Mott transition: DFT+*U* vs DFT+DMFT

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emergent behavior

The effectiveness of this message may be indicated by the fact that I heard it quoted recently by a leader in the field of materials science, who urged the participants at a meeting dedicated to "fundamental problems in condensed matter physics" to accept that there were few or no such problems and that nothing was left but extensive science, which he seemed to equate with device engineering.

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

4 August 1972, Volume 177, Number 4047

Philp Warren Anderson

Nobel Prize in Physics 1977

SCIENCE

http://www.emergentuniverse.org/

scheme of lecture

- metal or insulator
  - one-electron picture
  - what is the gap?
- the Hubbard model
  - some exact limits
  - Mott transition: DMFT approach
    - Hubbard dimer
      - Hartree-Fock solution
      - self-consistent Anderson molecule ?
    - the Anderson model
  - Mott transition: Hartree-Fock vs DMFT
- DFT+DMFT & DFT+U

metal or insulator

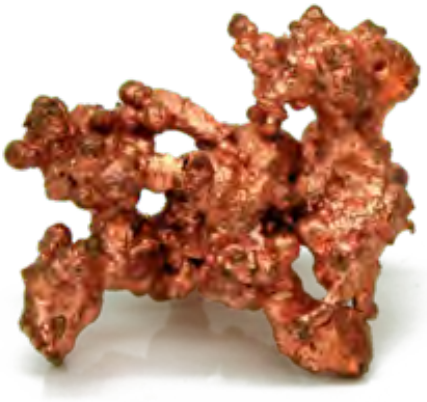
the independent electron picture

metal or insulator

some examples

diamond

silicon

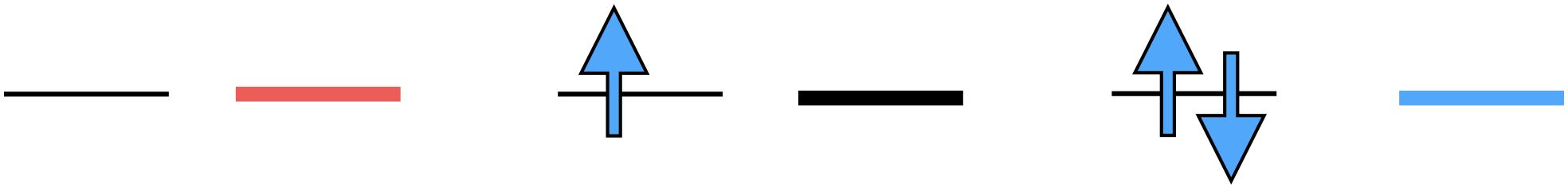


copper

photos from wikipedia

independent-electron picture

each level is filled with max two electrons

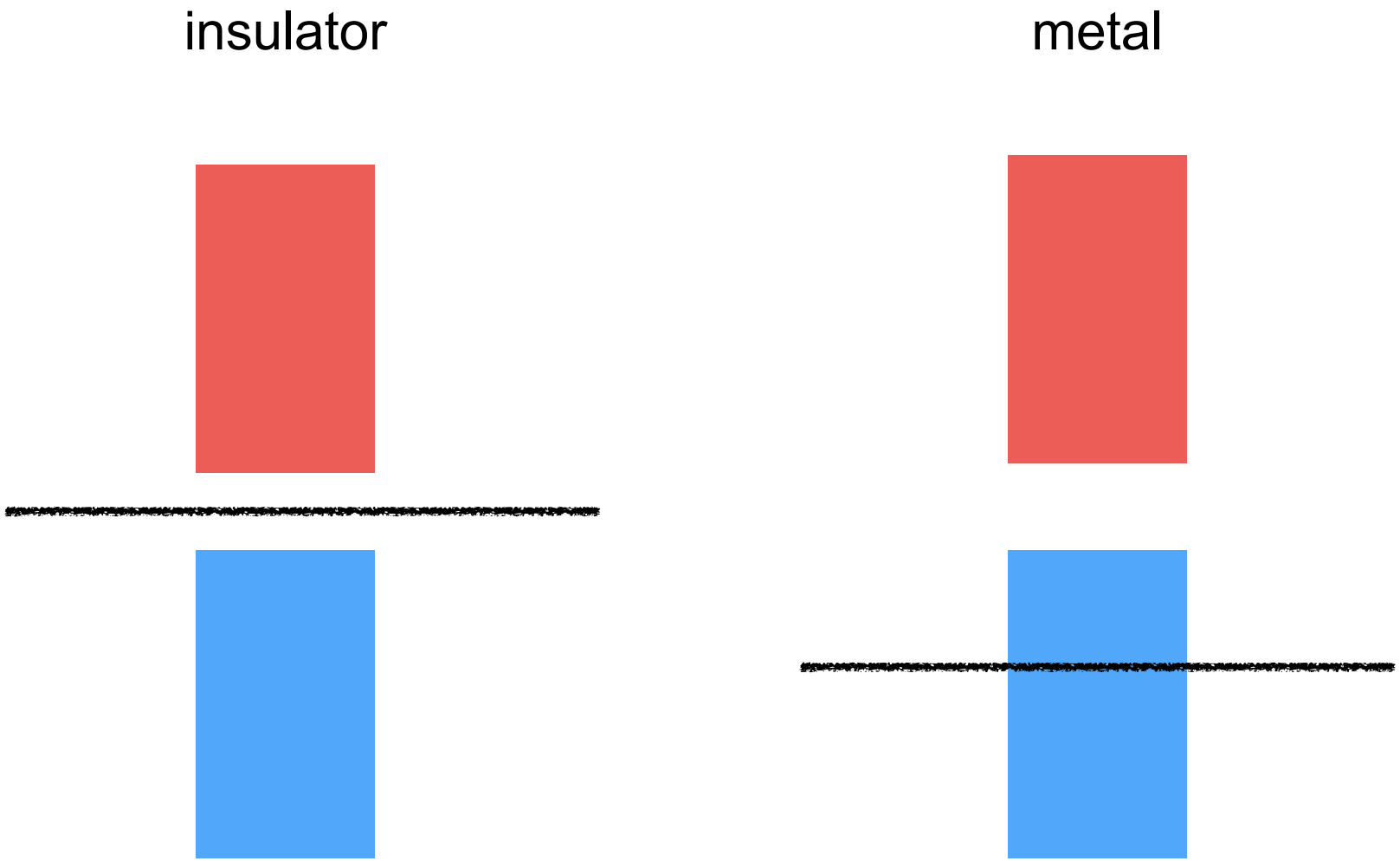


even number of electrons might result in a gapped system

independent-electron picture

odd number of electrons yield a system with no gap

independent-electron picture



an insulator is a system with a **gap**

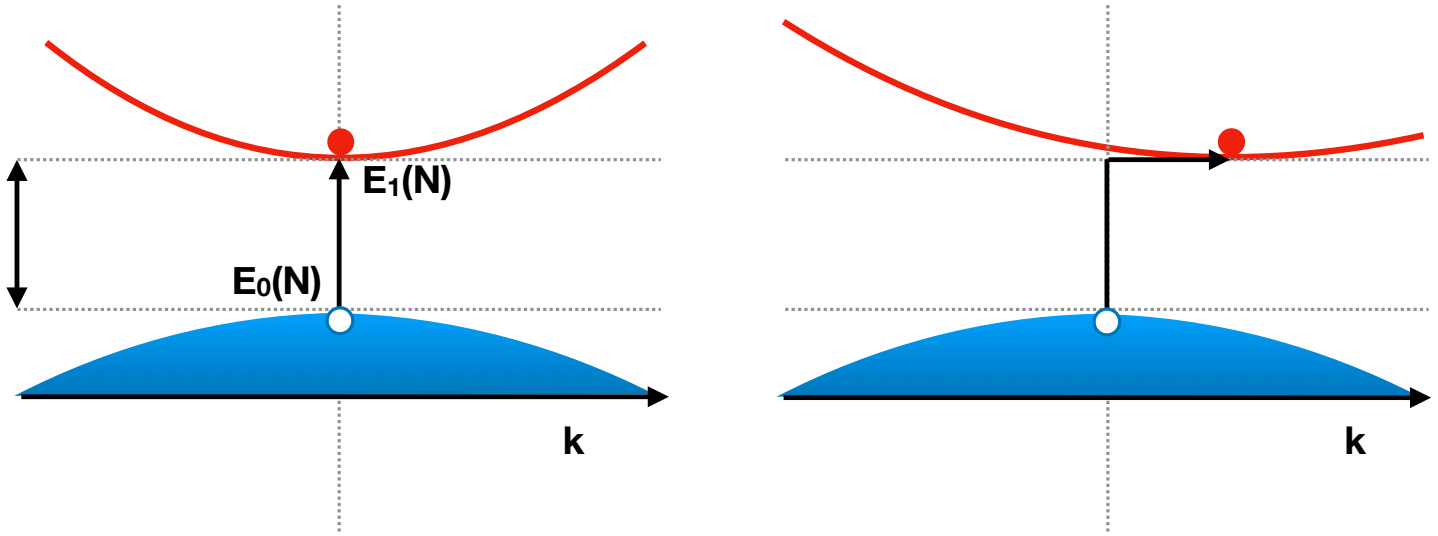
what is the gap?

it depends on the experimental tool used

the band gap

absorption spectroscopy

$$E_1(N)-E_0(N)$$



attention: one electron picture. Not considered: excitons, …

gap in spectral function

photoemission, inverse photoemission

$$E_0(N+1)-E_0(N) + E_0(N-1)-E_0(N)$$

electron affinity ionization energy

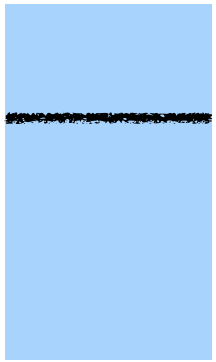
one-electron picture

$$E_0(N-1) \sim E_0(N)$$

$$E_0(N+1) \sim E_1(N)$$

the spectral-function gap equals the band gap

for some systems this approach fails

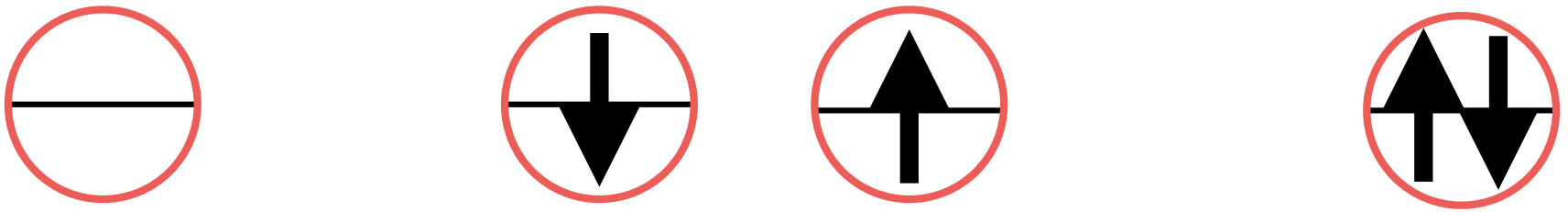
theory	experiments
metal	insulator/bad metal
	?
$E_1(N)-E_0(N)=0$	$E_1(N)-E_0(N)>0$
$E_0(N+1)+E_0(N-1)-2E_0(N)=0$	$E_0(N+1)+E_0(N-1)-2E_0(N)>0$

how can it happen?

a toy model: one-level atom

N electrons

N=0 N=1 N=2

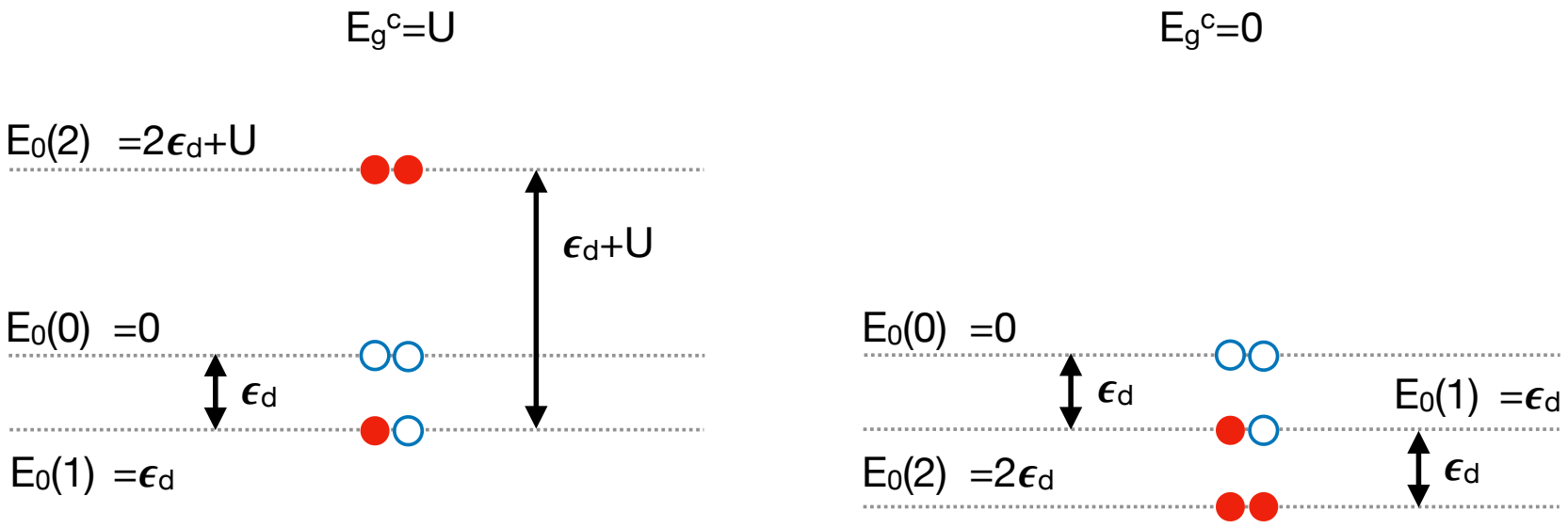


gap in spectral function

photoemission, inverse photoemission

$$E_0(N+1)-E_0(N) + E_0(N-1)-E_0(N)$$

many body vs one-electron picture



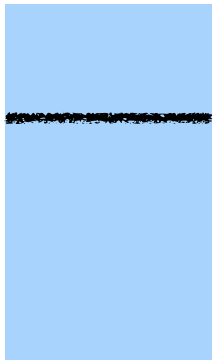
message

the gap can be finite for U>0

even if it is zero for U=0

but there is more than the gap..

