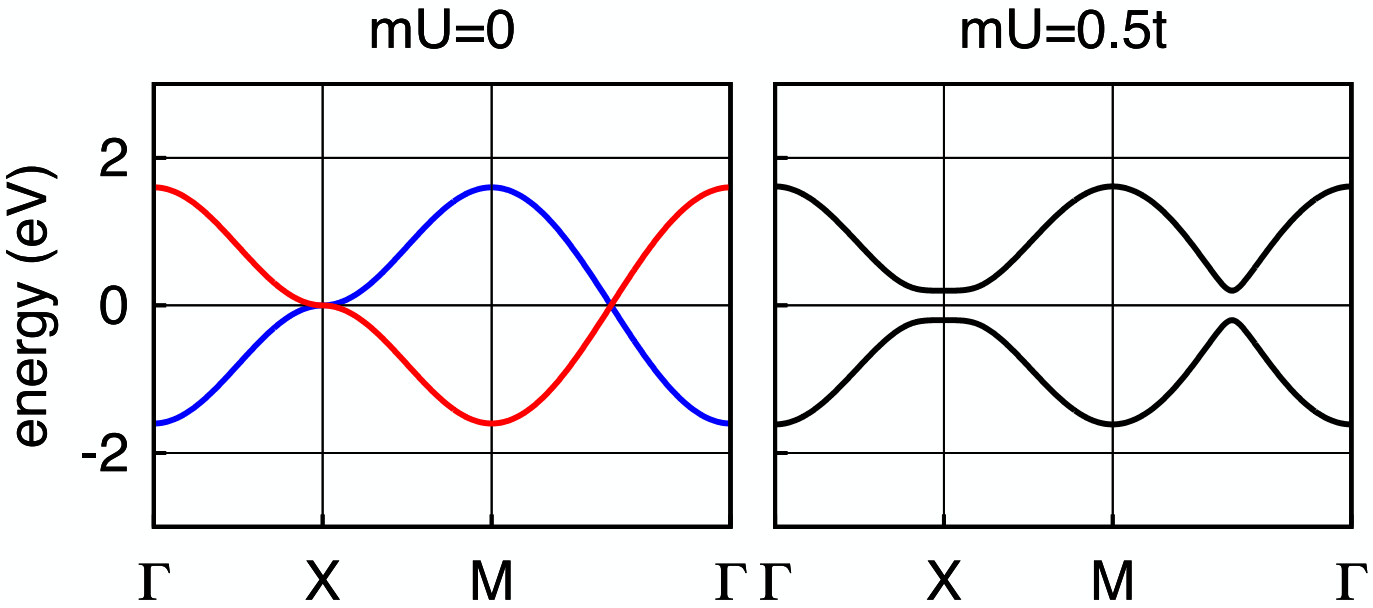
e.pavarini@fz-juelich.de

antiferromagnetic HF



CuO_2



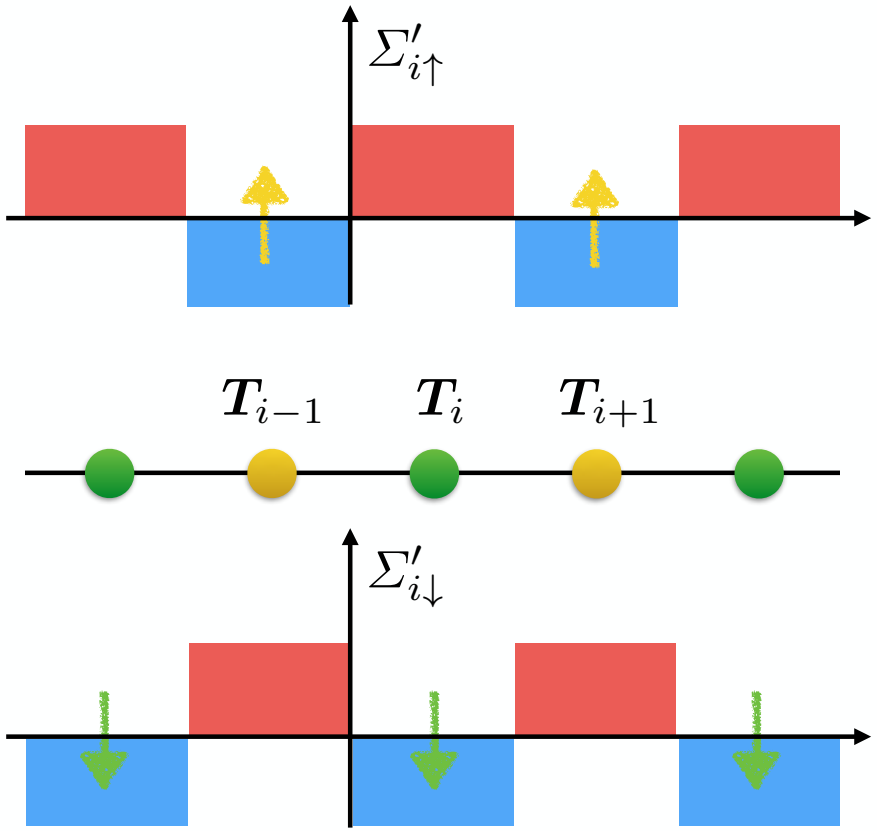


e.pavarini@fz-juelich.de

Mott transition: HF vs DMFT

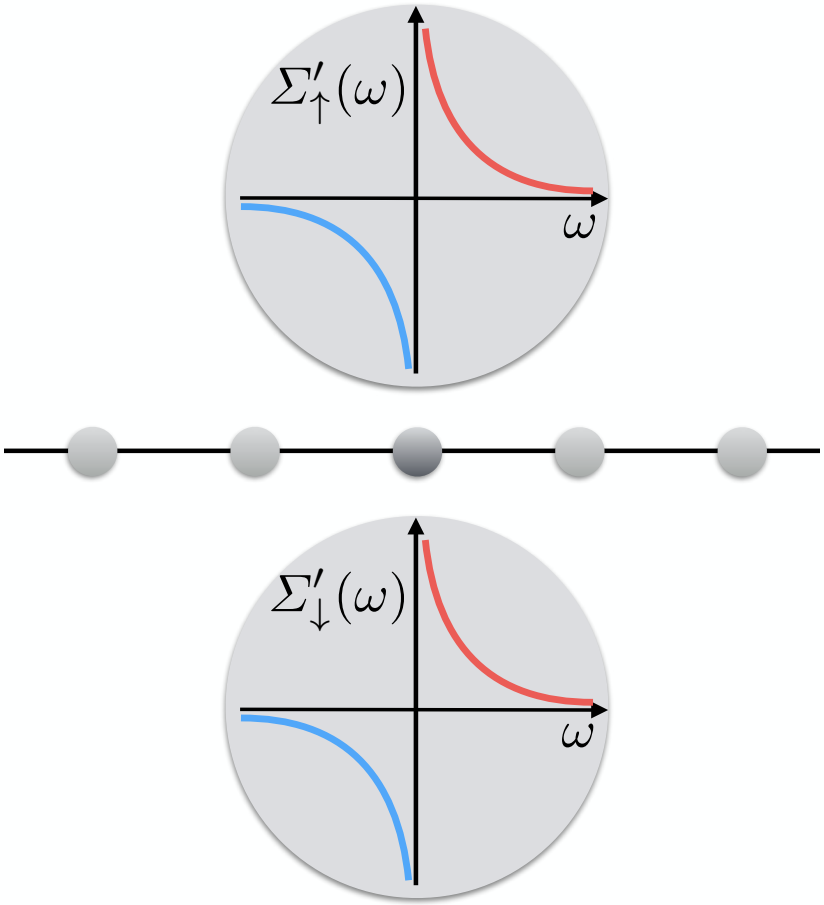
LDA+*U*

Hartree-Fock



LDA+DMFT

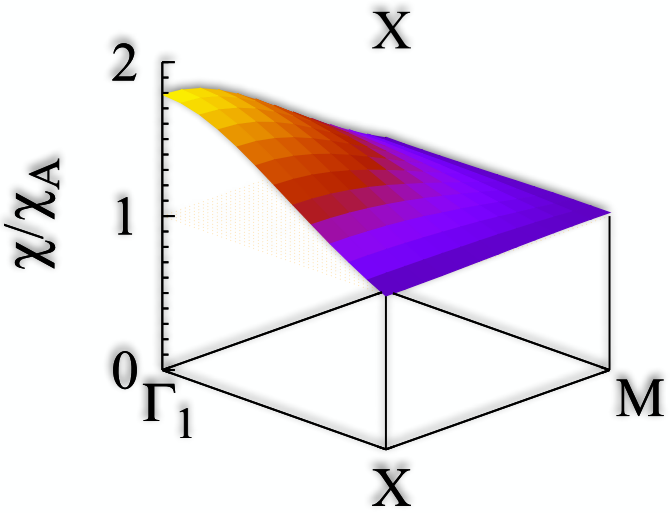
DMFT



see also my lecture notes in correl17

e.pavarini@fz-juelich.de

linear response functions



e.pavarini@fz-juelich.de

magnetic susceptibility tensor

$$\chi_{\hat{S}^i_\nu \; \hat{S}^{i'}_{\nu'}}(\boldsymbol{\tau}) \quad = \quad \langle \mathcal{T} \Delta \hat{S}^i_\nu(\tau_1, \tau_2) \Delta \hat{S}^{i'}_{\nu'}(\tau_3, \tau_4) \rangle_0,$$

$$\hat{S}^i_\nu(\tau_1, \tau_2) \quad = \quad \sum_{\boldsymbol{\alpha}} p^\nu_{\boldsymbol{\alpha}} \; c^\dagger_{i\alpha'}(\tau_2) c_{i\alpha}(\tau_1) \qquad\qquad p^z_{\boldsymbol{\alpha}} = -g\mu_B \langle \sigma' | \hat{\sigma}_z | \sigma' \rangle,$$

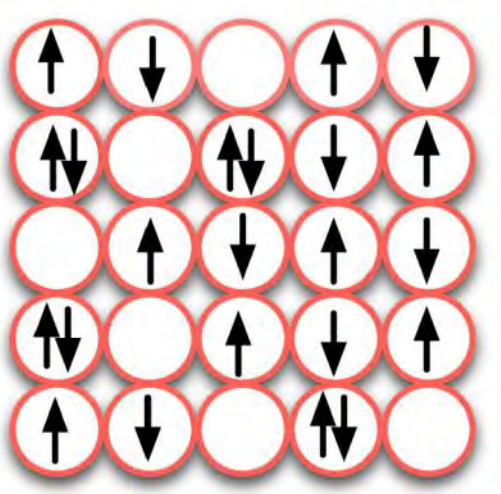
two-particle Green functions

e.pavarini@fz-juelich.de

Hubbard model

atomic hoppings atomic

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



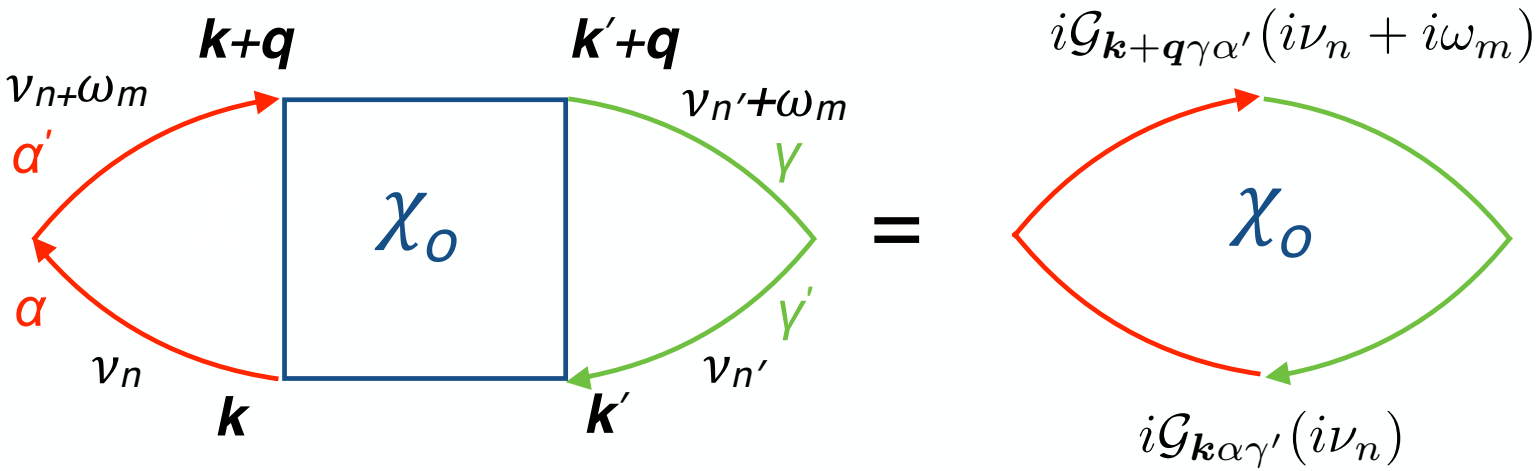
at half filling:

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

e.pavarini@fz-juelich.de

U=0: the non-interacting case

Wick's theorem holds

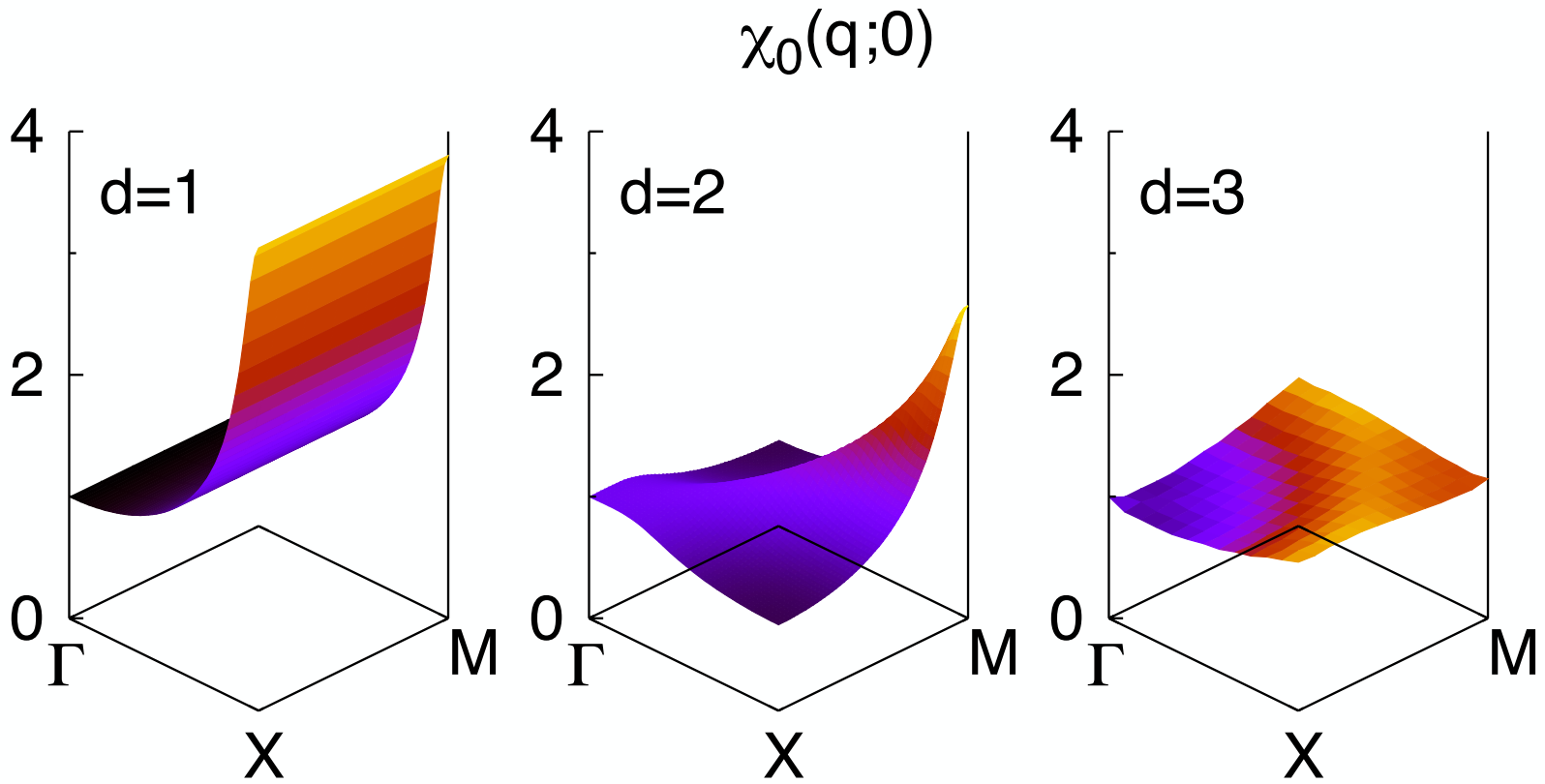


$$[\chi_0(\boldsymbol{q}; i\omega_m)]_{\boldsymbol{k}L_\alpha, \boldsymbol{k}'L_\gamma} = -\beta N_{\boldsymbol{k}} \mathcal{G}_{\boldsymbol{k}\alpha\gamma'}(i\nu_n) \mathcal{G}_{\boldsymbol{k}'+\boldsymbol{q}\alpha'\gamma}(i\nu_{n'} + i\omega_m) \delta_{n,n'} \delta_{\boldsymbol{k},\boldsymbol{k}'}$$

Hubbard model, U=0, n=1

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

T ~ 350 K



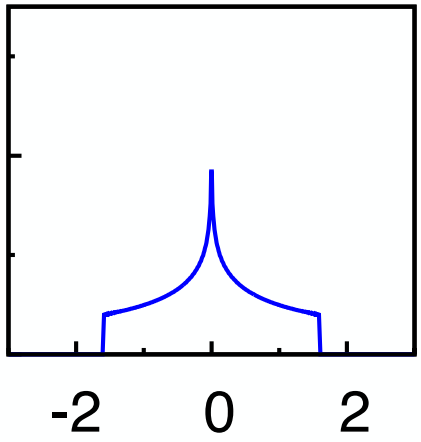
weakly T dependent (except close to van-Hove singularities/divergencies)

e.pavarini@fz-juelich.de

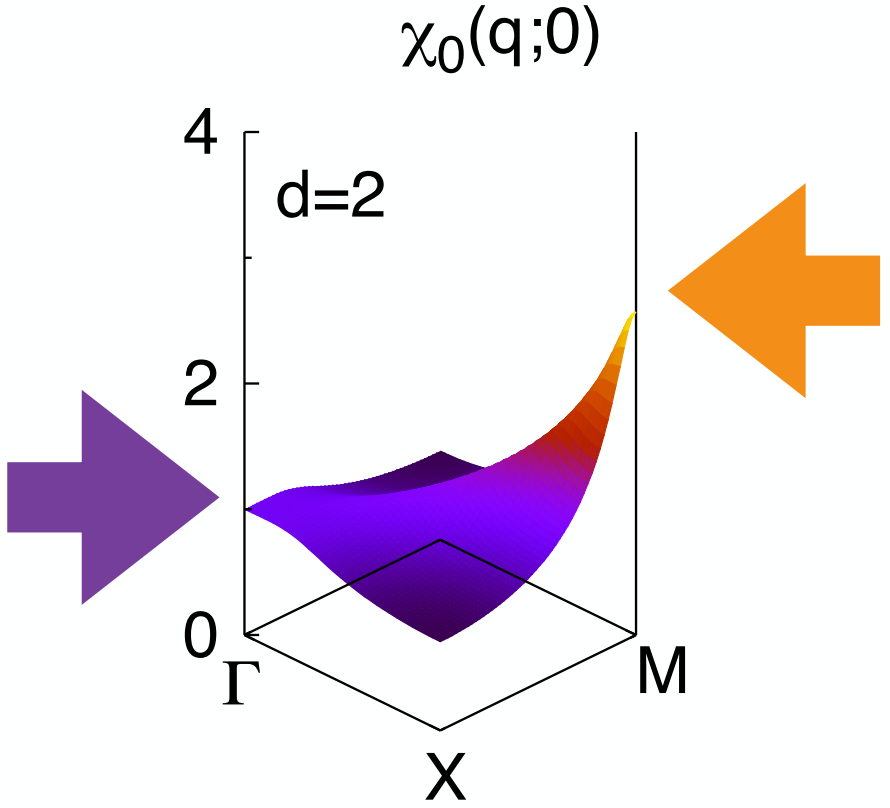
Hubbard model, U=0, n=1

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

T ~ 350 K



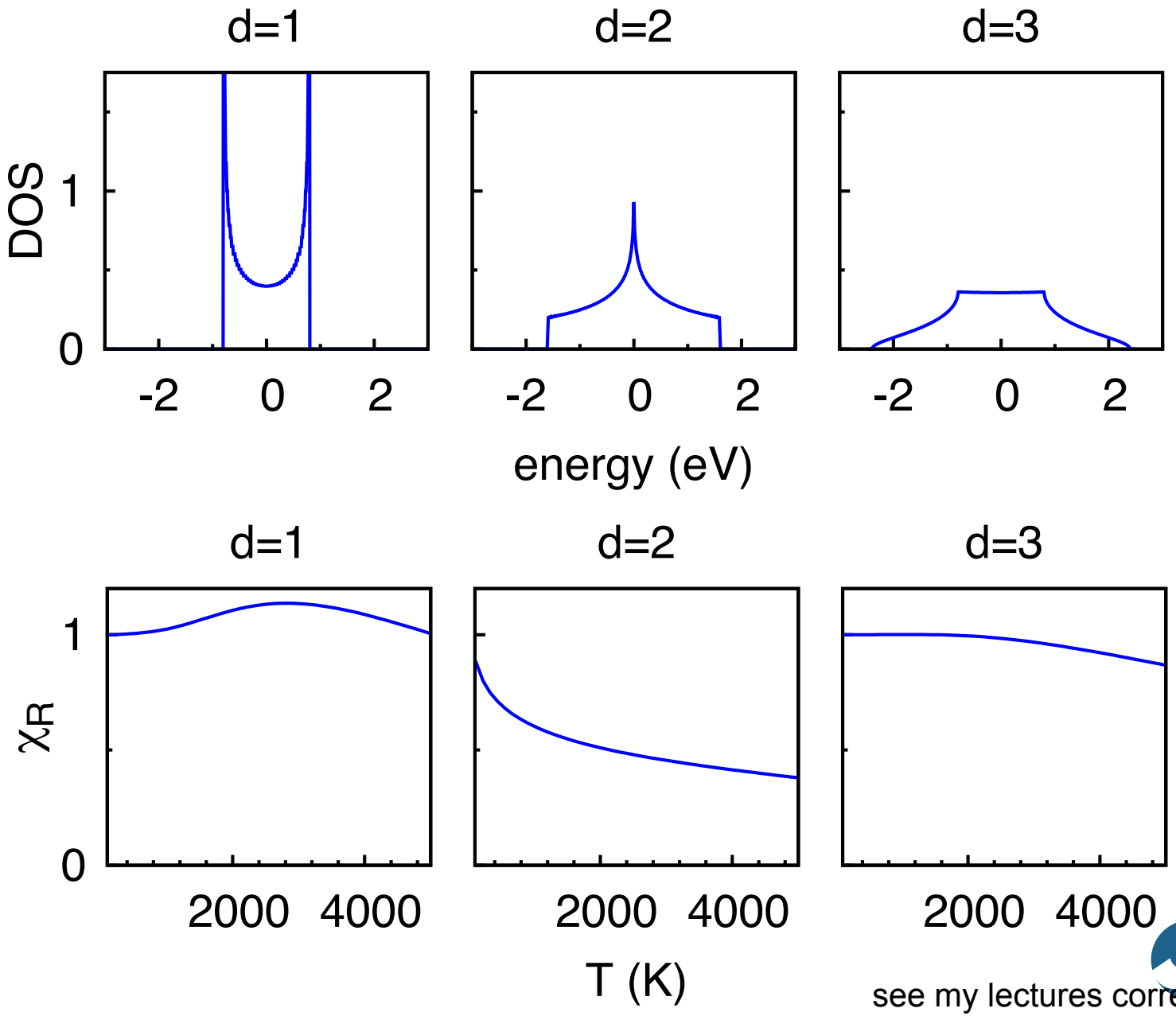
proportional to density of states (Pauli)



nesting vector

weakly T dependent (except close to van-Hove singularities/divergencies)

q=0 finite temperature



see my lectures correl12 and correl15

Hubbard model, atomic limit

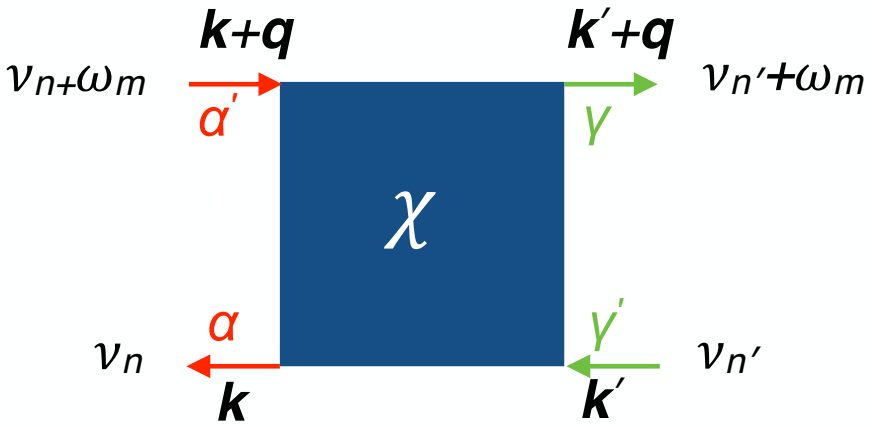
$$\chi_{zz}(\mathbf{0};0) = (g\mu_B S)^2 \frac{1}{k_B T} = \frac{C_{1/2}}{T}$$