for some systems this approach fails

theory	experiments
metal	insulator/bad metal
	?
$E_1(N)-E_0(N)=0$	$E_1(N)-E_0(N)>0$
$E_0(N+1)+E_0(N-1)-2E_0(N)=0$	$E_0(N+1)+E_0(N-1)-2E_0(N)>0$

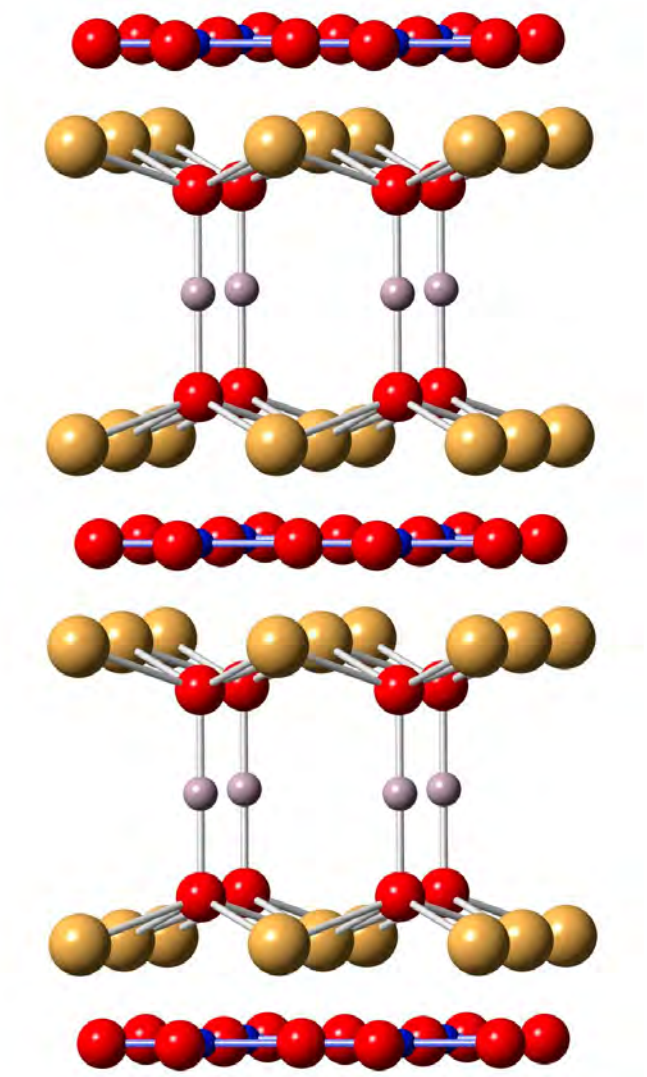
the Hubbard model

Hubbard model

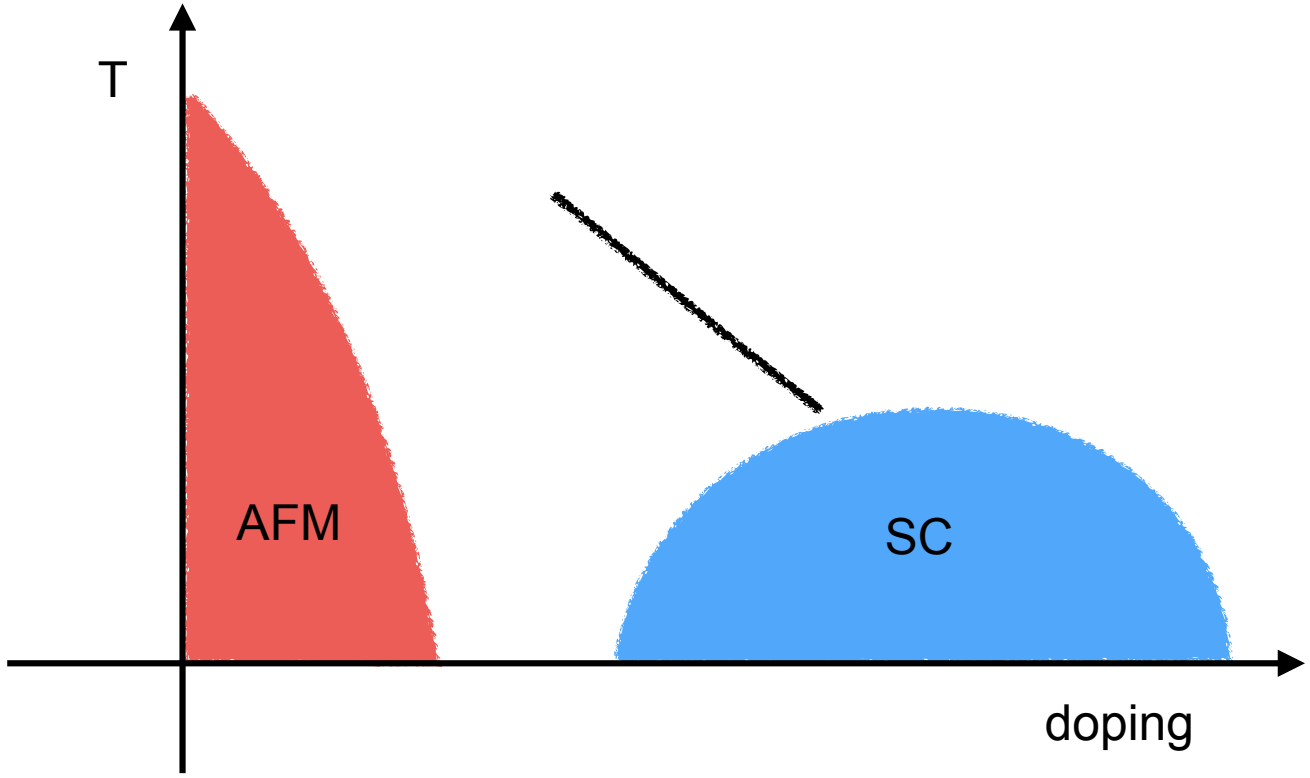
atomic hoppings atomic

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

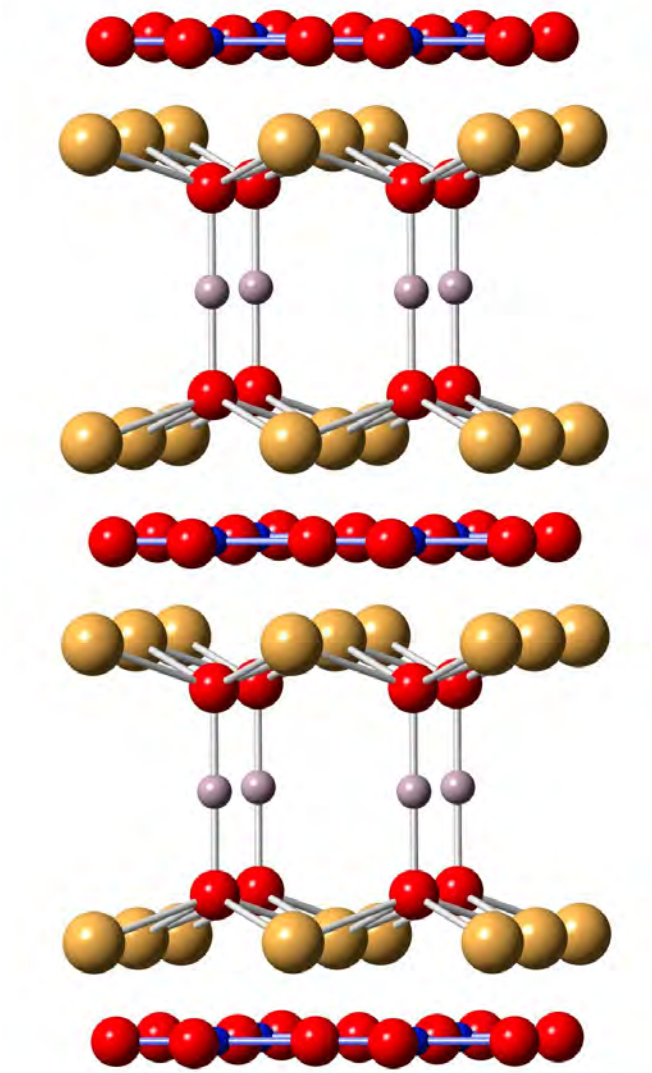
high-T_c superconducting cuprates



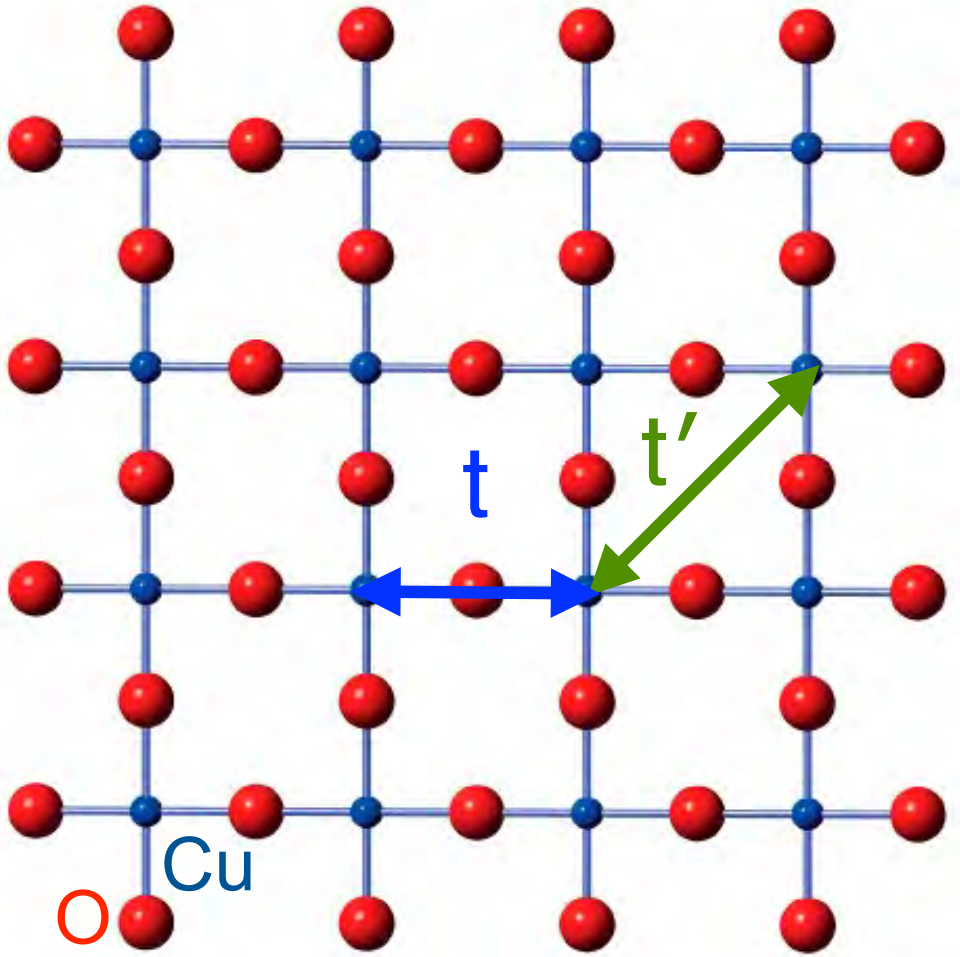
$HgBa_2CuO_4$



high-T_c superconducting cuprates



$HgBa_2CuO_4$



CuO_2 planes

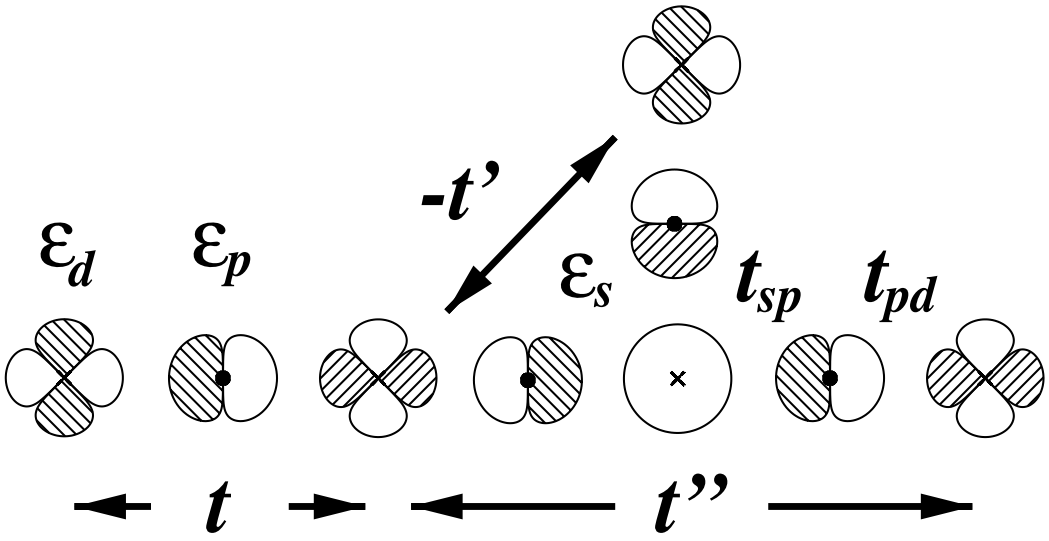
high-T_c superconducting cuprates

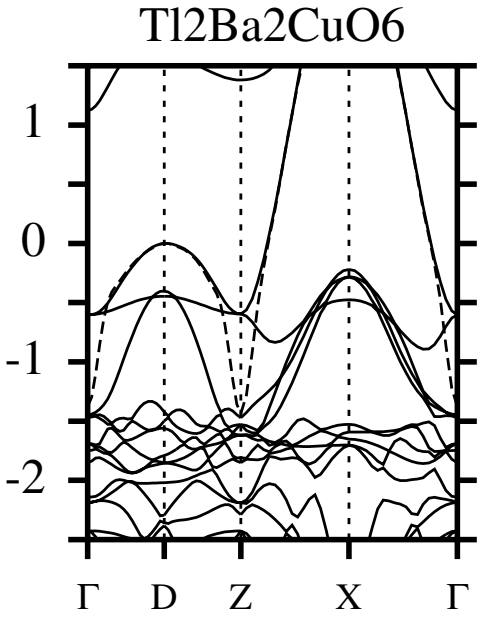
VOLUME 87, NUMBER 4 PHYSICAL REVIEW LETTERS 23 JULY 2001

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

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

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



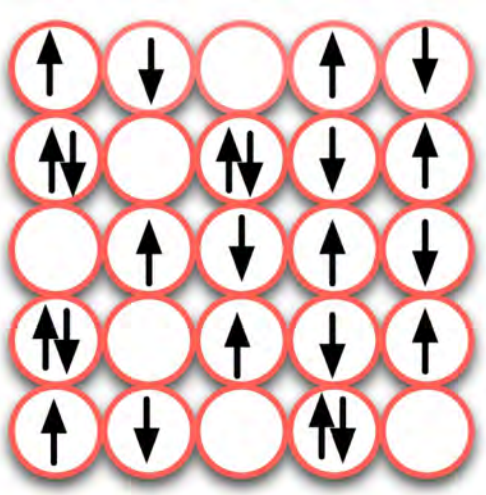


Hubbard model

half filling

atomic hoppings atomic

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



Hubbard model

some exact limits at half filling

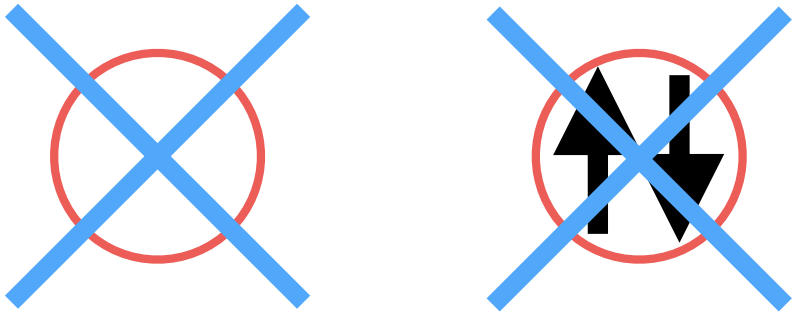
1. *t=0*
2. *t/U small*
3. *U=0*

1. the *t=0* limit

atomic limit (*t=0*) & half filling

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

half filling



atomic limit (*t=0*) & half filling

$\lvert N,S,S_z\rangle$			N	S	$E(N)$
$\lvert 0,0,0\rangle$	$=$	$\lvert 0\rangle$	0	0	0
$\lvert 1,\frac{1}{2},\uparrow\rangle$	$=$	$c^\dagger_{i\uparrow}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 1,\frac{1}{2},\downarrow\rangle$	$=$	$c^\dagger_{i\downarrow}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 2,0,0\rangle$	$=$	$c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}\lvert 0\rangle$	2	0	$2\varepsilon_d+U$

S=1/2

$$\hat{H}_d+\hat{H}_U=\varepsilon_d\sum_i n_i+U\sum_i\left[-\left(\hat{S}^i_z\right)^2+\frac{n_i^2}{4}\right]$$

emergence of the local spins!

half filling: highly degenerate states, 2^{Ns} degrees of freedom

insulating behavior

local spins, Curie paramagnetism

t=0 Hubbard model

$$\chi_{zz}(\mathbf{0};0) \sim \frac{(g\mu_B)^2}{k_B T}\left\{\frac{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\ \left(S_z^i\right)^2\right]}{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\right]} - \left[\frac{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\ S_z^i\right]}{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\right]}\right]^2\right\}$$

$$= \frac{C_{1/2}}{T}\frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

$$U = E(N_i+1) + E(N_i-1) - 2E(N_i)$$

infinite U limit: the spin S=1/2

only S=1/2 part of Hilbert space remains

2. the small *t/U* limit

perturbation theory

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

half filling: N=1 electrons per site

n_D = number of doubly occupied sites

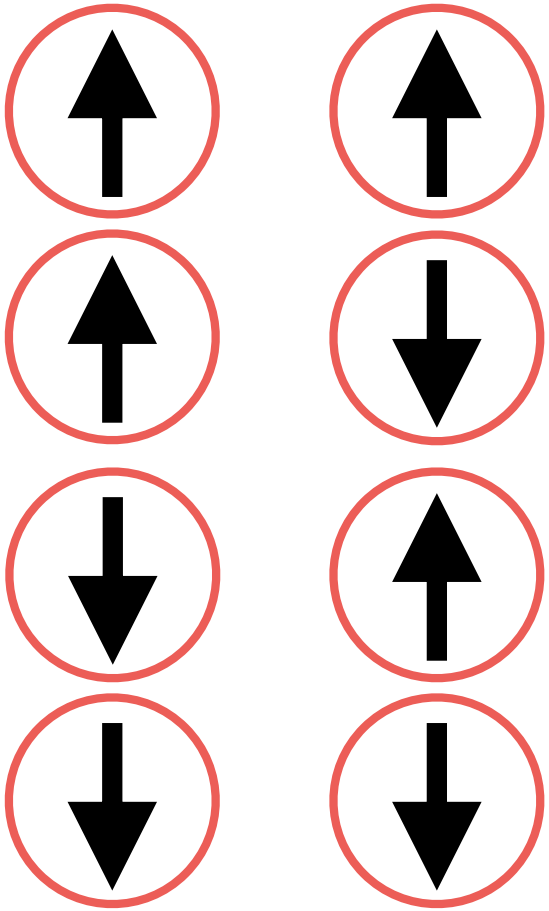
idea: divide Hilbert space into $n_D=0$ and $n_D>0$ sector

next downfold high energy $n_D>0$ sector

two sites

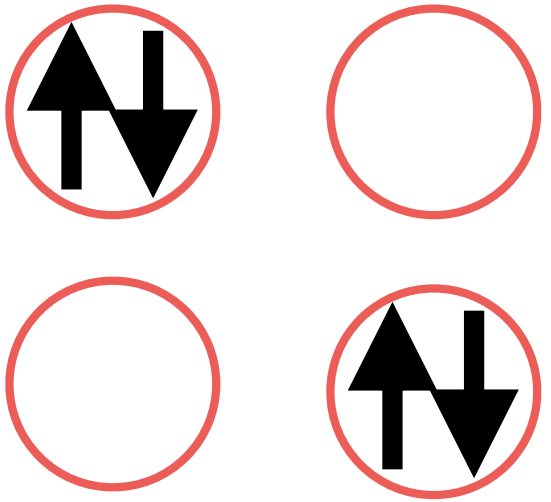
N=1 per site; $N_{tot}=2$

n_D=0 sector



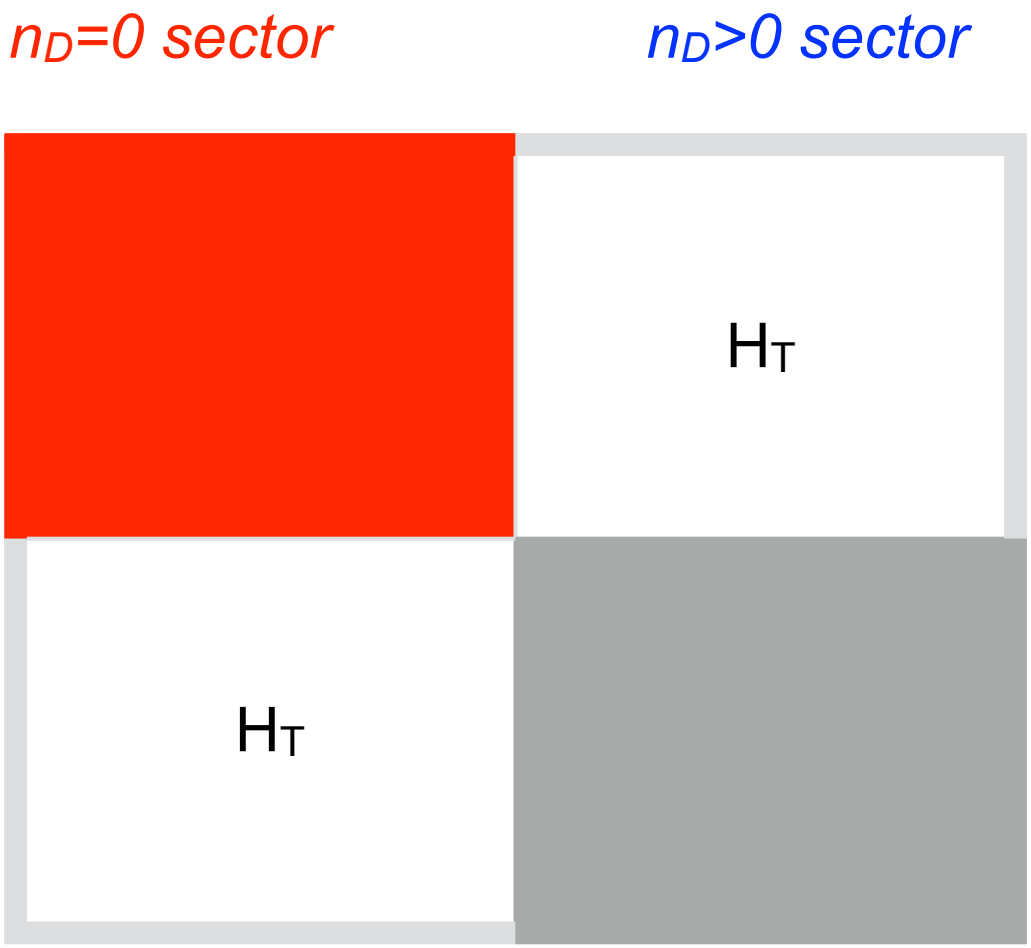
site 1 site 2

n_D=1 sector



site 1 site 2

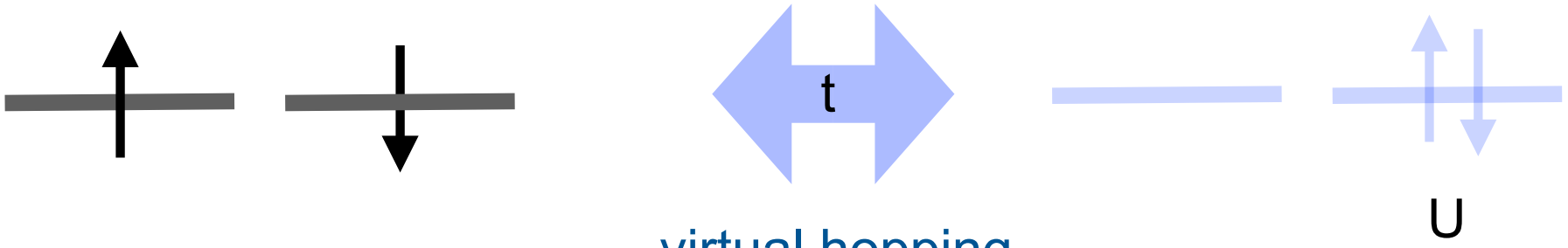
Hilbert space



next downfold high energy $n_D>0$ sector

low-energy model

eliminate states with a doubly occupied site



virtual hopping

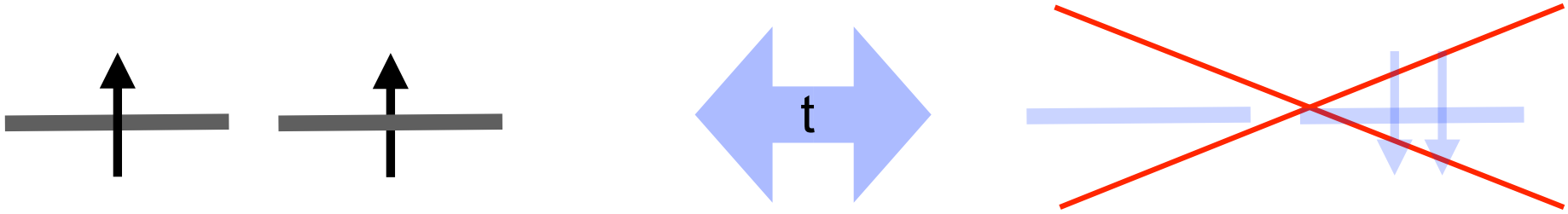
energy gain

$$\Delta E_{\uparrow\downarrow} \sim -\sum_I \langle\uparrow,\downarrow|H_T|I\rangle\langle I\left|\frac{1}{E(2)+E(0)-2E(1)}\right|I\rangle\langle I|H_T|\uparrow,\downarrow\rangle \sim -\frac{2t^2}{U}.$$