$$C_{1/2} = \frac{(g\mu_B)^2 S(S+1)}{3k_B}$$

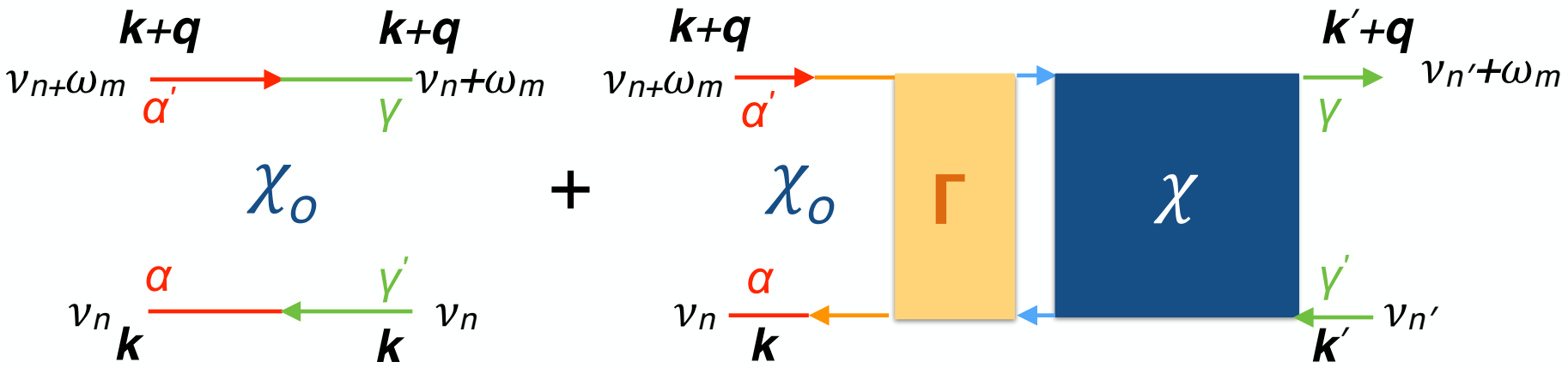
Curie susceptibility

e.pavarini@fz-juelich.de

Bethe-Salpeter equation



=

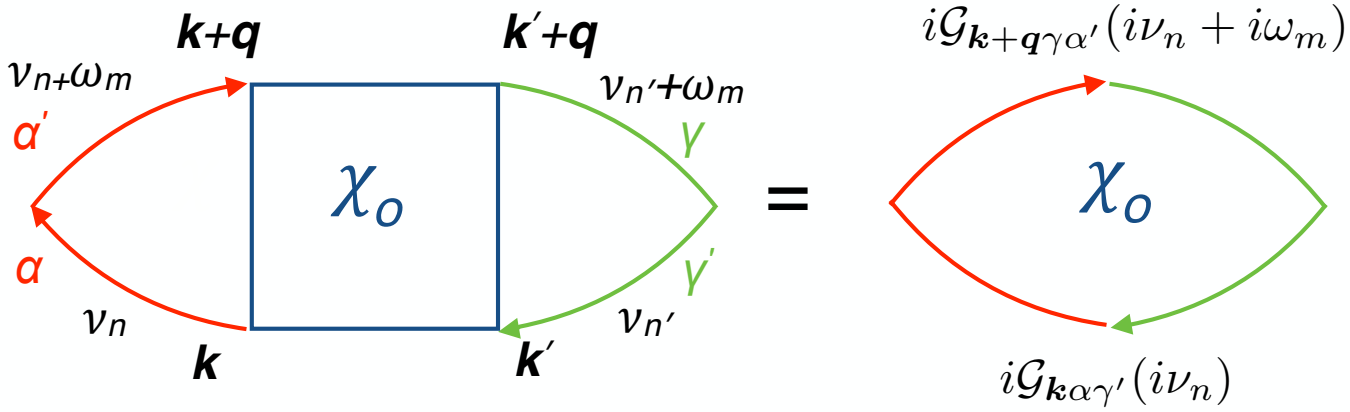


e.pavarini@fz-juelich.de

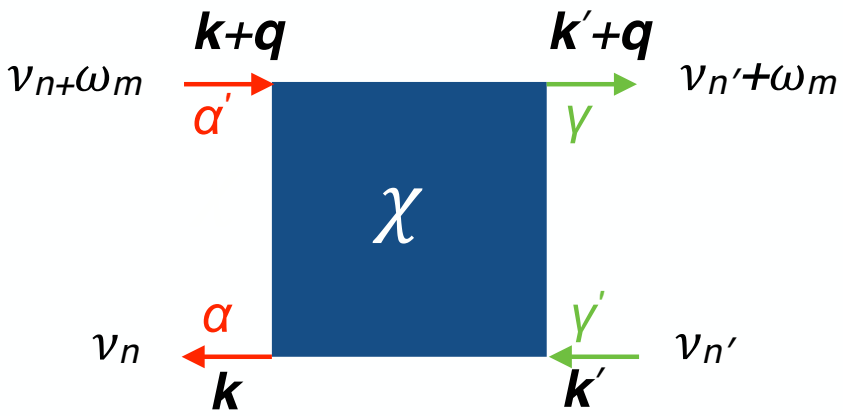
susceptibility in DMFT

1. perturbation around DMFT solution

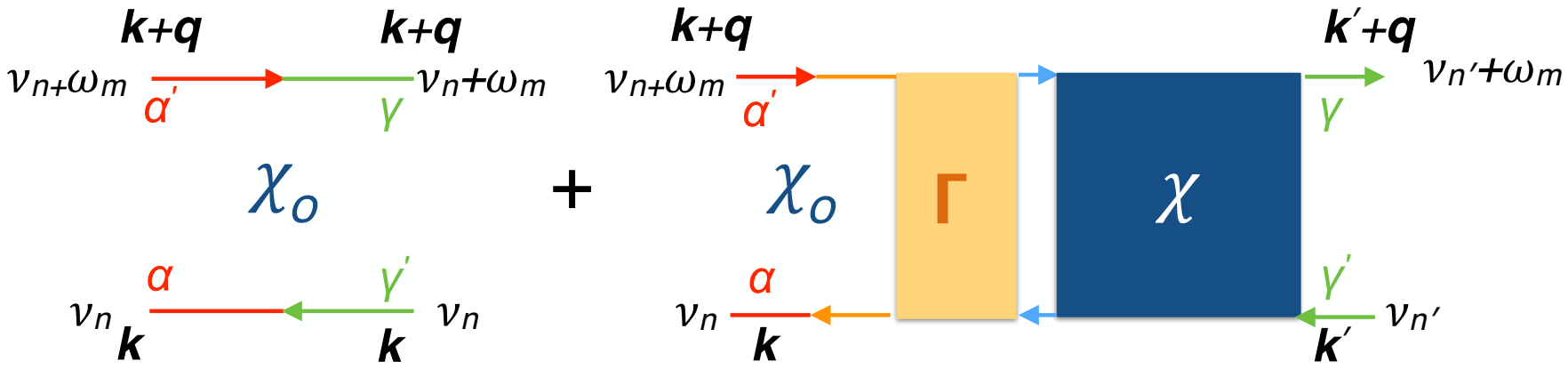
$$[\chi_0(\boldsymbol{q}; i\omega_m)]_{L_\alpha, L_\gamma} = -\beta\delta_{nn'} \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} G^{\mathrm{DMFT}}_{\alpha\gamma'}(\boldsymbol{k}; i\nu_n) G^{\mathrm{DMFT}}_{\alpha'\gamma}(\boldsymbol{k}+\boldsymbol{q}; i\nu_n + i\omega_m)$$



what about the vertex?



=



e.pavarini@fz-juelich.de

local-vertex approximation

vertex in BS equation local in infinite dimensions

$$[\chi(\boldsymbol{q}; i\omega_m)]_{L_\alpha, L_\gamma} = [\chi_0(\boldsymbol{q}; \omega_m) + \chi_0(\boldsymbol{q}; i\omega_m) \Gamma(i\omega_m) \chi(\boldsymbol{q}; i\omega_m)]_{L_\alpha, L_\gamma}$$

define local susceptibilities

$$[\chi_0(i\omega_m)]_{L_\alpha^{ic}, L_\gamma^{ic}} = \frac{1}{N_{\boldsymbol{q}}} \sum_{\boldsymbol{q}} [\chi_0(\boldsymbol{q}; i\omega_m)]_{L_\alpha^{ic}, L_\gamma^{ic}} ,$$

$$[\chi(i\omega_m)]_{L_\alpha^{ic}, L_\gamma^{ic}} = \frac{1}{N_{\boldsymbol{q}}} \sum_{\boldsymbol{q}} [\chi(\boldsymbol{q}; i\omega_m)]_{L_\alpha^{ic}, L_\gamma^{ic}}$$

e.pavarini@fz-juelich.de

local-vertex approximation

2. solve local BS equation

$$[\Gamma(i\omega_m)]_{L_\alpha,L_\gamma} = [\chi_0^{-1}(i\omega_m)]_{L_\alpha,L_\gamma} - [\chi^{-1}(i\omega_m)]_{L_\alpha,L_\gamma}$$

local susceptibility: from quantum impurity solver

3. solve ***q***-dependent BS equation

$$[\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma} = [\chi_0(\boldsymbol{q};\omega_m) + \chi_0(\boldsymbol{q};i\omega_m)\Gamma(i\omega_m)\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma}$$

q-dependence here from non-interacting part

e.pavarini@fz-juelich.de

Hubbard Model in Infinite Dimensions: A Quantum Monte Carlo Study

M. Jarrell

Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221

(Received 5 December 1991)

An essentially exact solution of the infinite-dimensional Hubbard model is made possible by a new self-consistent Monte Carlo procedure. Near half filling antiferromagnetism and a pseudogap in the single-particle density of states are found for sufficiently large values of the intrasite Coulomb interaction. At half filling the antiferromagnetic transition temperature obtains its largest value when the intrasite Coulomb interaction $U \approx 3$.

PACS numbers: 75.10.Jm, 71.10.+x, 75.10.Lp, 75.30.Kz

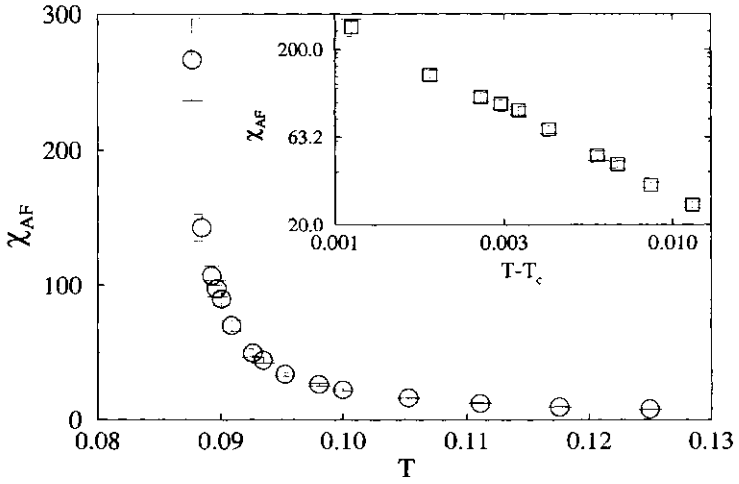


FIG. 3. Antiferromagnetic susceptibility $\chi_{AF}(T)$ vs temperature T when $U=1.5$ and $\epsilon=0.0$. The logarithmic scaling behavior is shown in the inset. The data close to the transition fit the form $\chi_{AF} \propto |T-T_c|^{\nu}$ with $T_c=0.0866 \pm 0.0003$ and $\nu=-0.99 \pm 0.05$. The points at $U=0$ reflect exactly known limits.

DMFT for 1- and 2- particle GFs

Green Function

k-dependent Dyson equation matrix

$$G(\boldsymbol{k}; i\nu_n) = G_0(\boldsymbol{k}; i\nu_n) + G_0(\boldsymbol{k}; i\nu_n)\Sigma(\boldsymbol{k}; i\nu_n)G(\boldsymbol{k}; i\nu_n)$$

local self-energy approximation

$$\Sigma(\boldsymbol{k}; i\nu_n) \to \Sigma(i\nu_n)$$

local Dyson equation

$$G(i\nu_n) = G_0(i\nu_n) + G_0(i\nu_n)\Sigma(i\nu_n)G(i\nu_n)$$

Susceptibility

q-dependent Bethe-Salpeter equation matrix

$$\chi(\boldsymbol{q}; i\omega_m) = \chi_0(\boldsymbol{q}; i\omega_m) + \chi_0(\boldsymbol{q}; i\omega_m)\Gamma(\boldsymbol{q}; i\omega_m)\chi(\boldsymbol{q}; i\omega_m)$$

local vertex approximation

$$\Gamma(\boldsymbol{q}; i\omega_m) \to \Gamma(i\omega_m)$$

local Bethe-Salpeter equation

$$\chi(i\omega_m) = \chi_0(i\omega_m) + \chi_0(i\omega_m)\Gamma(i\omega_m)\chi(i\omega_m)$$

Example: Mott insulators in small t/U limit

in the *t=0* limit

$$G(i\nu_n) = \frac{1}{i\nu_n + \mu - \Sigma(i\nu_n)} \qquad \Sigma(i\nu_n) = \mu + \frac{U^2}{4}\frac{1}{i\nu_n}$$

small *t/U* limit: approximate form for the self-energy

$$\Sigma(i\nu_n) = \mu + \frac{r_U U^2}{4}\frac{1}{i\nu_n}$$

e.pavarini@fz-juelich.de

Mott insulators: small t/U limit

bubble term

$$\chi_0(\boldsymbol{q};0) \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U}U}\left[1 - \frac{1}{2}\frac{J_{\mathbf{0}}}{\sqrt{r_U}U} - \frac{1}{4}\frac{J_{\boldsymbol{q}}}{\sqrt{r_U}U}\right]$$

$$J_{\boldsymbol{q}} = 2J[\cos q_x + \cos q_y], \quad J \propto t^2/U$$

local magnetic susceptibility

$$\chi_{zz}(\boldsymbol{q};0) = (g\mu_B)^2 \frac{1}{4k_BT}\frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

e.pavarini@fz-juelich.de

Bethe-Salpeter equation

$$\Gamma \sim \frac{1}{\chi^0_{zz}(0)} - \frac{1}{\chi_{zz}(0)} \sim \frac{1}{(g\mu_B)^2}\left[4\sqrt{r_U}U\left(1+\frac{1}{2}\frac{J_{\mathbf{0}}}{\sqrt{r_U}U}\right) - 4k_BT\right]$$

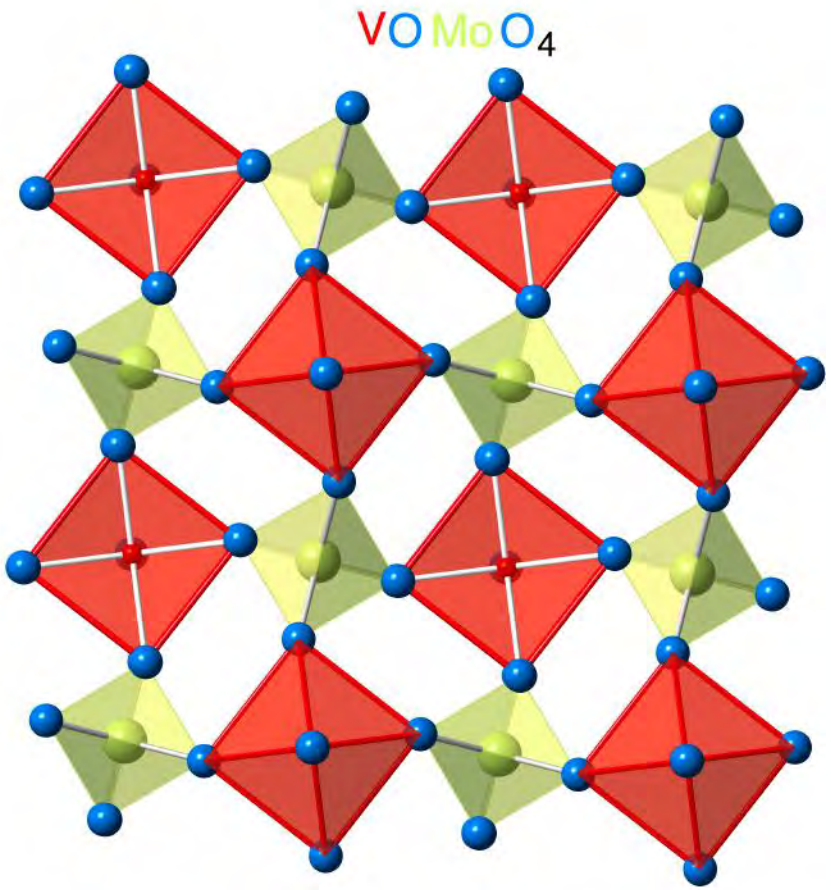
local vertex

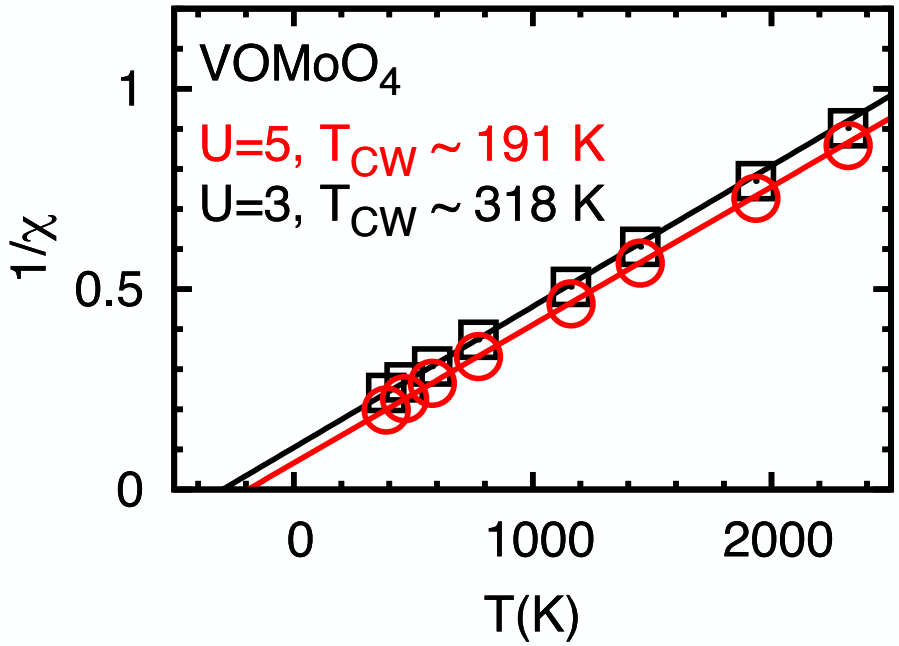
$$\chi_{zz}(\boldsymbol{q};0) = \frac{1}{[\chi^0_{zz}(\boldsymbol{q};0)]^{-1} - \Gamma} \sim (g\mu_B)^2 \frac{1}{4}\frac{1}{k_BT + J_{\boldsymbol{q}}/4} = \frac{(g\mu_B)^2}{k_B}\frac{1}{4}\frac{1}{T - T_{\boldsymbol{q}}}$$