=t =1/U =t

low energy model

energy gain only for antiferromagnetic arrangement



Pauli principle

$$\frac{1}{2}\Gamma \sim (\Delta E_{\uparrow\uparrow} - \Delta E_{\uparrow\downarrow}) = \frac{1}{2}\frac{4t^2}{U}$$

$$H_S = \frac{1}{2}\Gamma \sum_{\langle ii' \rangle} \left[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} - \frac{1}{4} n_i n_{i'} \right]$$

insulating behavior

a canonical transformation

Hubbard model

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

here for simplicity $\varepsilon_d = 0$

half filling: N=1 per site

PHYSICAL REVIEW B VOLUME 37, NUMBER 16 1 JUNE 1988

t/U expansion for the Hubbard model

A. H. MacDonald, S. M. Girvin, and D. Yoshioka*
Department of Physics, Indiana University, Bloomington, Indiana 47405
(Received 8 January 1988)

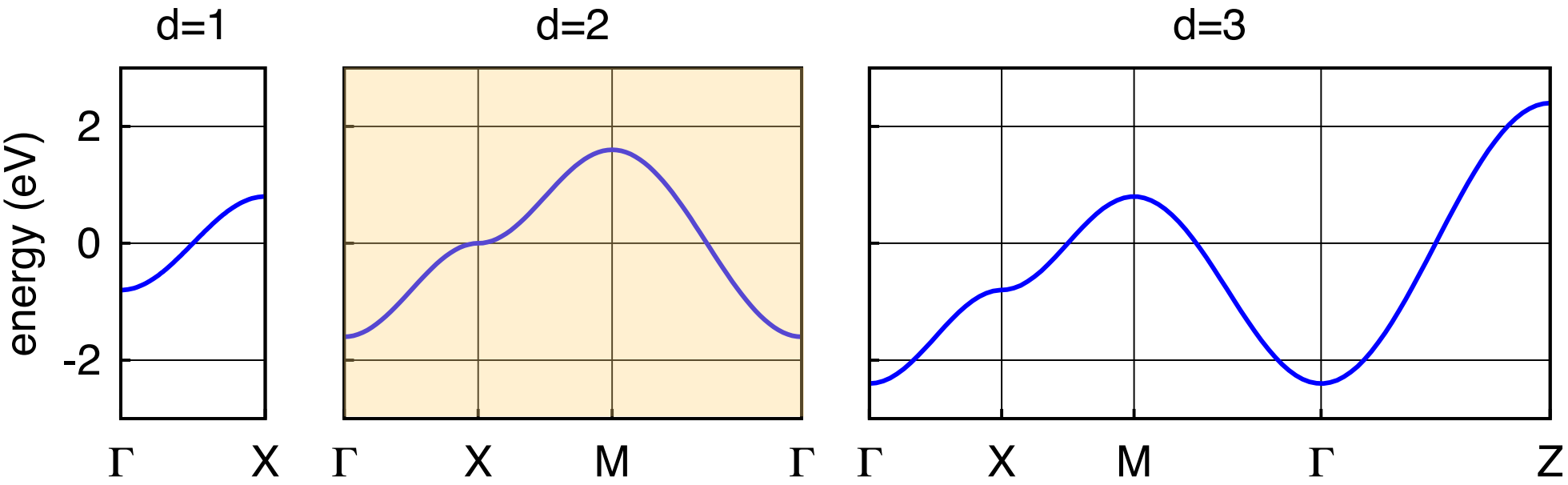
3. the *U=0* case: band limit

the *U=0* limit

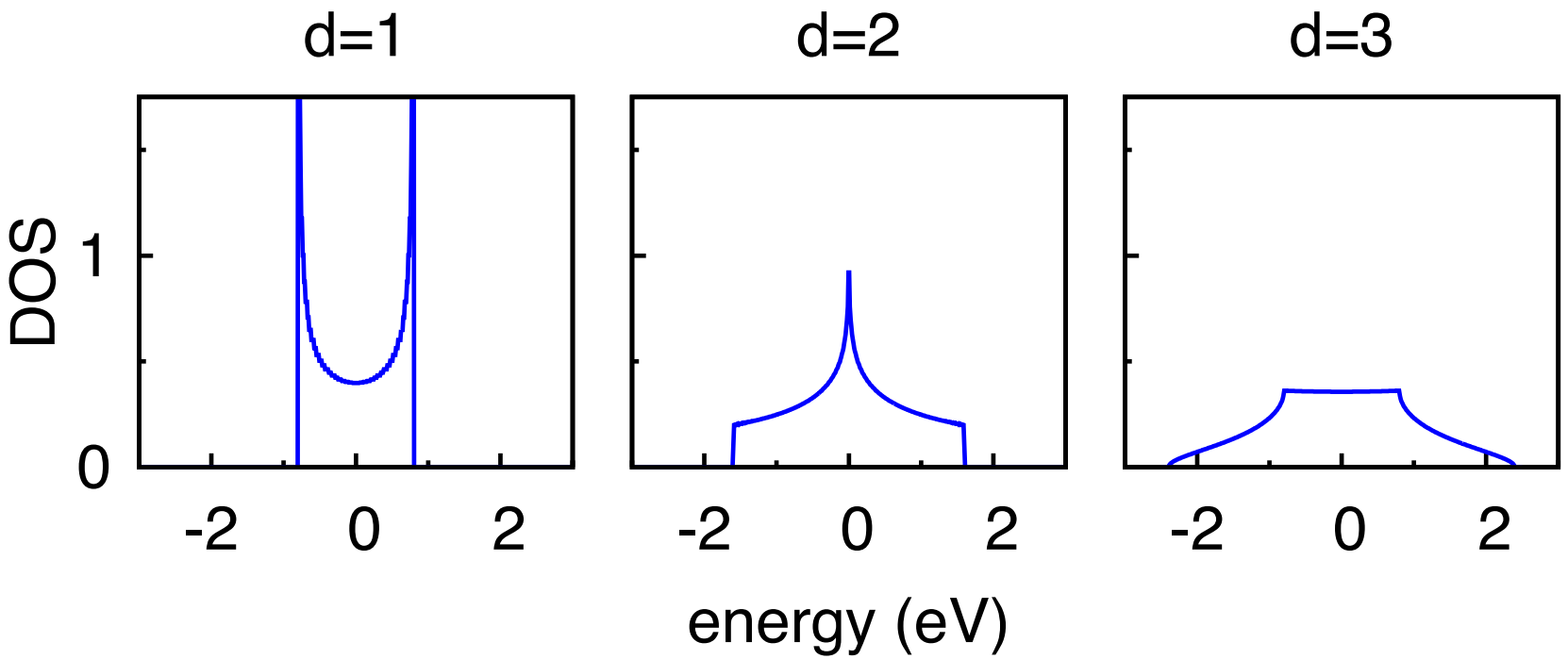
$$H_d + H_T = \sum_{\boldsymbol{k}} \sum_{\sigma} [\varepsilon_d + \varepsilon_{\boldsymbol{k}}] c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$$

hypercubic lattice

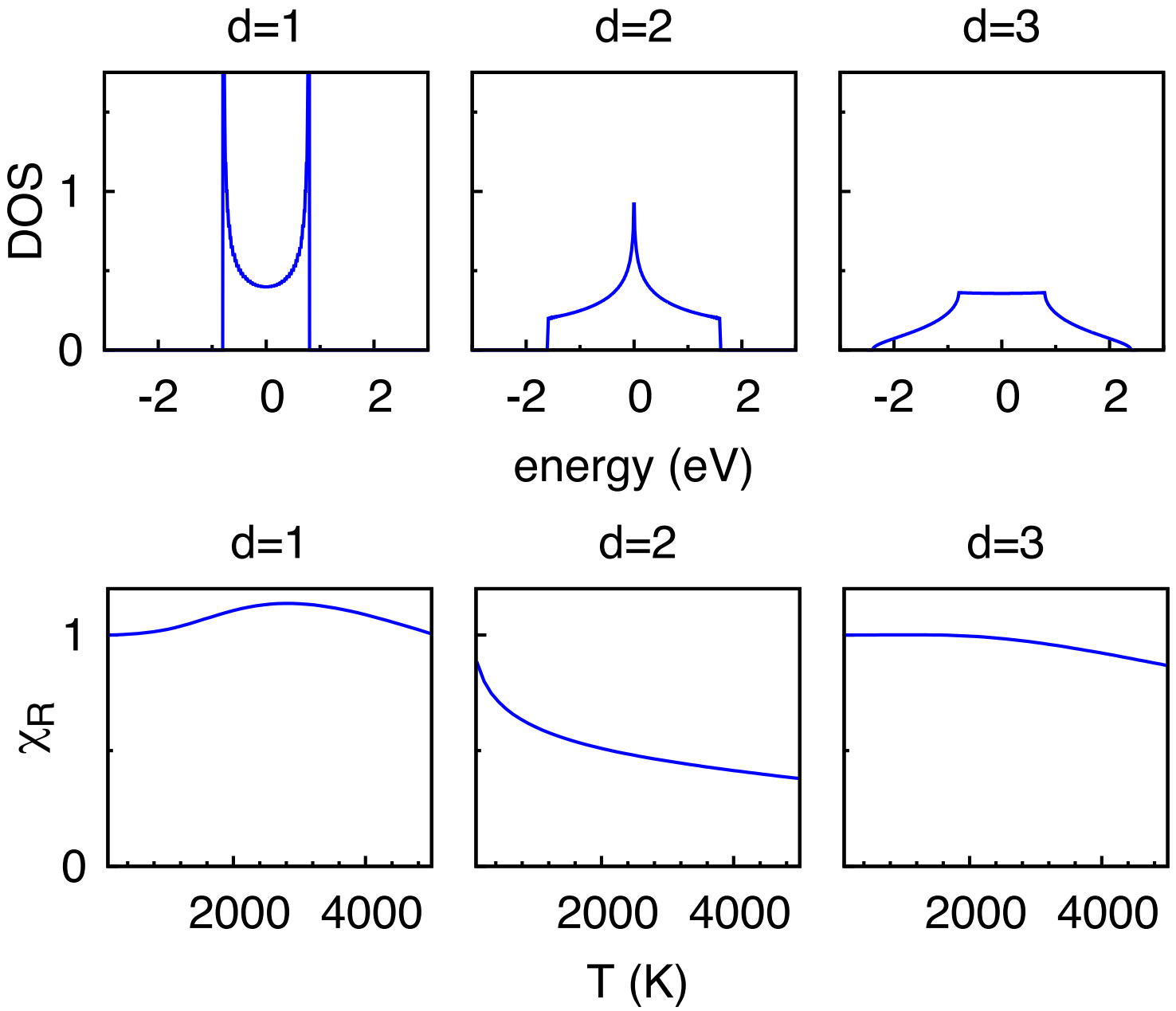
$$\varepsilon_{\boldsymbol{k}} = -2t \sum_{\nu=1}^{d} \cos(k_{r_\nu} a)$$



density of states



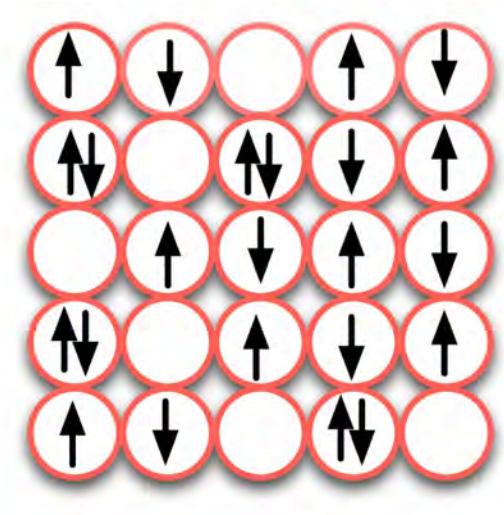
delocalized spins, Pauli paramagnetism



Hubbard model at half-filling

atomic hoppings atomic

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

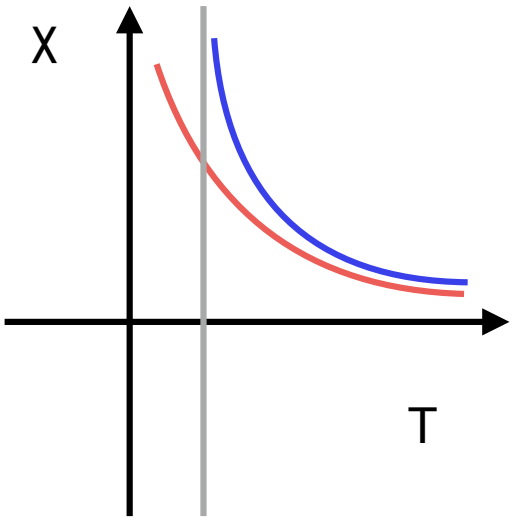


1. *t=0*: collection of atoms, **insulator**
2. *t/U small*: interacting spins, **insulator**
3. *U=0*: half-filled band, **metal**

magnetism (schematic)

t=0

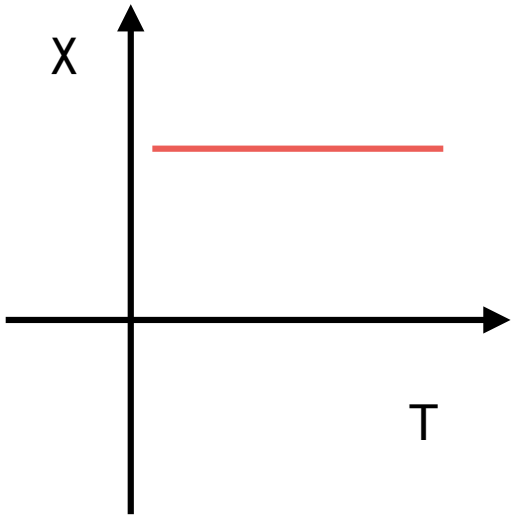
Curie-Weiss paramagnetism



local moments

U=0

Pauli paramagnetism (no van-Hove)



no local moments

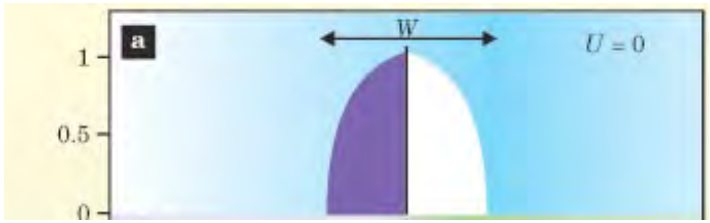
REMARK: van-Hove singularities can also give strong T dependence

message so far

the Hubbard model at half-filling has all essential ingredients

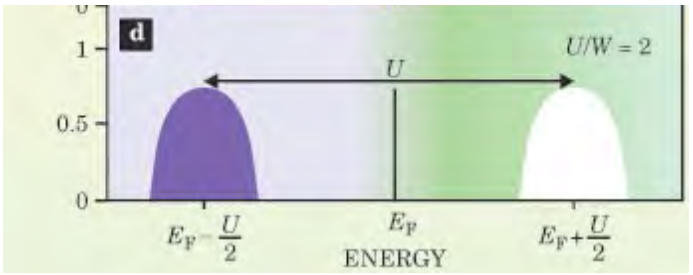
small U/t

band metal, Fermi-liquid



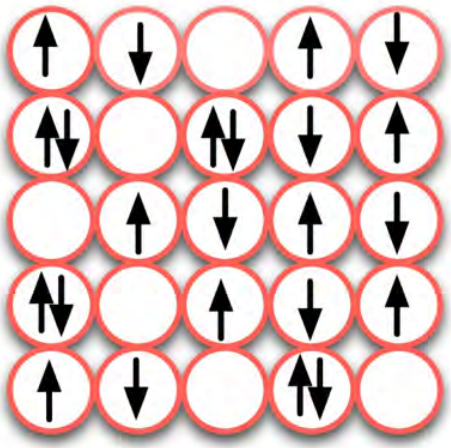
small t/U

local moments, insulator



but how can we describe the transition?

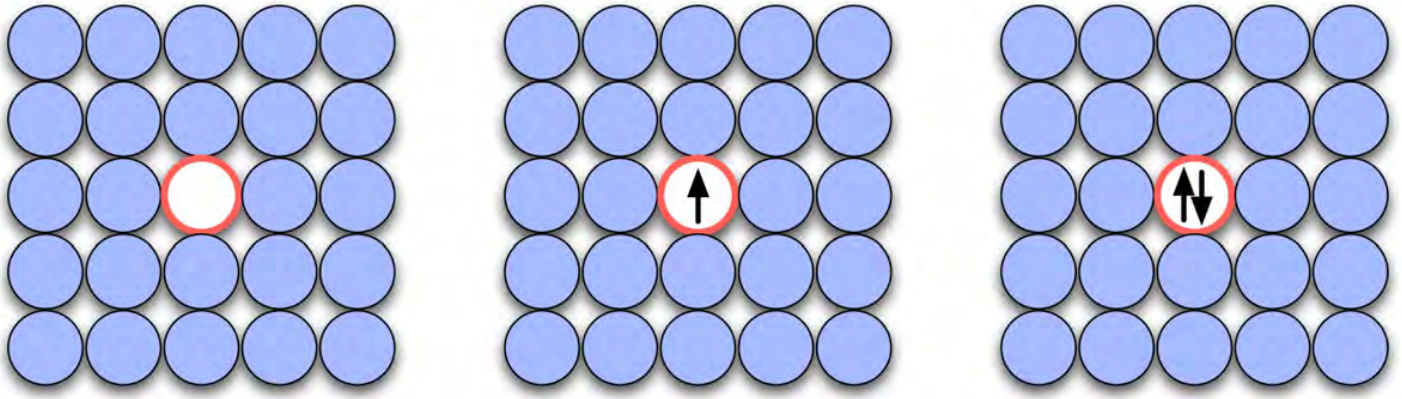
dynamical mean-field theory



$G^{i,j}$

H^{LDA}

$U^{i,i}$



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

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

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

self-consistency loop

lattice model

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

impurity model (Anderson model) with self-consistent bath

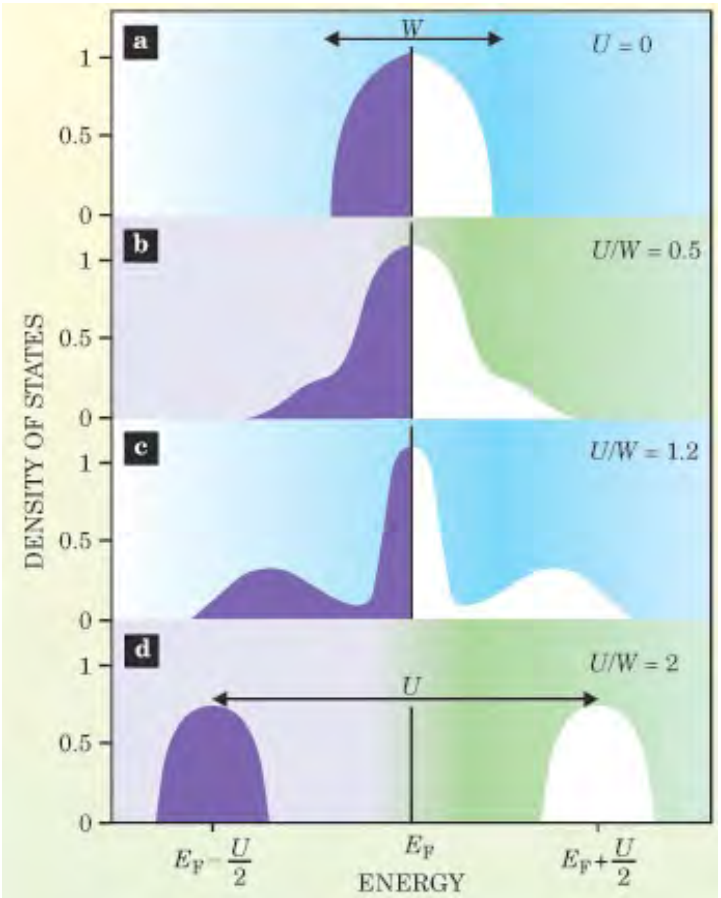
$$H_{\mathrm{A}} = \sum_\sigma \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_\sigma \varepsilon_f n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}$$

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

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

metal-insulator transition

Bethe lattice



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

metallic phase

$$\mathrm{Re}\Sigma(\omega + i0^+) = U/2 + (1 - 1/Z)\omega + O(\omega^3), \qquad (226)$$

$$\mathrm{Im}\Sigma(\omega + i0^+) = -B\omega^2 + O(\omega^4). \qquad (227)$$

The quasiparticle residue Z defines the renormalized Fermi energy of the problem:

$$\epsilon_F^* \equiv ZD \qquad (228)$$

This is also the Kondo temperature of the impurity model. Since the self-energy is momentum independent, Z directly yields the effective mass of quasiparticles (Müller-Hartmann, 1989c):

$$\frac{m^*}{m} = \frac{1}{Z} = 1 - \frac{\partial}{\partial\omega}\mathrm{Re}\Sigma(\omega + i0^+)|_{\omega=0}. \qquad (229)$$

insulating phase

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

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

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

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

everything clear ?

- local Green function
- Anderson model
- relation Hubbard model Anderson model
- impurity Green function
- why mean-field theory
- non-local effects
- difference between static and dynamical mean-field
- how do we go from models to real materials

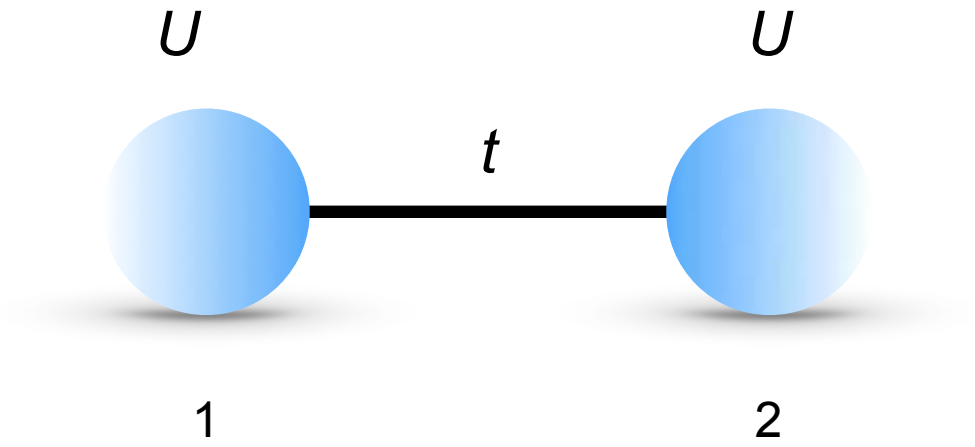
a step back

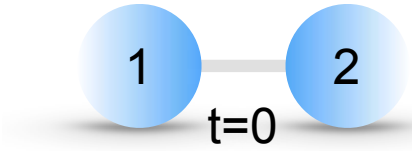
a simpler version of the model

the Hubbard dimer

the Hubbard dimer

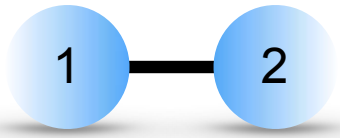
$$\hat{H} = \varepsilon_d \sum_{i\sigma} n_{i\sigma} - t \sum_{\sigma} \left[c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right] + U \sum_{i=1,2} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}.$$





t=0: exact diagonalization

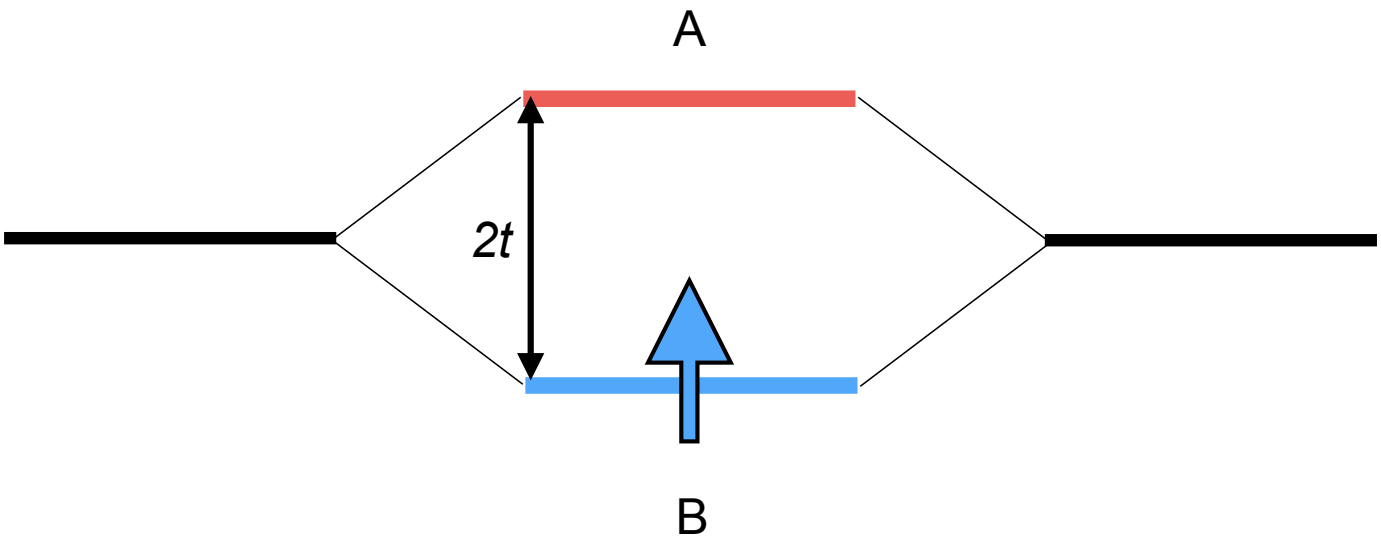
$\lvert N,S,S_z\rangle$			N	S	$E(N,S)$
$\lvert 0,0,0\rangle$	$=$	$\lvert 0\rangle$	0	0	0
$\lvert 1,1/2,\sigma\rangle_1$	$=$	$c^\dagger_{1\sigma}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 1,1/2,\sigma\rangle_2$	$=$	$c^\dagger_{2\sigma}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 2,1,1\rangle$	$=$	$c^\dagger_{2\uparrow}c^\dagger_{1\uparrow}\lvert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