Curie-Weiss behavior

e.pavarini@fz-juelich.de

$VOMoO_4$

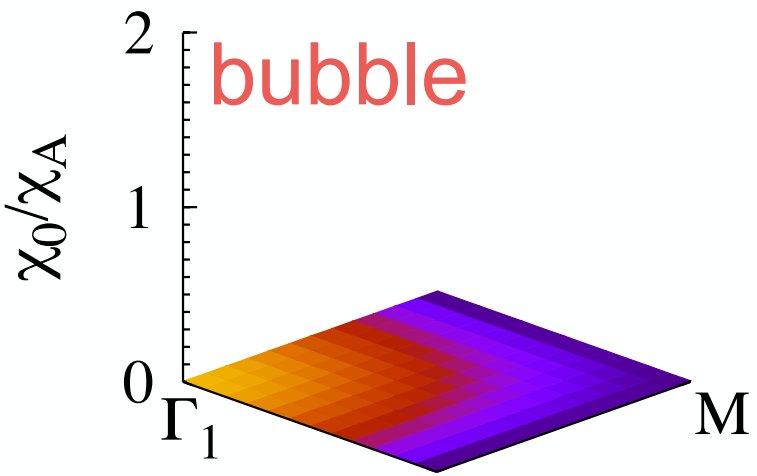


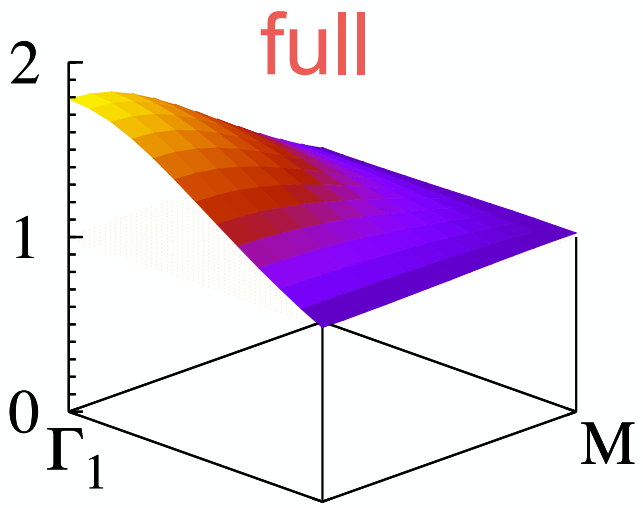


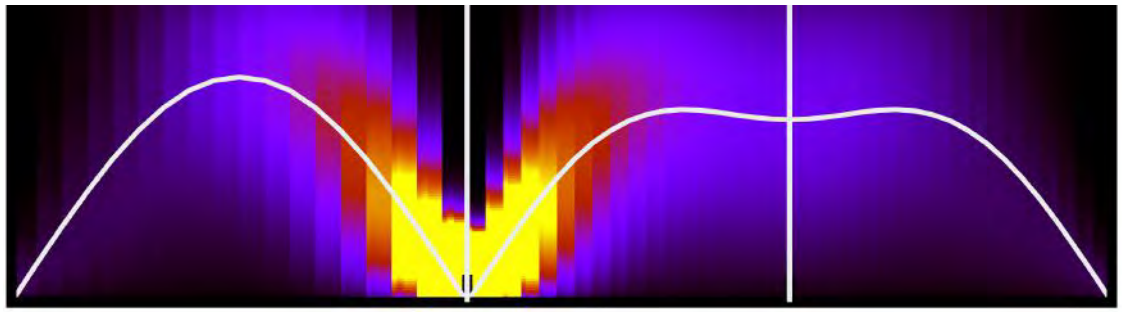
e.pavarini@fz-juelich.de

A. Kiani and E. Pavarini, Phys. Rev. B **94**, 075112 (2016)

static and dynamical response







e.pavarini@fz-juelich.de

A. Kiani and E. Pavarini, Phys. Rev. B **94**, 075112 (2016); J. Musshoff and E. Pavarini, to be published.

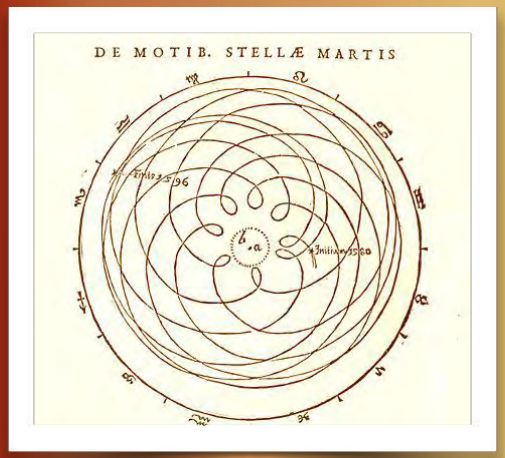
so what!

the one-band Hubbard model
is not enough for understanding materials

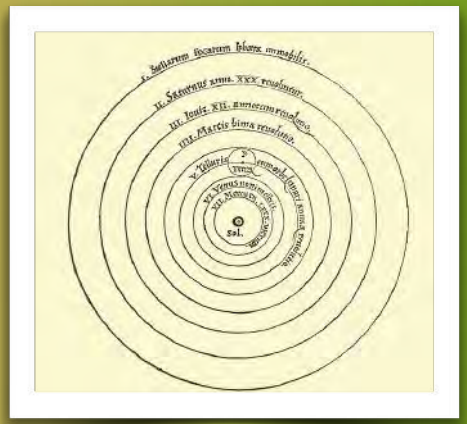
e.pavarini@fz-juelich.de

from models to materials

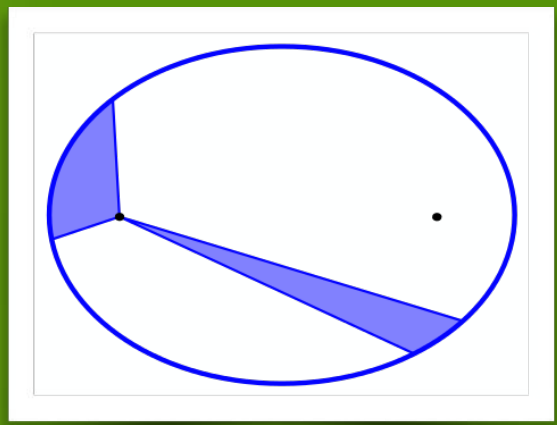
geocentric model



heliocentric model (circles)



heliocentric model (Kepler)



photos from wikipedia

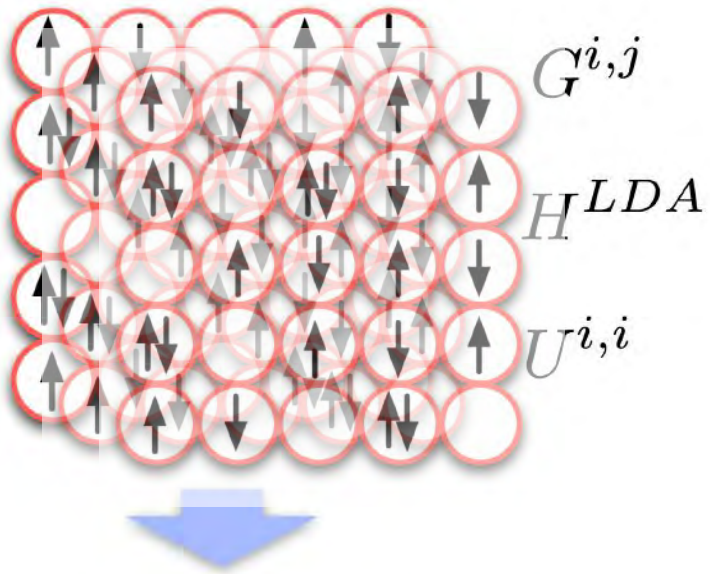
e.pavarini@fz-juelich.de

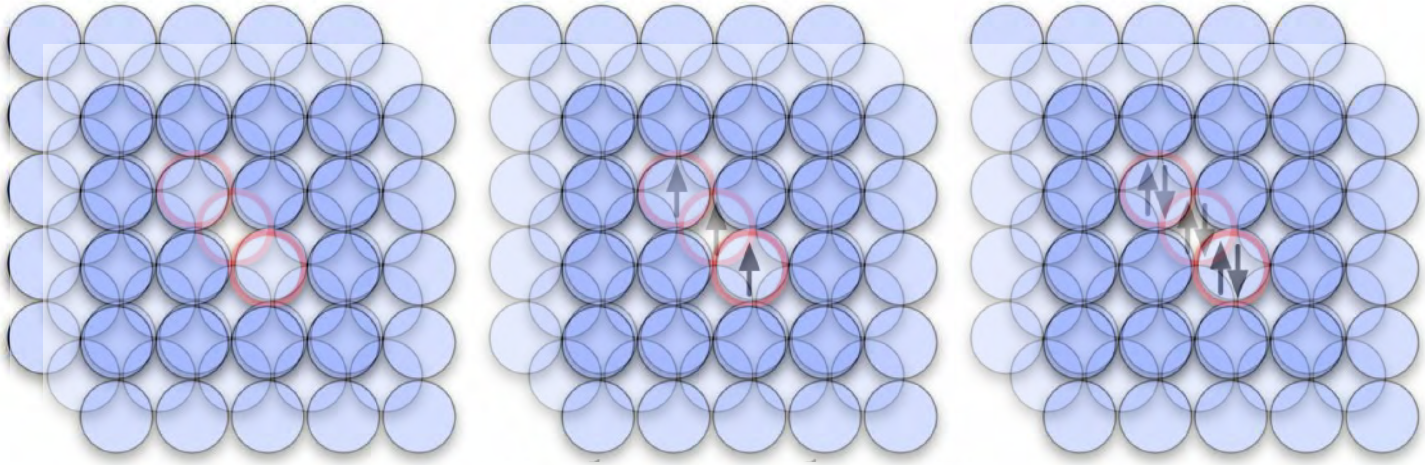
multi-band Hubbard model

e.pavarini@fz-juelich.de

DMFT for multi-band models

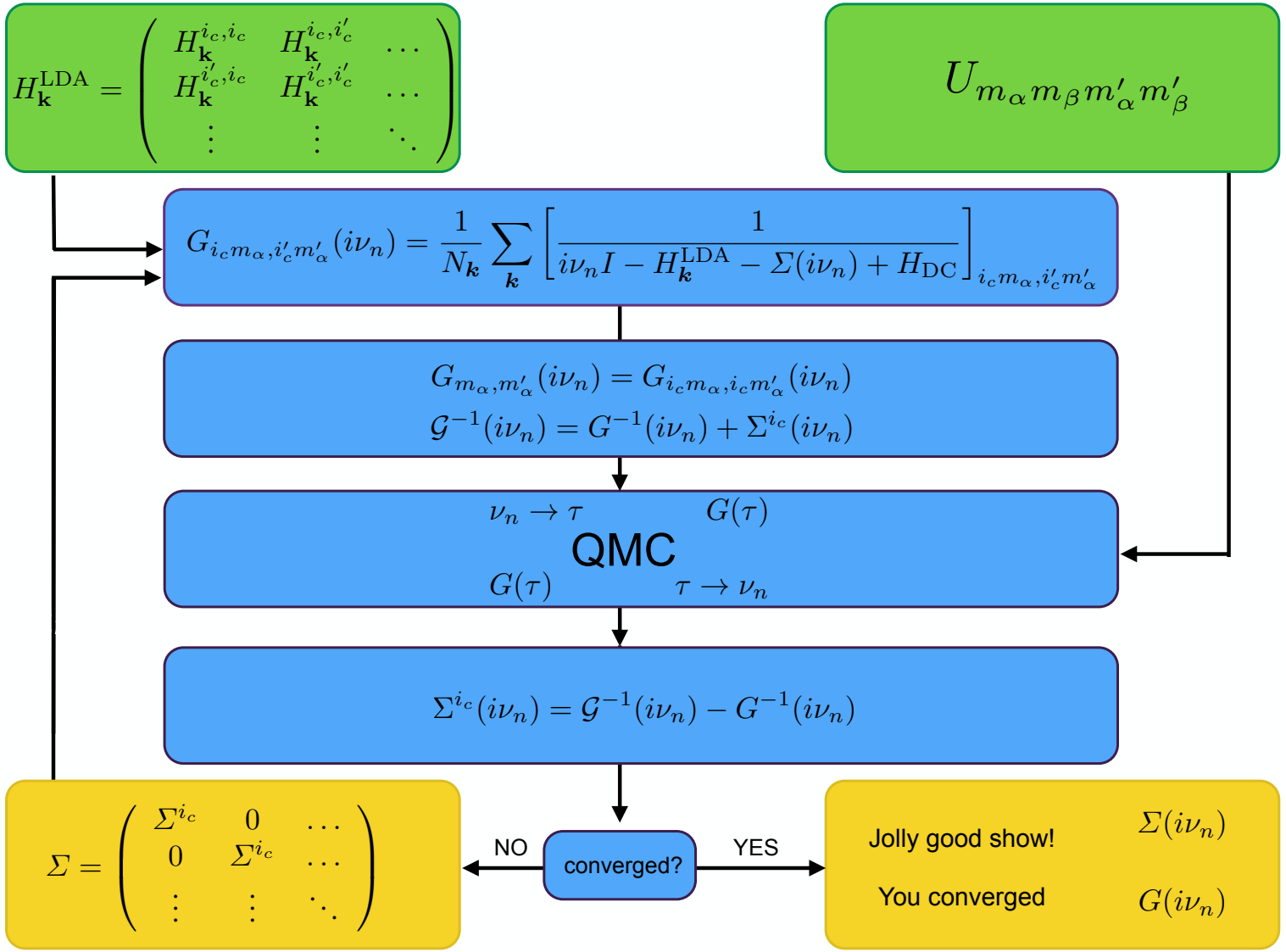
$$\hat{H}_e = -\sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}$$





e.pavarini@fz-juelich.de

in principle, only more indices



e.pavarini@fz-juelich.de

in practice, QMC-based solvers

computational time

limited number of orbitals/site

finite temperature

sign problem

some *interactions* are worse than others

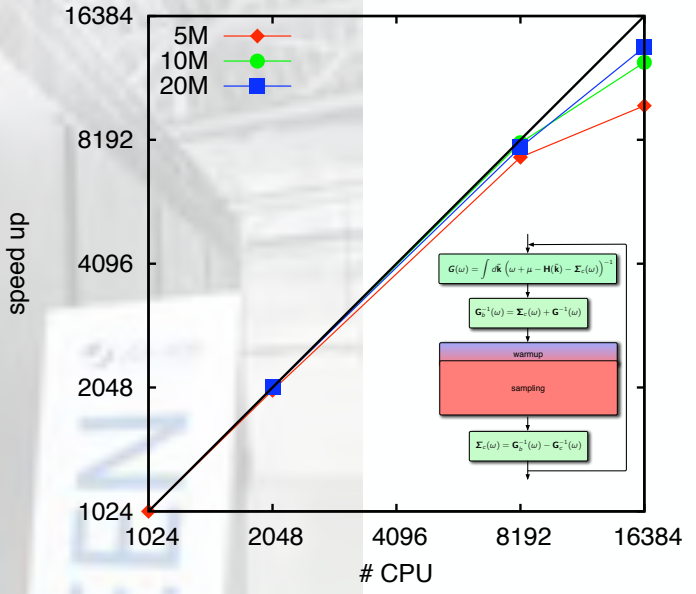
some *bases* are worse than others

e.pavarini@fz-juelich.de

flexible and efficient solvers

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

self-energy matrix in spin-orbital space

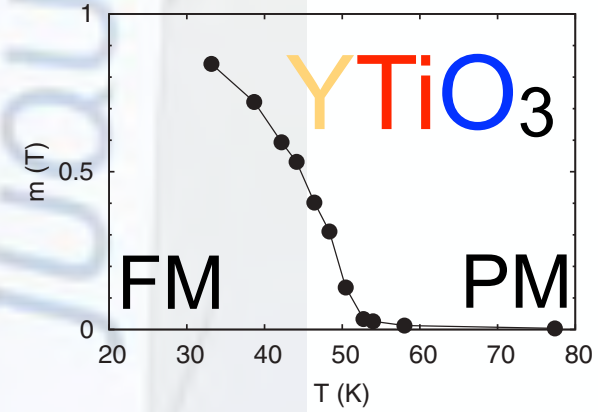


DMFT and cDMFT

generalized quantum impurity solvers:

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

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



sign problem: smart adapted basis choice

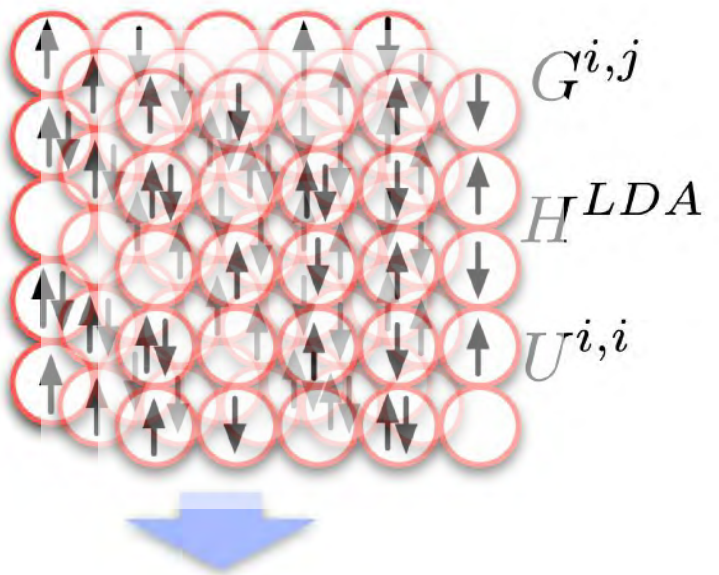
e.pavarini@fz-juelich.de

JÜLICH
FORSCHUNGSZENTRUM

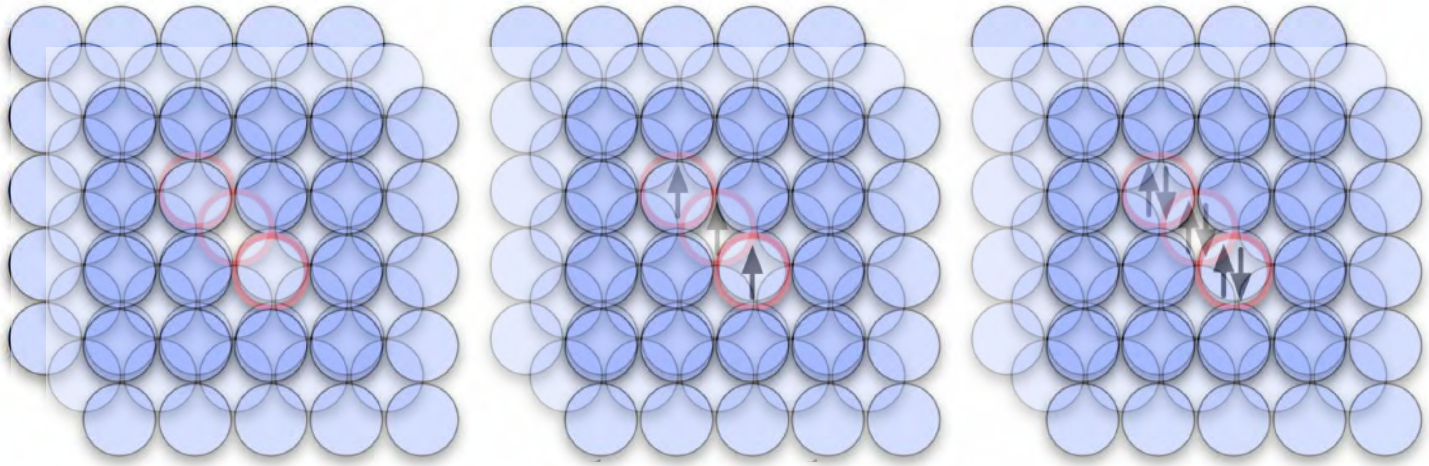
we need **minimal** material-specific models

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



e.pavarini@fz-juelich.de

let’s take a step backwards

e.pavarini@fz-juelich.de

the theory of almost everything

Born-Oppenheimer approximation, non-relativistic

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

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

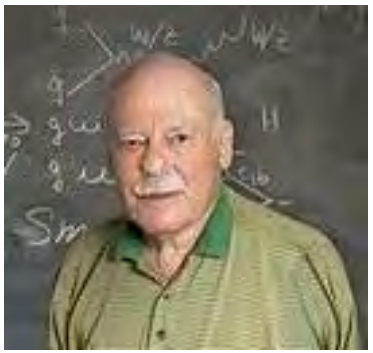
$$\hat{H}_e \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E_\alpha \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

linear combination of Slater determinants

bad news: the exact solution is not an option

e.pavarini@fz-juelich.de

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@fz-juelich.de

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

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

density-functional theory

1964

PHYSICAL REVIEW VOLUME 136, NUMBER 3B 9 NOVEMEBR 1964

Inhomogeneous Electron Gas*

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

This paper deals with the ground state of an inter… electron gas in an external potential $v(\mathbf{r})$. It is proved that there exists a universal functional of the … pression $E \equiv \int v(\mathbf{r})n(\mathbf{r})d\mathbf{r} + F[n(\mathbf{r})]$ has as its minimum … $v(\mathbf{r})$. 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

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)

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

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

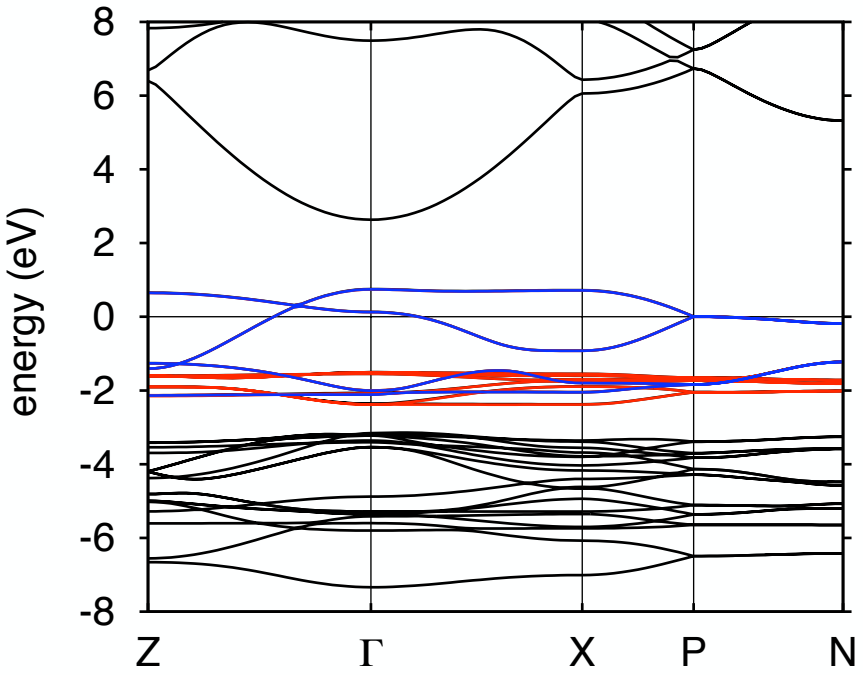
$$v_R(\boldsymbol{r}) = -\sum_\alpha \frac{Z_\alpha}{|\boldsymbol{r} - \boldsymbol{R}_\alpha|} + \int d\boldsymbol{r}' \frac{n(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} + \frac{\delta E_{\mathrm{xc}}[n]}{\delta n} = v_{en}(\boldsymbol{r}) + v_H(\boldsymbol{r}) + v_{xc}(\boldsymbol{r})$$

(in practice: LDA,GGA,…)

e.pavarini@fz-juelich.de

unexpected successes of DFT

Kohn-Sham eigenvalues as elementary excitations!



band structures, material trends, prediction

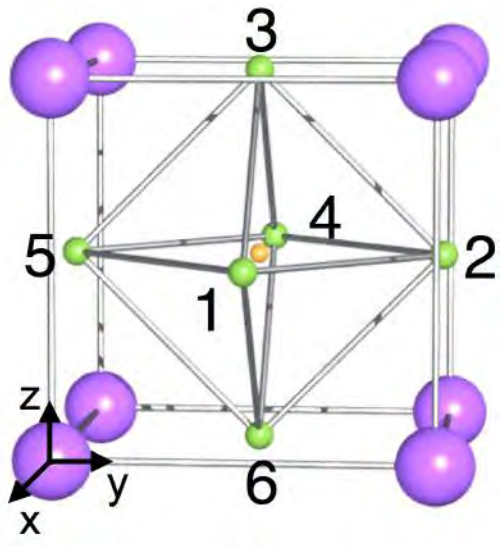
e.pavarini@fz-juelich.de

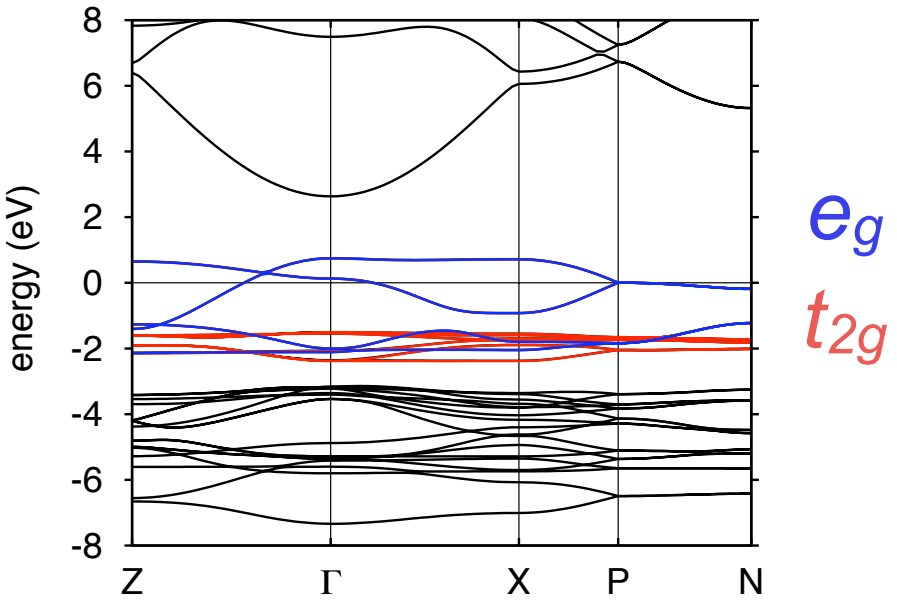
but *very deep problems* remain

$KCuF_3$

one-electron picture: it is a metal!

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





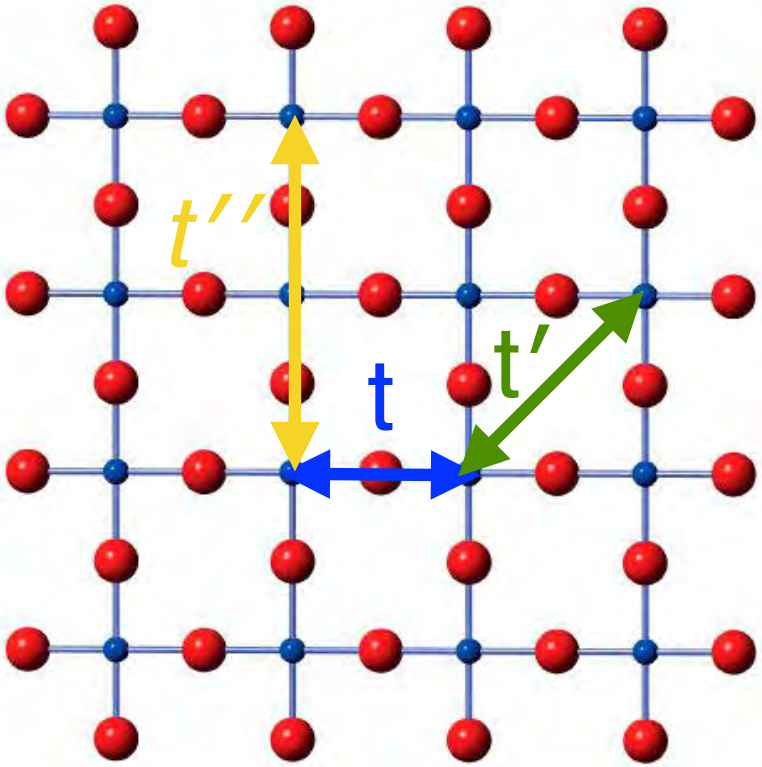
e.pavarini@fz-juelich.de

origin of failures: one-electron picture

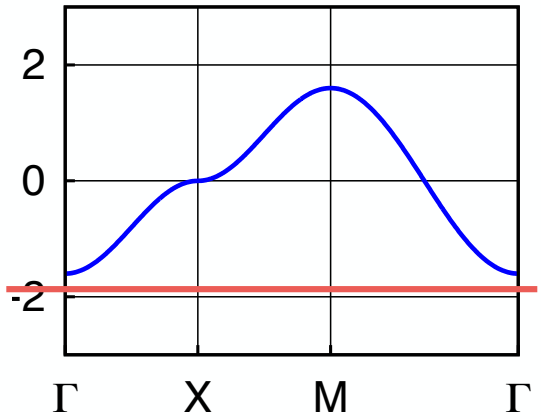
E. Pavarini, E. Koch, A.I. Lichtenstein, Phys. Rev. Lett. **101**, 266405 (2008)

electron counting argument

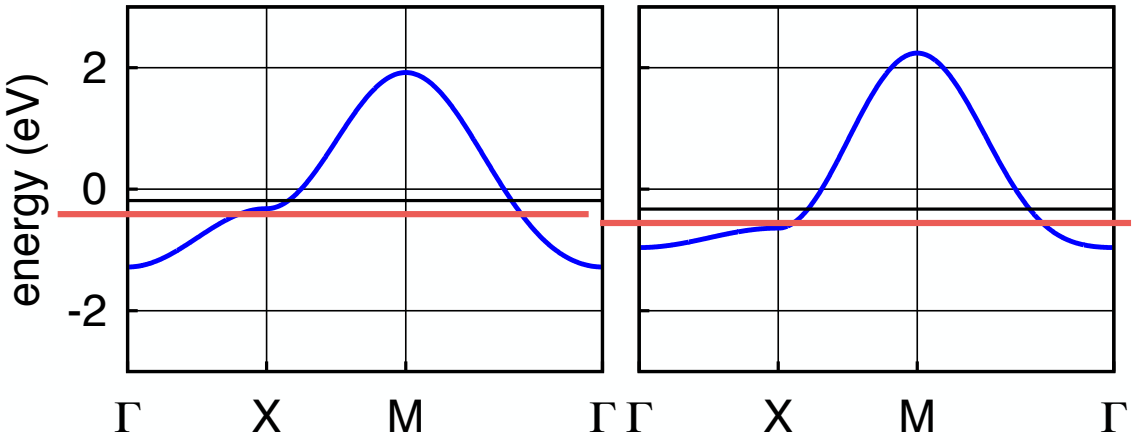
one electron per site



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



t′/t= =0.2 t′/t= =0.4



``*symmetry protected*''
metallic state

how can we exploit the successes of LDA

for strongly correlated materials ?