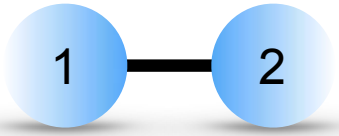


finite *t*: exact diagonalization

N=1

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





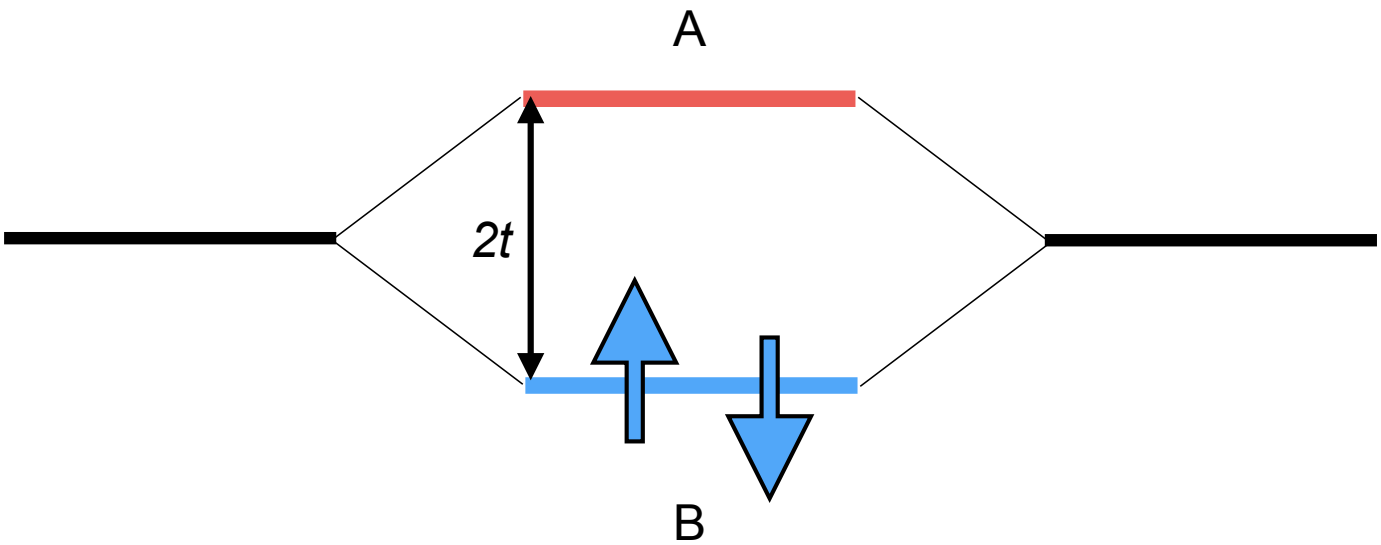
finite *t*: exact diagonalization

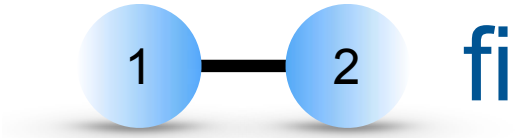
half filling (N=2)

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

ground state is a singlet

U=0

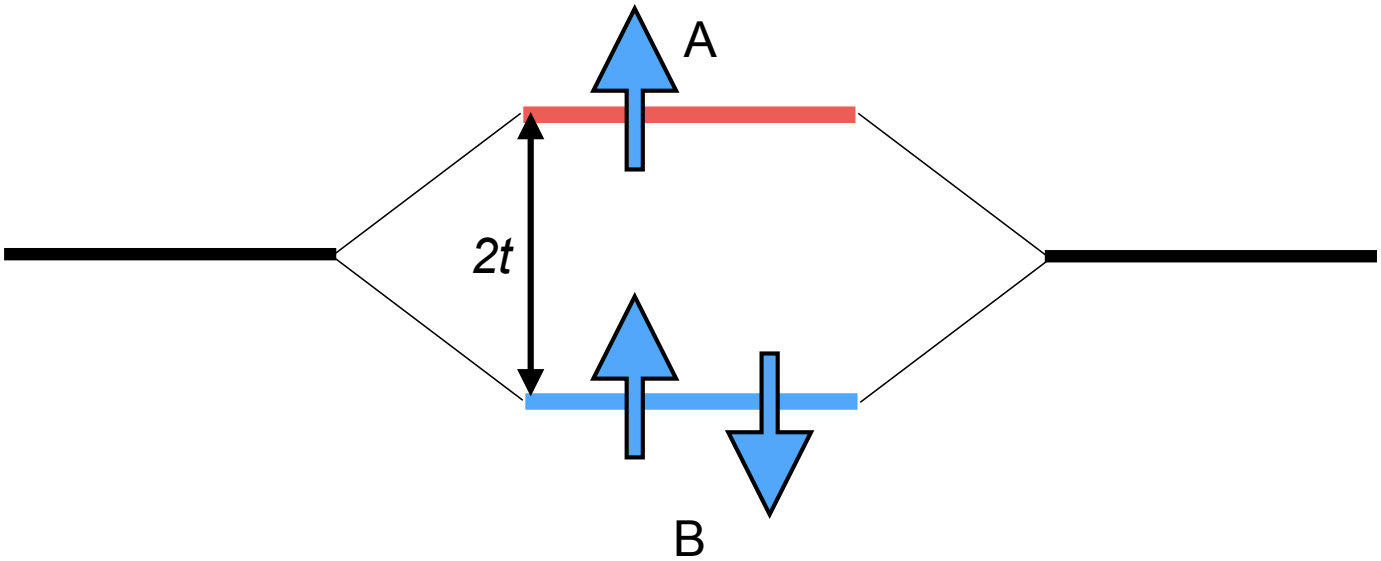




finite *t*: exact diagonalization

N=3

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



the gap is finite

$E_0(N+1)-E_0(N)$ + $E_0(N-1)-E_0(N)$

$$E_g^c(V) = -2t + \sqrt{U^2 + 16t^2}$$

small *t*

$$E_g^c(V) \sim U - 2t$$

atomic limit

small *U*

$$E_g^c(V) \sim 2t$$

one-electron limit

local Green function

definition

$$G_{ii,\sigma}(i\nu_n) = -\int_0^\beta d\tau e^{i\nu_n\tau}\langle \mathcal{T} c_{i\sigma}(\tau)c^\dagger_{i\sigma}(0)\rangle,$$

Lehmann representation

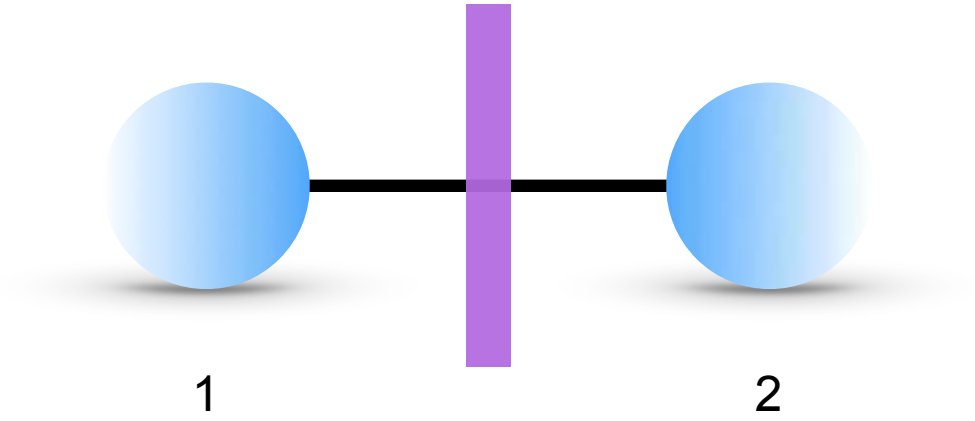
$$G_{ii,\sigma}(i\nu_n) = \frac{1}{Z}\sum_{nn'N} e^{-\beta(E_n(N)-\mu N)}\left[\frac{|\langle n'N-1|c_{i\sigma}|nN\rangle|^2}{i\nu_n - [E_n(N) - E_{n'}(N-1) - \mu]}\right.$$
$$\left. + \frac{|\langle n'N+1|c^\dagger_{i\sigma}|nN\rangle|^2}{i\nu_n - [E_{n'}(N+1) - E_n(N) - \mu]}\right]$$

we need *N*, *N+1* and *N-1* states

symmetries

bonding (**k**=0) and antibonding (**k**=pi) combination

diagonalize quadratic hermitian operators



use symmetries

bonding (**k**=0) and antibonding (**k**=pi) combination of operators

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

$$G_{\pm\pm,\sigma}(i\nu_n) = -\int_0^\beta d\tau e^{i\nu_n \tau} \langle \mathcal{T} c_{\pm\sigma}(\tau) c^\dagger_{\pm\sigma}(0) \rangle,$$

$$G_{11,\sigma}(i\nu_n) = \frac{1}{2} \left[G_{++,\sigma} + G_{--,\sigma} \right]$$

non-interacting case

$$G^0_{11,\sigma}(i\nu_n) = \frac{1}{2}\sum_{\alpha=\pm}\frac{1}{i\nu_n - (\varepsilon_\alpha - \mu)} = \frac{1}{i\nu_n - (\varepsilon_d + F^0(i\nu_n) - \mu)},$$

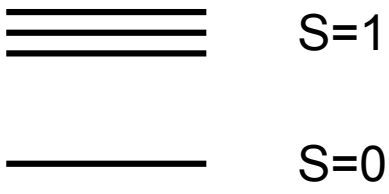
$$F^0(i\nu_n) = \frac{t^2}{i\nu_n - (\varepsilon_d - \mu)},$$

hybridization function

interacting case

(small t/U limit, low temperature)

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



we assume that the triplet-singlet energy difference negligible

interacting case

(small t/U limit, low temperature)

$$G_{11,\sigma}(i\nu_n) \sim \frac{1}{4}\sum_{\alpha=\pm}\left[\frac{1}{i\nu_n-(\varepsilon_\alpha-\mu)}+\frac{1}{i\nu_n-(\varepsilon_\alpha+U-\mu)}\right]$$

$$=\frac{1}{2}\sum_{\alpha=\pm}\frac{1}{i\nu_n-(\varepsilon_\alpha-\mu+\Sigma_{\alpha\alpha}(i\nu_n))}.$$

$$\Sigma_{\alpha\alpha}(i\nu_n)=\frac{U}{2}+\frac{U^2}{4}\frac{1}{i\nu_n-(\varepsilon_\alpha+\frac{1}{2}U-\mu)}.$$

some rewriting

local Green function

$$G_{11,\sigma}(i\nu_n) = \left[\frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma_{l\sigma}(i\nu_n) + F_\sigma(i\nu_n))}\right].$$

local self-energy

$$\Sigma_l(i\nu_n) = \frac{1}{2}(\Sigma_{++}(i\nu_n) + \Sigma_{--}(i\nu_n)),$$

$$= \frac{U}{2} + \frac{U^2}{4}\,\frac{1}{i\nu_n - (\varepsilon_d + \frac{1}{2}U - \mu + \frac{t^2}{(i\nu_n - (\varepsilon_d + \frac{1}{2}U - \mu))})},$$

some rewriting

hybridization function

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

non-local self-energy

$$\begin{aligned}\Delta\Sigma_{l\sigma}(i\nu_n) &= \frac{1}{2}(\Sigma_{++}(i\nu_n) - \Sigma_{--}(i\nu_n)) \\ &= \frac{U^2}{4}\,\frac{t}{(i\nu_n - (\varepsilon_d + \frac{1}{2}U - \mu))^2 - t^2},\end{aligned}$$

message: the self-energy is NOT local

U=0 vs finite *U*

$$G^0_{11,\sigma}(i\nu_n) = \frac{1}{2}\sum_{\alpha=\pm}\frac{1}{i\nu_n - (\varepsilon_\alpha - \mu)} = \frac{1}{i\nu_n - (\varepsilon_d + F^0(i\nu_n) - \mu)},$$

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

$$G_{11,\sigma}(i\nu_n) = \left[\frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma_{l\sigma}(i\nu_n) + F_\sigma(i\nu_n))}\right].$$

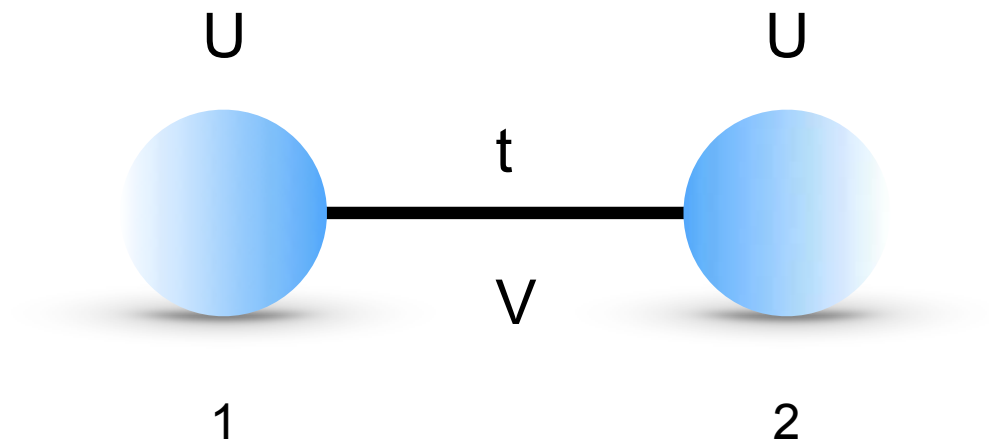
$$E_g^c = -2t + \sqrt{U^2 + 16t^2} \quad \sim U\text{-}2t$$

non-local Coulomb interaction

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

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

$J_V=0$



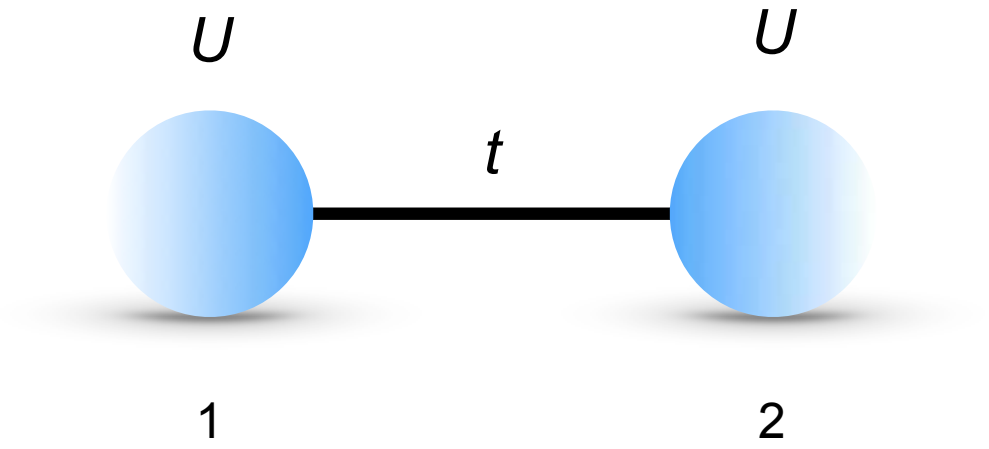
half-filling, the states

V=U: uncorrelated Hamiltonian

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

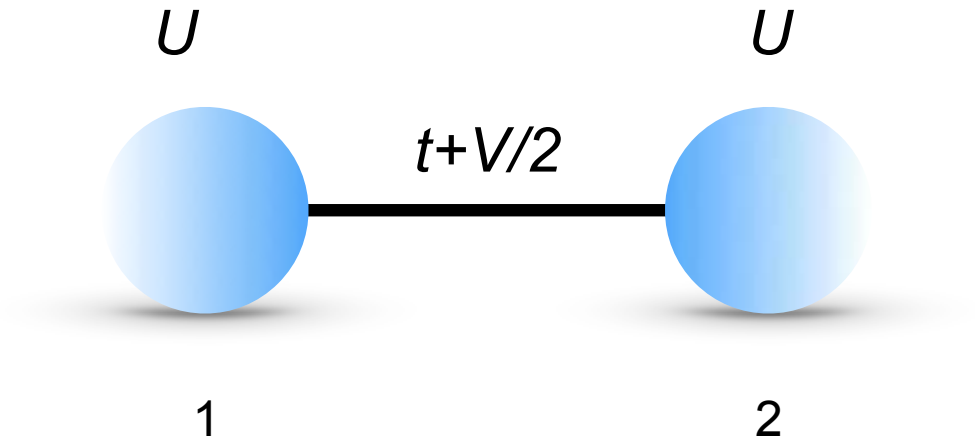
half-filling, the gap

$$E_g^c(V) = -2t + V + \sqrt{(U-V)^2 + 16t^2}.$$



***U* large**, *V* small, *U*-*V* large

***U* large**, *V*=*U*, *U*-*V* small



message

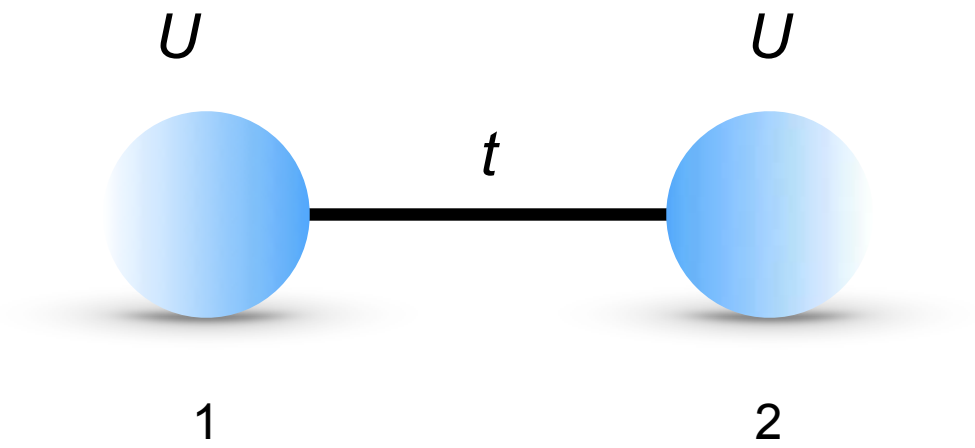
long-range Coulomb term reduce the effects of correlations

strong-correlation effects arise from local Coulomb term

this does NOT mean that the self-energy is local

exact solution: conclusions

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

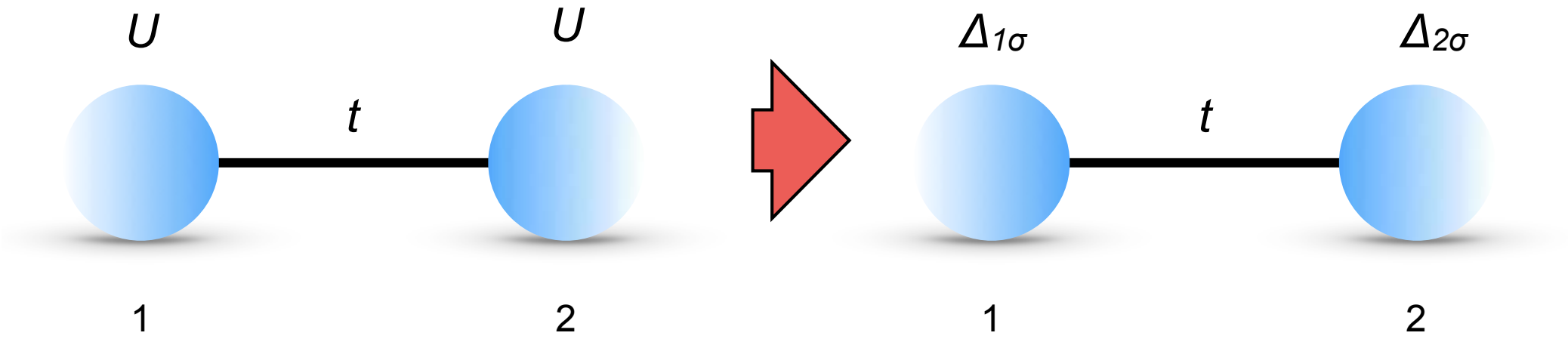


- self-energy: local + non-local
- gap is U-2t for small t ("*insulating*")
- gap is 2t for small U (artefact, "*metallic*")

static mean-field vs exact

the Hartree-Fock approach

$$\hat{H}_U = U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \rightarrow \hat{H}_U^{\mathrm{HF}} = U \sum_i [\hat{n}_{i\uparrow}\bar{n}_{i\downarrow} + \hat{n}_{i\downarrow}\bar{n}_{i\uparrow} - \bar{n}_{i\uparrow}\bar{n}_{i\downarrow}],$$



ferro and antiferro case, $n_1=n_2=n$

ferro

$$m_+ = \frac{1}{2}(m_1 + m_2)$$

anti-ferro

$$m_- = \frac{1}{2}(m_1 - m_2)$$

$$\Delta_{1\sigma}^{\mathrm{F}} = U\left(\frac{n}{2} + \sigma m_+\right)$$

$$\Delta_{2\sigma}^{\mathrm{F}} = U\left(\frac{n}{2} + \sigma m_+\right)$$

$$\Delta_{1\sigma}^{\mathrm{AF}} = U\left(\frac{n}{2} + \sigma m_-\right)$$

$$\Delta_{2\sigma}^{\mathrm{AF}} = U\left(\frac{n}{2} - \sigma m_-\right)$$

this term is like an energy-independent self-energy

$$\Sigma_{ii,\sigma}(i\nu_n) = \Delta_{i\sigma}.$$

Hartree-Fock Hamiltonian

$$\delta n = 0$$

$$\hat{H}_{\mathrm{HF}} = \sum_{i\sigma} \left(\varepsilon_d + \Delta_{i\sigma}\right) \hat{n}_{i\sigma} - t \sum_{\sigma} \left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right) - \Delta_0$$

$$\Delta_0 = 2U \left[\frac{n^2}{4} - m_+^2 - m_-^2 \right]$$

$$\Delta_{i\sigma} = U \left[(-1)^{\sigma} \left(m_+ + (-1)^{i-1} m_- \right) + \frac{1}{2} n \right].$$

this term is like an energy-independent self-energy

$$\Sigma_{ii,\sigma}(i\nu_n) = \Delta_{i\sigma}.$$

relation to exact self-energy

exact

$$\Sigma_l(i\nu_n) = \frac{1}{2}(\Sigma_{++}(i\nu_n) + \Sigma_{--}(i\nu_n)),$$

$$= \frac{U}{2} + \frac{U^2}{4}\,\frac{1}{i\nu_n - (\varepsilon_d + \frac{1}{2}U - \mu + \frac{t^2}{(i\nu_n - (\varepsilon_d + \frac{1}{2}U - \mu))})},$$

HF is the high-frequency limit in the paramagnetic case

$$\Sigma_{ii,\sigma}(i\nu_n) = \Delta_{i\sigma} = \frac{U}{2}$$

it is also the self-energy in first order perturbation theory

self-energy, antiferro half-filling

Green function matrix in bonding-antibonding basis

$$G_\sigma(i\nu_n) = \frac{1}{2}\begin{bmatrix} i\nu_n - (\varepsilon_d - t - \mu + \frac{1}{2}\sum_i \Sigma_{i\sigma}(i\nu_n)) & \frac{1}{2}\sum_i (-1)^{i-1}\Sigma_{i\sigma}(i\nu_n) \\ \frac{1}{2}\sum_i (-1)^{i-1}\Sigma_{i\sigma}(i\nu_n) & i\nu_n - (\varepsilon_d + t - \mu + \frac{1}{2}\sum_i \Sigma_{i\sigma}(i\nu_n)) \end{bmatrix}^{-1}.$$

diagonal elements are identical

off-diagonal elements: coupling of bonding and antibonding!

symmetry reduction

gap at half-filling, antiferro

$$E_g^{\mathrm{HF}} = 2\Delta_1(t,U) = 2\sqrt{(m_- U)^2 + t^2} = U$$

$$m_- = 0 \quad \text{or} \quad m_- = \frac{1}{2}\sqrt{1 - \frac{4t^2}{U^2}}.$$

eigenstates, antiferro

$\|2\rangle_l$	$E_l(2)$
$\|2\rangle_5 = \frac{1}{\sqrt{2}}\left[\|2,0,0\rangle_0 + a_2\|2,1,0\rangle - \frac{a_1}{\sqrt{2}}\left[\|2,0,0\rangle_1 + \|2,0,0\rangle_2\right]\right]$	$\varepsilon_0(2) + 2\Delta_1(t,U)$
$\|2\rangle_4 = \frac{1}{\sqrt{2}}\left[\|2,0,0\rangle_1 - \|2,0,0\rangle_2\right]$	$\varepsilon_0(2)$
$\|2\rangle_3 = \|2,1,1\rangle$	$\varepsilon_0(2)$
$\|2\rangle_2 = \|2,1,-1\rangle$	$\varepsilon_0(2)$
$\|2\rangle_1 = a_1\|2,1,0\rangle + a_2\frac{1}{\sqrt{2}}\left[\|2,0,0\rangle_1 + \|2,0,0\rangle_2\right]$	$\varepsilon_0(2)$
$\|2\rangle_0 = \frac{1}{\sqrt{2}}\left[\|2,0,0\rangle_0 - a_2\|2,1,0\rangle + \frac{a_1}{\sqrt{2}}\left[\|2,0,0\rangle_1 + \|2,0,0\rangle_2\right]\right]$	$\varepsilon_0(2) - 2\Delta_1(t,U)$

$$\Delta_1(t,U) = \sqrt{(m\_U)^2 + t^2}$$

states, ferro

$\|2\rangle_l$	$E_l(2)$
$\|2\rangle_5 = \|2,1,-1\rangle$	$\varepsilon_0^+(2) + 2Um_+$
$\|2\rangle_4 = \frac{1}{\sqrt{2}}\left[\|2,0,0\rangle_0 - \frac{1}{\sqrt{2}}\left[\|2,0,0\rangle_1 + \|2,0,0\rangle_2\right]\right]$	$\varepsilon_0^+(2) + 2t$
$\|2\rangle_3 = \frac{1}{\sqrt{2}}\left[\|2,0,0\rangle_1 - \|2,0,0\rangle_2\right]$	$\varepsilon_0^+(2)$
$\|2\rangle_2 = \|2,1,\quad 0\rangle$	$\varepsilon_0^+(2)$
$\|2\rangle_1 = \frac{1}{\sqrt{2}}\left[\|2,0,0\rangle_0 + \frac{1}{\sqrt{2}}\left[\|2,0,0\rangle_1 + \|2,0,0\rangle_2\right]\right]$	$\varepsilon_0^+(2) - 2t$
$\|2\rangle_0 = \|2,1,\quad 1\rangle$	$\varepsilon_0^+(2) - 2Um_+$