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

e.pavarini@fz-juelich.de

let us go back once more 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!

e.pavarini@fz-juelich.de

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

e.pavarini@fz-juelich.de

in *theory* all basis are identical

in *practice* some bases are better than others

e.pavarini@fz-juelich.de

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

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

e.pavarini@fz-juelich.de

what do the parameters contain?

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

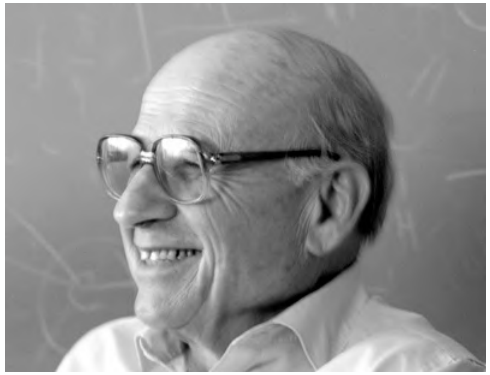
Hartree

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

potential

exchange-correlation

e.pavarini@fz-juelich.de



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

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

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

very good approach for weakly correlated systems

e.pavarini@fz-juelich.de

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

e.pavarini@fz-juelich.de

why LDA Wannier functions?

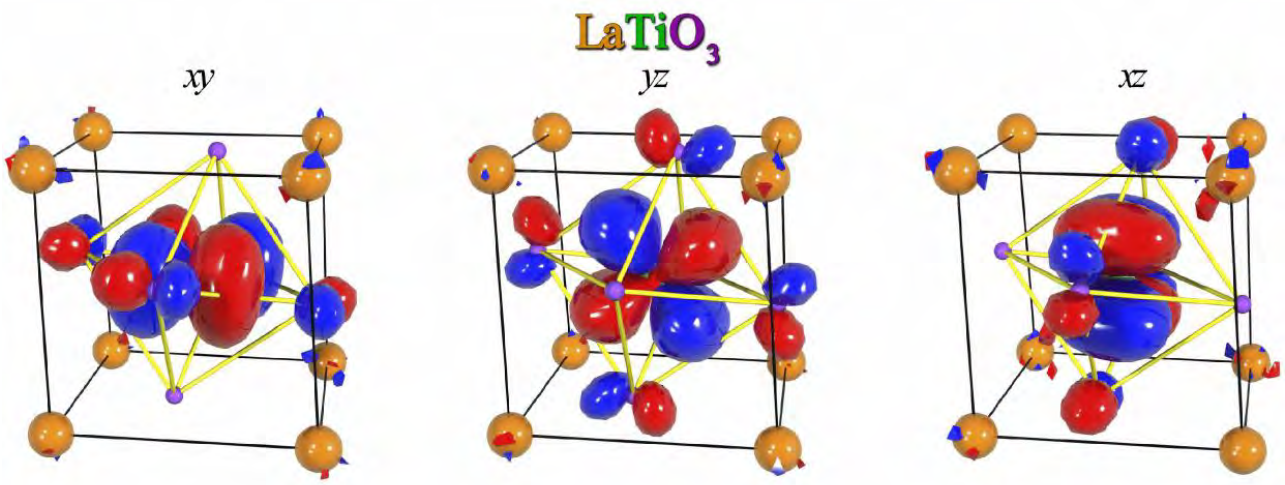
span exactly the one-electron Hamiltonian

can be constructed site-centered & orthogonal & localized

natural basis for **local** Coulomb terms

very good for weakly correlated systems

information on lattice and chemistry



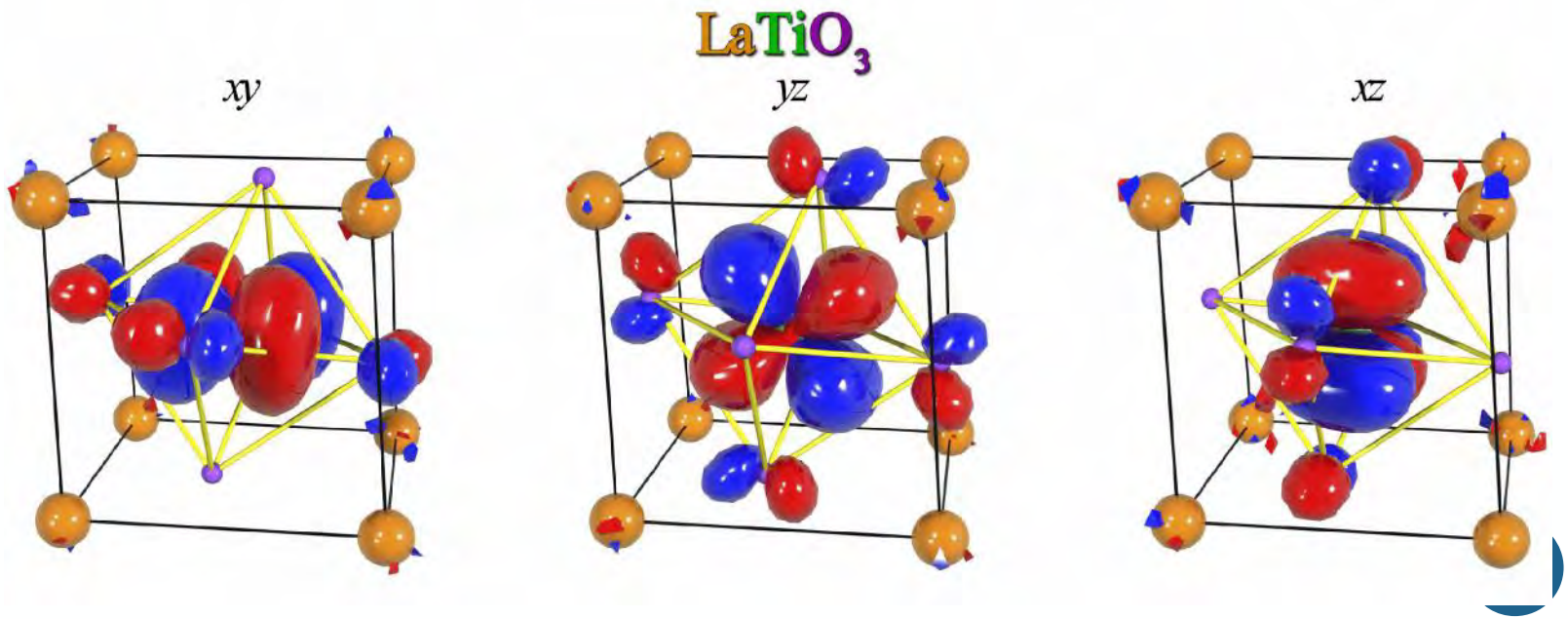
e.pavarini@fz-juelich.de

why LDA Wannier functions?

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

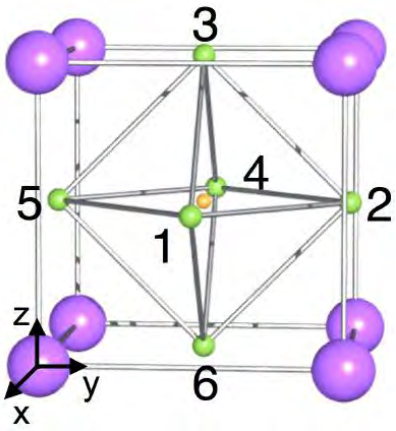
ΔU

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

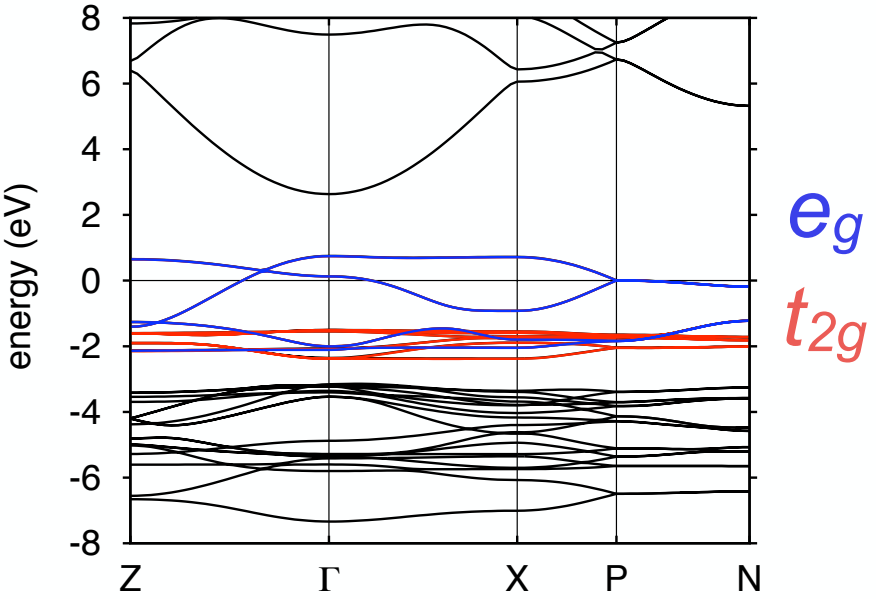


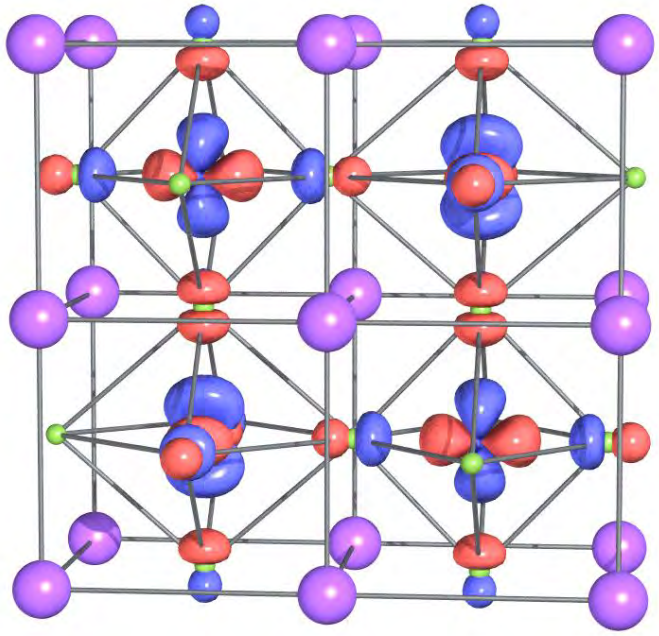
e.pavarini@fz-juelich.de

but *very deep problems* remain



$KCuF_3$

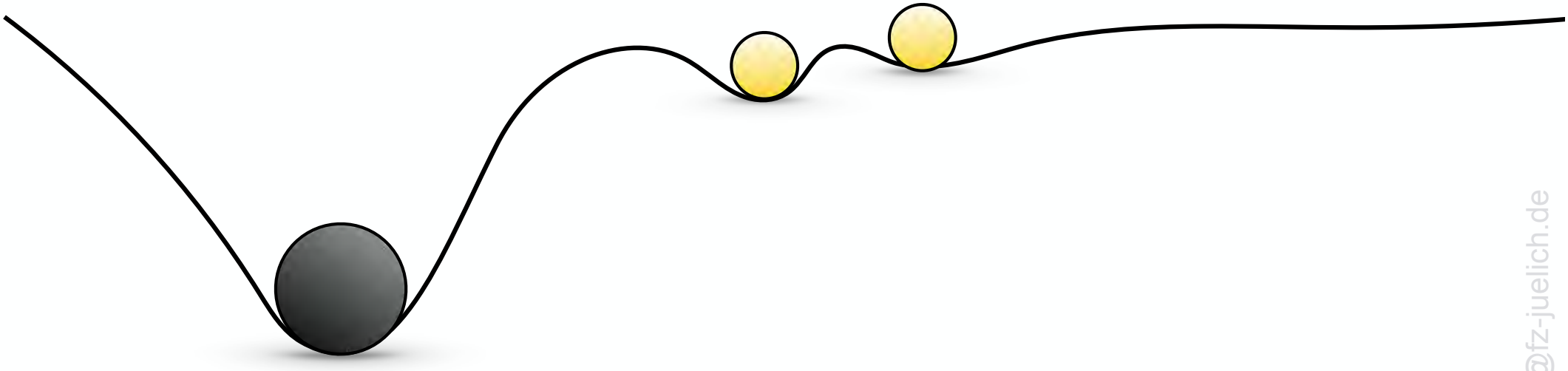




e.pavarini@fz-juelich.de

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

heavy electrons, light electrons

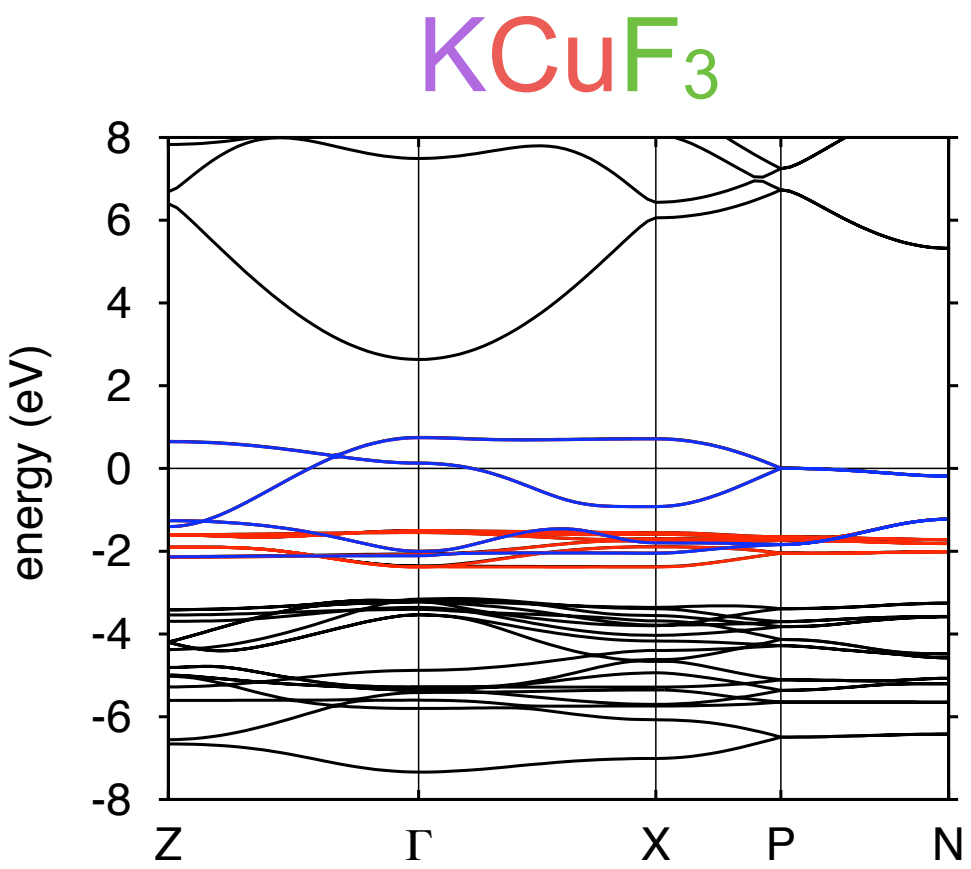


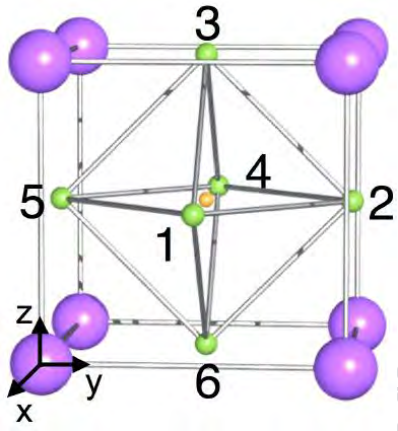
light electrons → LDA, GGA,…

heavy electrons → ΔU correction, DMFT

e.pavarini@fz-juelich.de

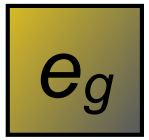
to downfold or not to downfold?





e.pavarini@fz-juelich.de

integrate out light electrons



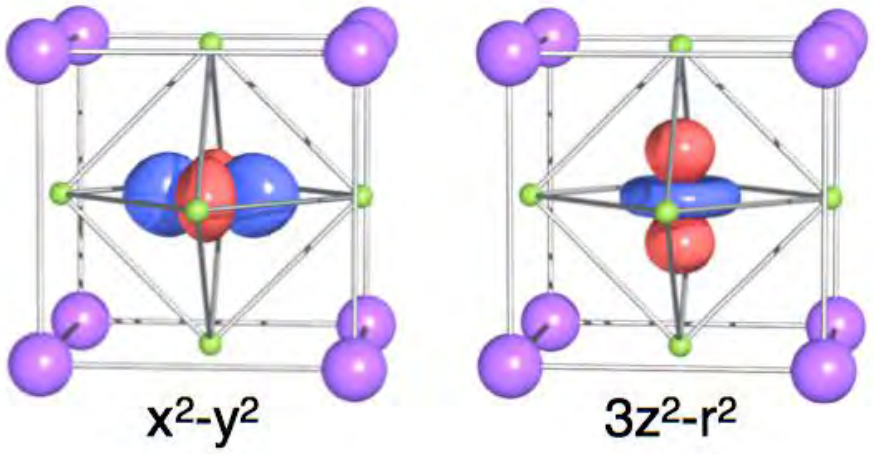
E. Pavarini, E. Koch, A.I. Lichtenstein, Phys. Rev. Lett. **101**, 266405 (2008)

should we downfold light electrons?

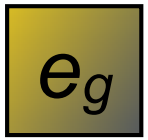
no downfolding

more parameters & H_{DC}

WF more localized

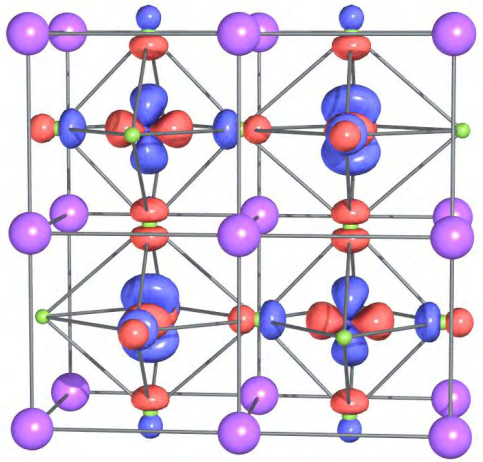


massive downfolding



fewer parameters & no H_{DC}

WF less localized

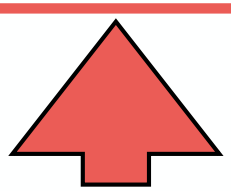


e.pavarini@fz-juelich.de

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

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

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

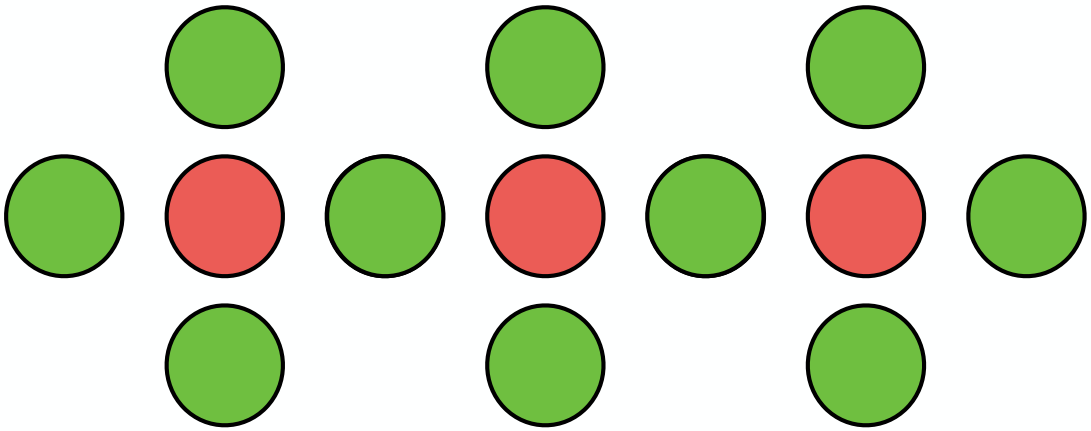
$$\psi_{im\sigma}(\boldsymbol{r})\overline{\psi_{i'm'\sigma'}}(\boldsymbol{r}) \sim \delta_{i,i'}\delta(\boldsymbol{r} - \boldsymbol{T}_i)$$

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

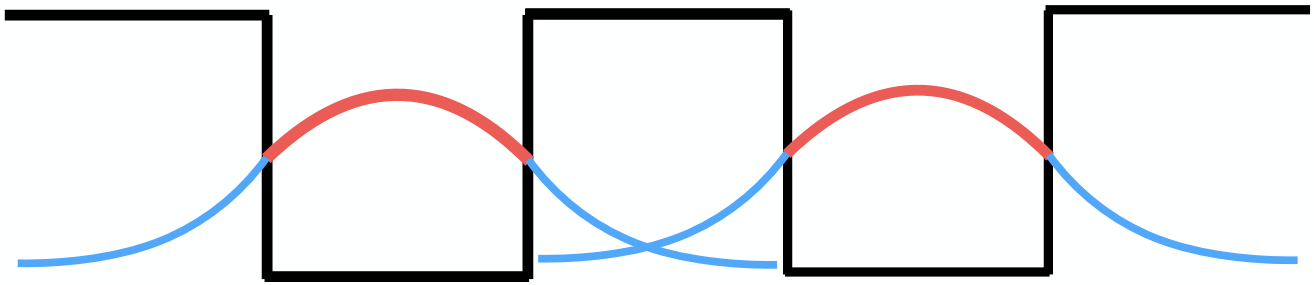
e.pavarini@fz-juelich.de

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?



e.pavarini@fz-juelich.de

screening effects

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

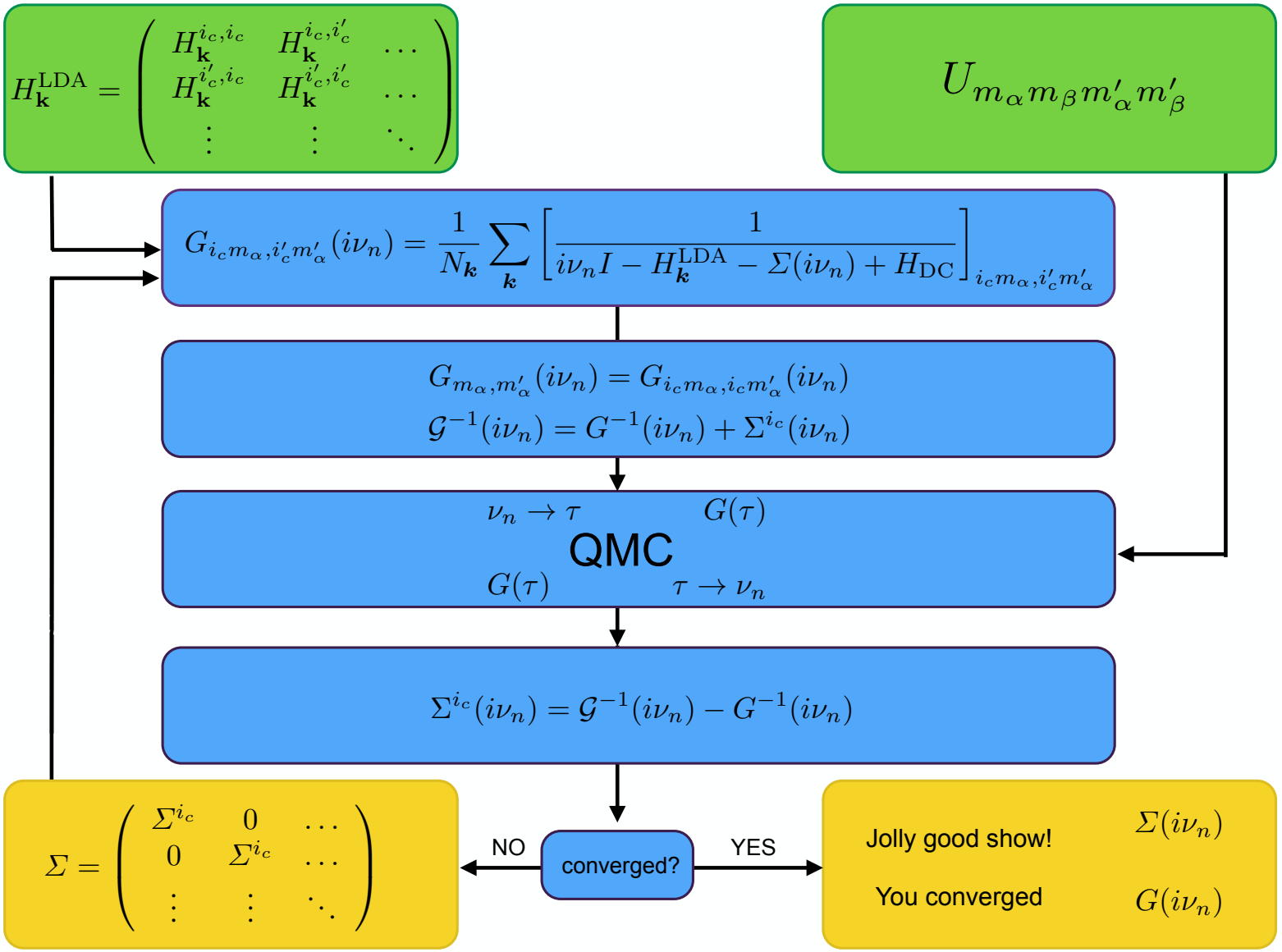
light electrons → DFT (LDA, GGA,…)

heavy electrons → *ΔU* correction, DMFT

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

e.pavarini@fz-juelich.de

LDA+DMFT



e.pavarini@fz-juelich.de

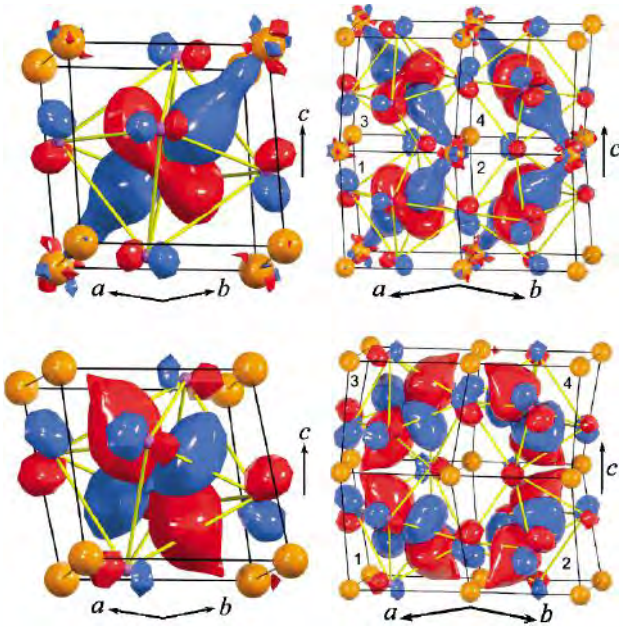
details matter!

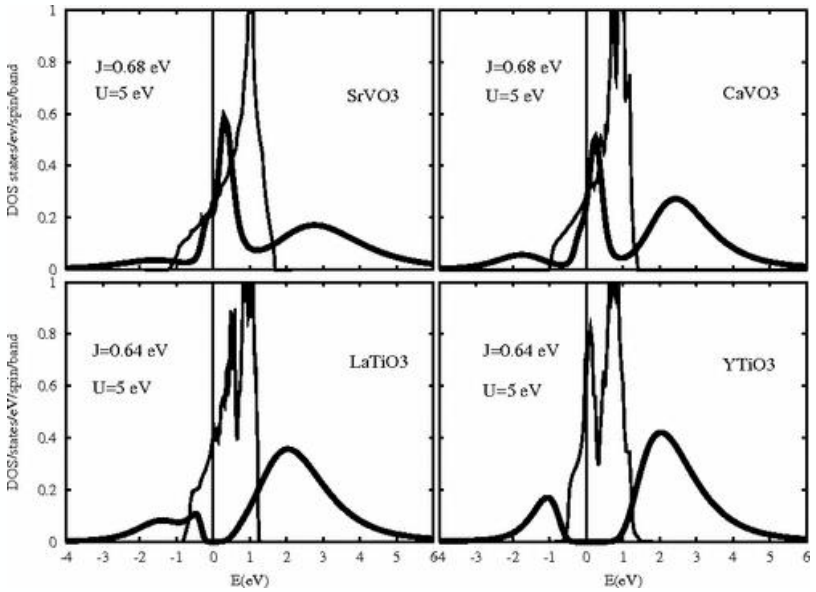
VOLUME 92, NUMBER 17 PHYSICAL REVIEW LETTERS week ending 30 APRIL 2004

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

t_{2g}^1

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





chemistry plays key role
non-cubic hoppings and crystal field Δ<<W

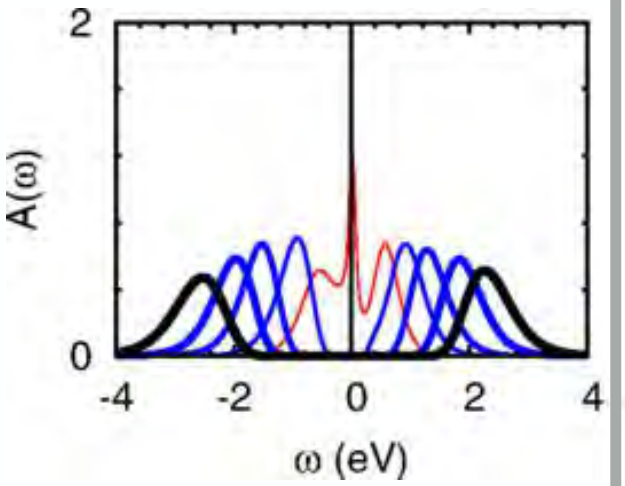
e.pavarini@fz-juelich.de

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

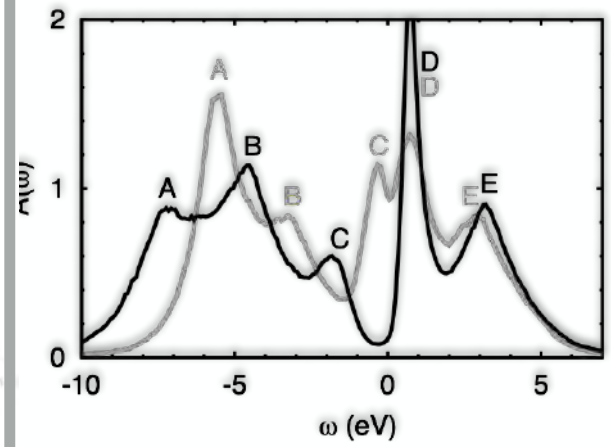
JÜLICH FORSCHUNGSZENTRUM

what can we do so far?

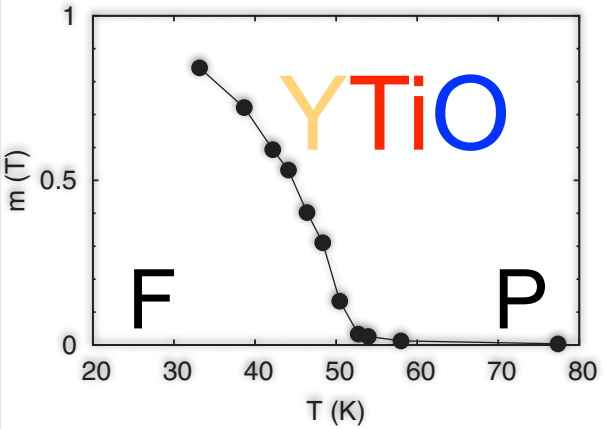
spectral functions



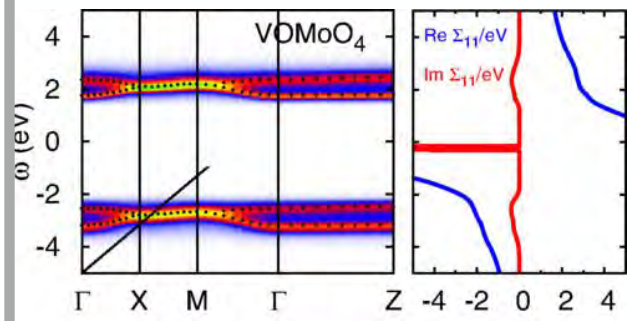
many orbitals



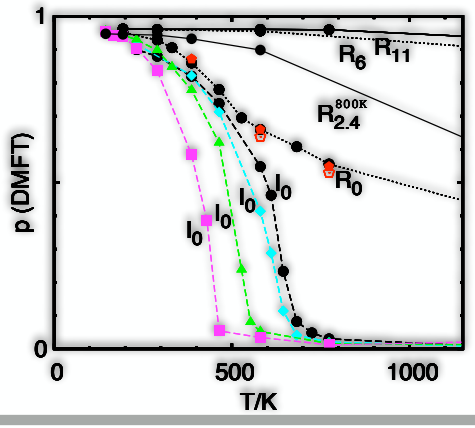
low T



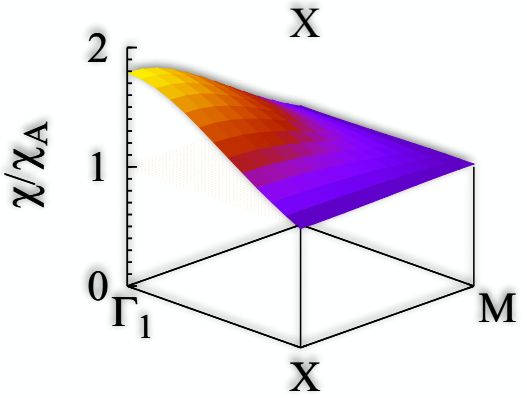
correlated bands



phase transitions



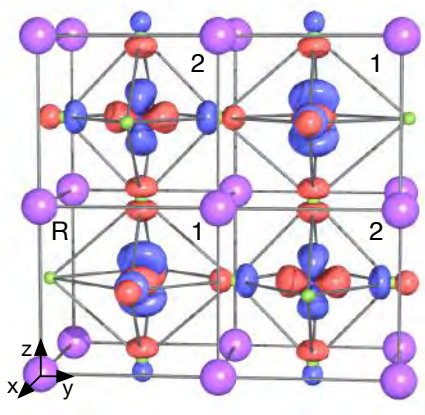
susceptibilities



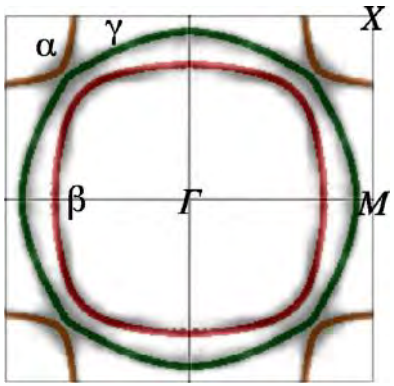
e.pavarini@fz-juelich.de

what can we do so far?

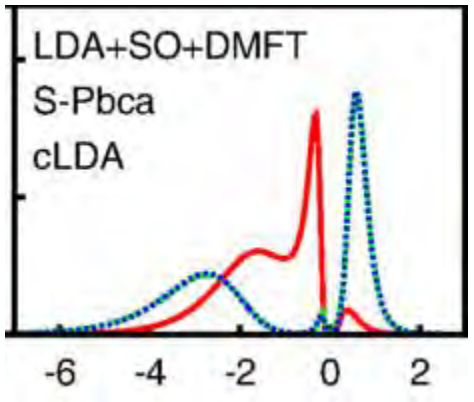
orbital order



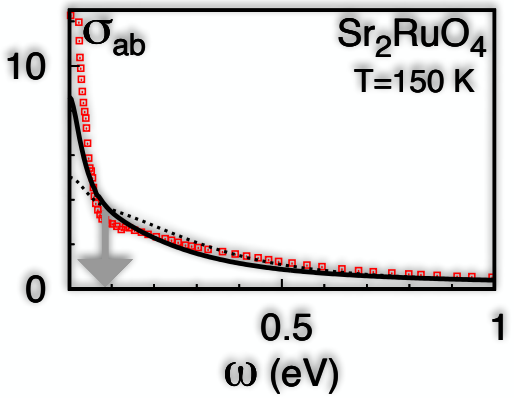
Fermi surface



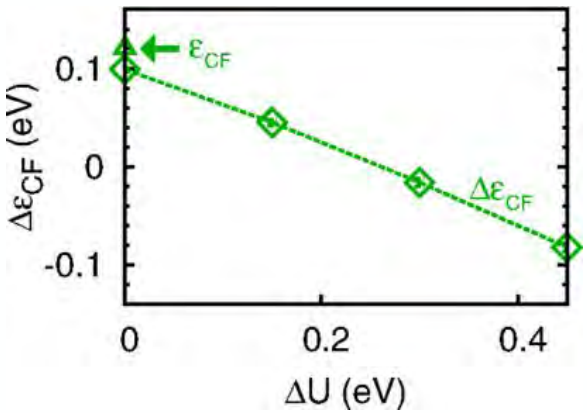
spin-orbit



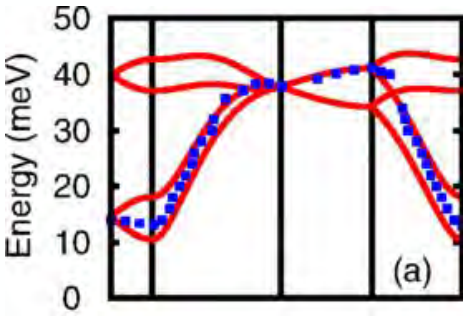
conductivity



realistic Coulomb



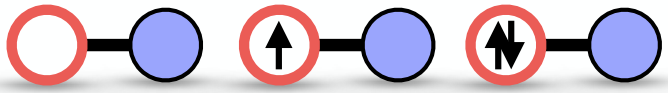
spin waves



e.pavarini@fz-juelich.de

DMFT

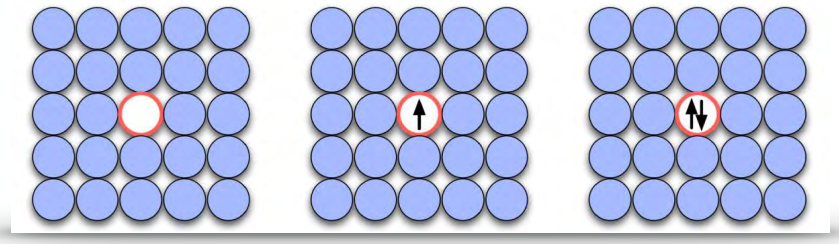
dimer



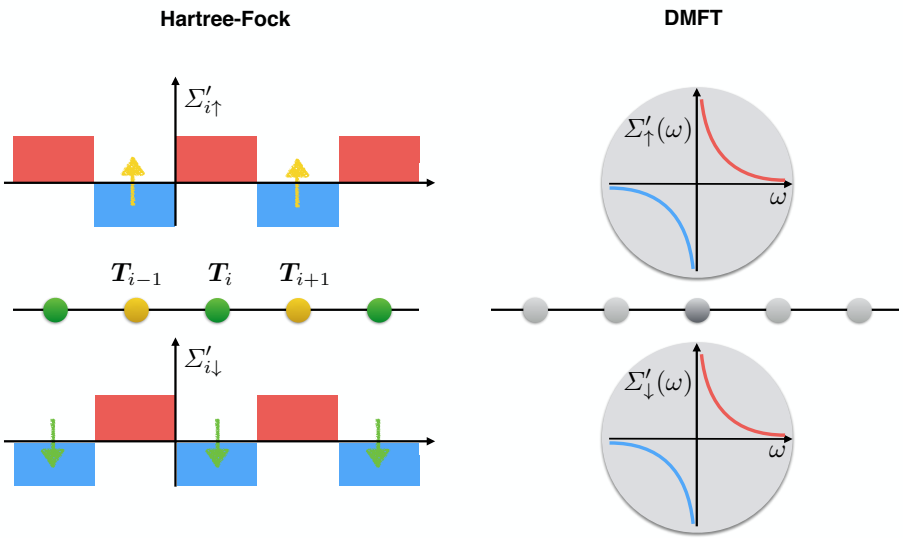
strong-correlations = large local U

U=V

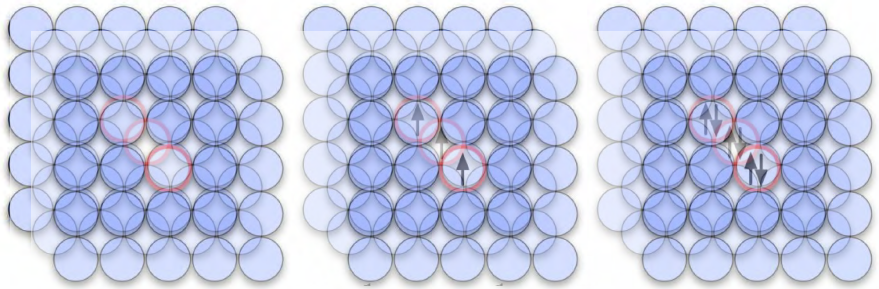
one band



DMFT vs HF



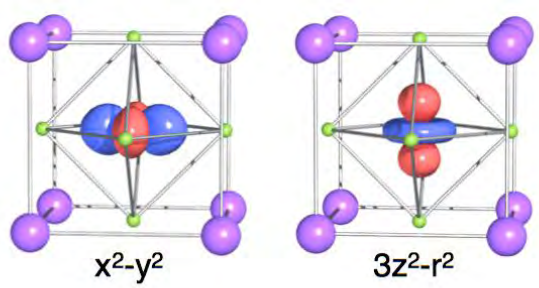
multiband



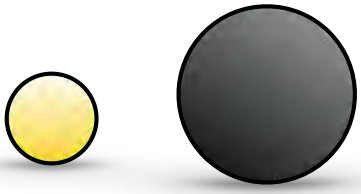
e.pavarini@fz-juelich.de

DMFT for materials

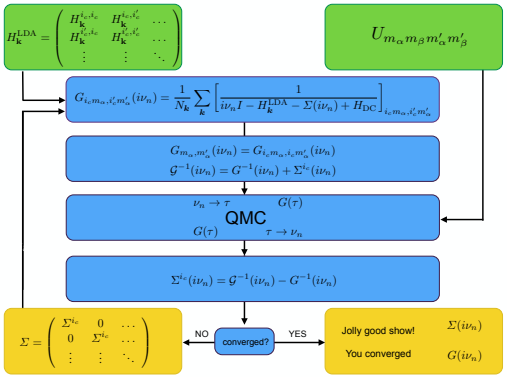
basis choice



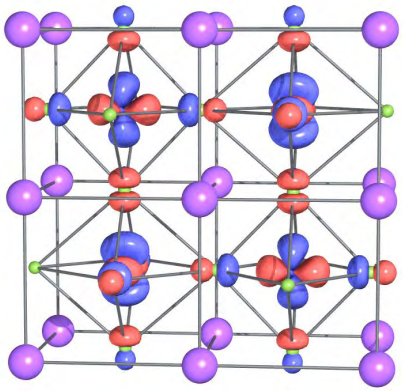
light & heavy electrons



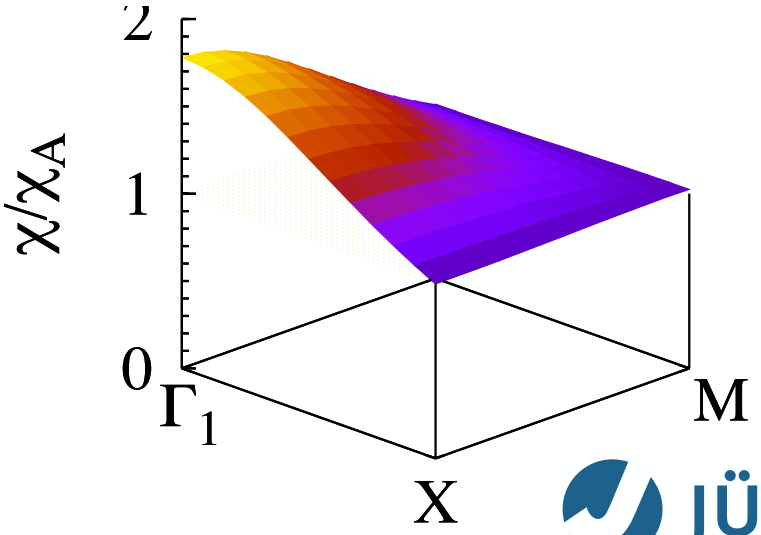
DMFT



downfolding, localization, double counting & screening



linear response functions



e.pavarini@fz-juelich.de

JÜLICH
FORSCHUNGSZENTRUM

thank you!

e.pavarini@fz-juelich.de