what is not so bad

1/2 the magnetic coupling

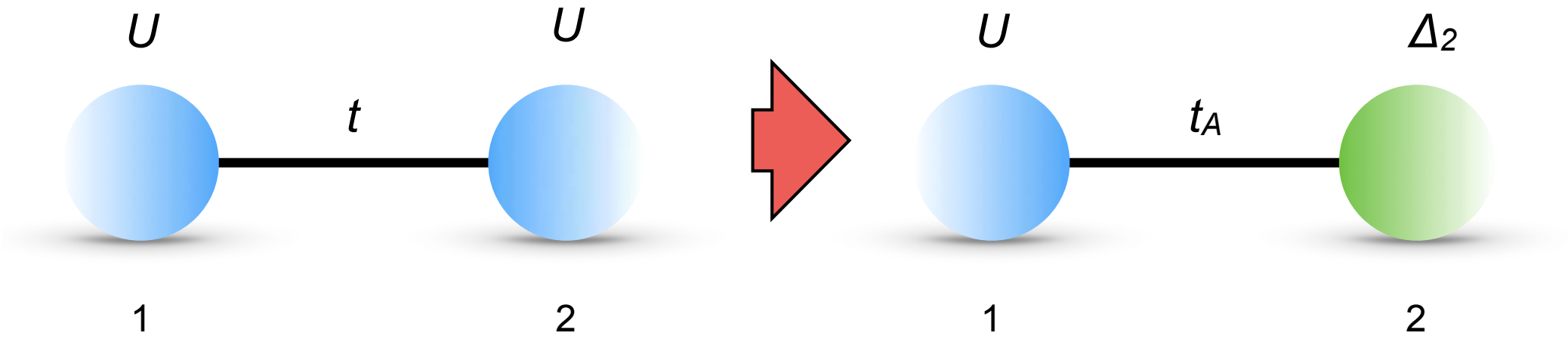
$$E_{AF} - E_F \sim -\frac{2t^2}{U},$$

Hartree-Fock: conclusions

- self-energy frequency independent (static)
- paramagnetic self-energy: high-frequency limit of exact self-energy
- charge gap is U — incorrect
- triplet-singlet energy difference is U — wrong
- AF excited spectrum incorrect
- F spectrum totally wrong
- AF-FM state difference for large U correct
- triplet-singlet mix — symmetry not respected

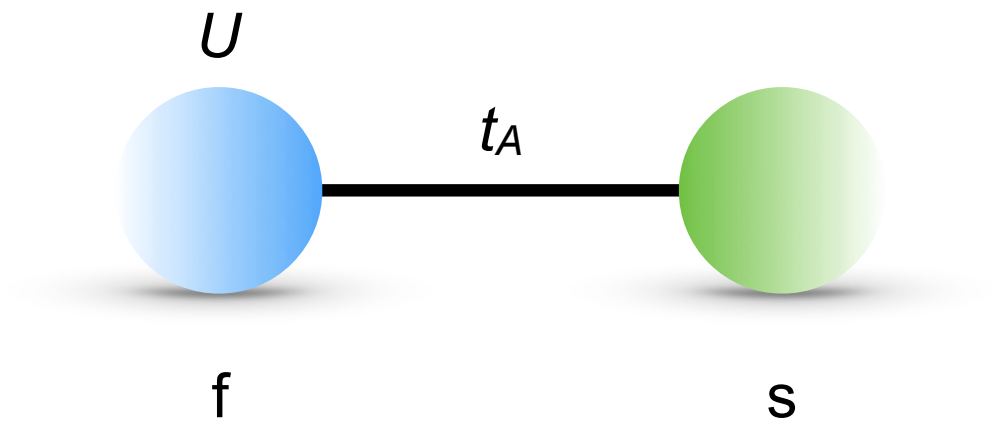
a better mean-field theory?

the Anderson molecule



the Anderson molecule

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



Hamiltonian at half-filling

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

singlet ground-state at half-filling

$$E_0(\omega) = \omega = \varepsilon_f + \varepsilon_s - \frac{2t_A^2}{2\varepsilon_f + U - \omega} - \frac{2t_A^2}{2\varepsilon_s - \omega}.$$

$$\omega = \varepsilon_f + \varepsilon_s - \Delta E,$$

$$\Delta E \sim -2t_A^2 \left[\frac{1}{\varepsilon_f} - \frac{1}{\varepsilon_f + U} \right] \equiv \Gamma.$$

Kondo energy gain

(real T_k exponentially small: Kondo effect **non-perturbative**)

$$T_k = De^{-2/\rho\Gamma}$$

the impurity Green function

non-interacting Anderson modecule

$$\mathcal{G}_{\sigma}^{-1}(i\nu_n) = \begin{pmatrix} i\nu_n - \varepsilon_f + \mu & t_A \\ t_A & i\nu_n - \varepsilon_s + \mu \end{pmatrix}^{-1}.$$

$$\mathcal{G}_{ff,\sigma}(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_f - \mu + \mathcal{F}(i\nu_n))},$$

$$\mathcal{F}(i\nu_n) = \frac{t_A^2}{i\nu_n - (\varepsilon_s - \mu)} = i\nu_n - \varepsilon_f + \mu - \mathcal{G}_{ff,\sigma}^{-1}(i\nu_n).$$

interacting Anderson modecule

$$G_{ff,\sigma}(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_f - \mu + \mathcal{F}(i\nu_n) + \Sigma_{ff}(i\nu_n))}.$$

compare to Hubbard dimer

non-interacting Hubbard dimer

$$G^0_{11,\sigma}(i\nu_n) = \frac{1}{2}\sum_{\alpha=\pm}\frac{1}{i\nu_n - (\varepsilon_\alpha - \mu)} = \frac{1}{i\nu_n - (\varepsilon_d + F^0(i\nu_n) - \mu)},$$

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

non-interacting Anderson modecule

$$\mathcal{G}_{ff,\sigma}(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_f - \mu + \mathcal{F}(i\nu_n))},$$

approximated Hubbard dimer?

interacting Hubbard dimer

$$G_{11,\sigma}(i\nu_n) = \left[\frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma_{l\sigma}(i\nu_n) + F_\sigma(i\nu_n))} \right].$$

non local self-energy is here

interacting Anderson modecule

$$G_{ff,\sigma}(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_f - \mu + \mathcal{F}(i\nu_n) + \Sigma_{ff}(i\nu_n))}.$$

approximated Hubbard dimer?

self-consistent condition

$$G_{ff}=G_{ii}$$

we need that

- non-local self-energy Hubbard dimer negligible
- local self-energy equals impurity self-energy
- hybridization function equals impurity hybridization function

for a molecule not really working…. but what about a soild?

DMFT

lattice model

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

impurity model (Anderson model)

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

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

self-consistency loop

the Anderson model

Anderson model

metal impurity

$$\hat{H}_{\mathrm{A}} = \sum_{\sigma}\sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} \hat{n}_{\boldsymbol{k}\sigma} + \sum_{\sigma} \varepsilon_f \hat{n}_{f\sigma} + U \hat{n}_{f\uparrow}\hat{n}_{f\downarrow}$$

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

hybridization

Kondo regime: $n_f \sim 1$

canonical transformation (Schrieffer-Wolff) to Kondo model

$$H_{\mathrm{K}} = \sum_{\sigma}\sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \Gamma \boldsymbol{S}_f \cdot \boldsymbol{s}_c(\boldsymbol{0}) = H_0 + H_{\Gamma}$$

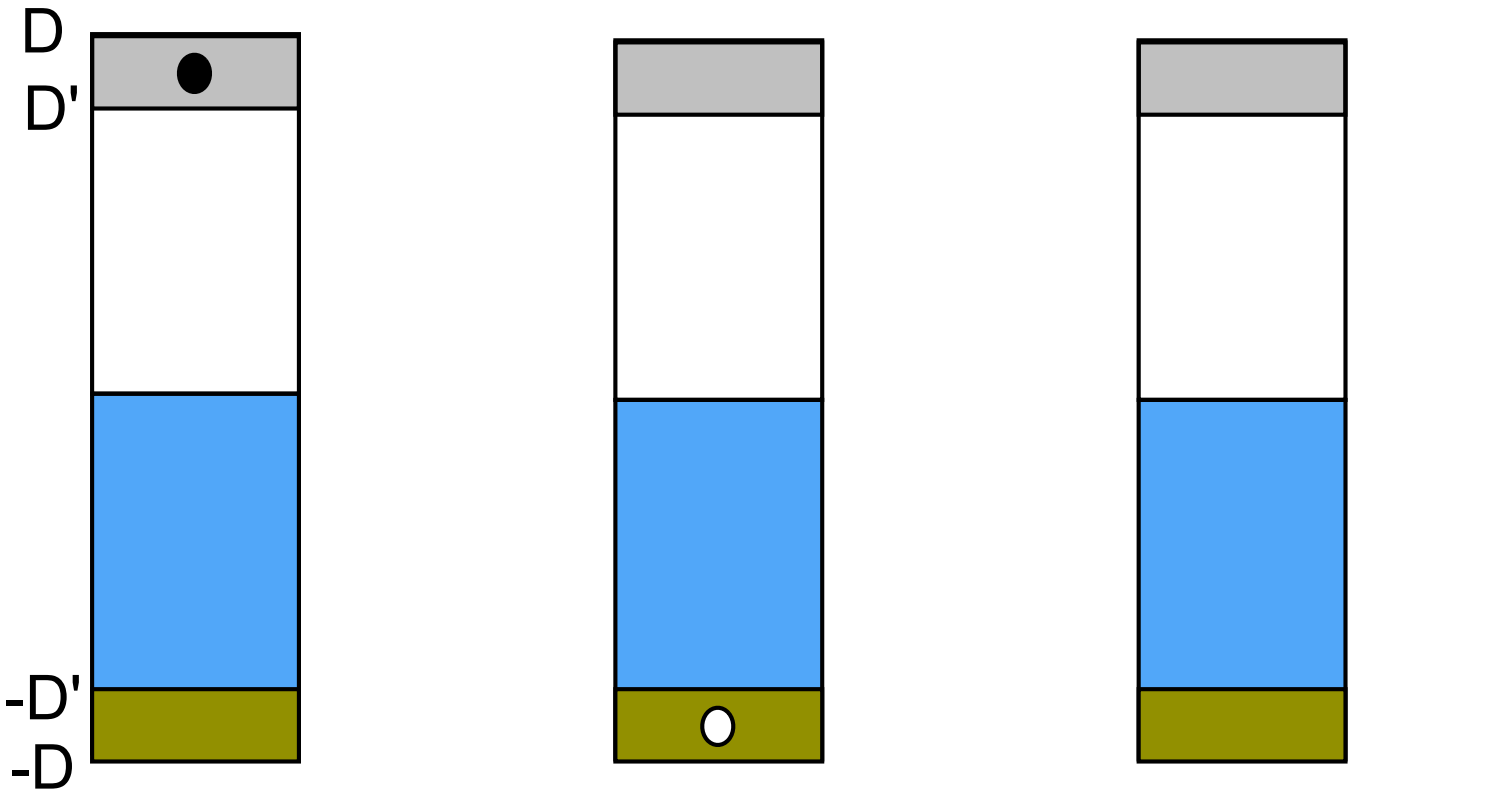
$$\Gamma \sim -2|V_{k_F}|^2 \left[\frac{1}{\varepsilon_f} - \frac{1}{\varepsilon_f + U} \right] > 0$$

antiferromagnetic coupling

poor-man scaling

eliminate high-energy states, i.e., the states with

- at least one electron in high-energy region
- at least one hole in high-energy region



- one electron
- one hole
- low-energy state

downfolding

electron case: projectors

$$P_H \sim \sum_{\sigma} \sum_{\boldsymbol{q}} c^{\dagger}_{\boldsymbol{q}\sigma} |FS\rangle\langle FS| c_{\boldsymbol{q}\sigma}$$

high-energy sector

$$P_L \sim \sum_{\sigma} \sum_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} |FS\rangle\langle FS| c_{\boldsymbol{k}\sigma}$$

low-energy sector

effect of downfolding high sector at second order

$$\delta H_L^{(2)} \sim P_L H_\Gamma P_H (\omega - P_H H_0 P_H)^{-1} P_H H_\Gamma P_L$$

electron contribution

$$\begin{aligned} \delta H_L^{(2)} &= -\frac{1}{2}\Gamma^2 \sum_{\boldsymbol{q}} \frac{1}{\omega - \varepsilon_{\boldsymbol{q}}} \boldsymbol{S}_f \cdot \boldsymbol{s}_c(\boldsymbol{0}) + \ldots \\ &\sim \frac{1}{4}\rho(\varepsilon_F)\Gamma^2 \, \frac{\delta D}{D} \boldsymbol{S}_f \cdot \boldsymbol{s}_c(\boldsymbol{0}) + \ldots \end{aligned}$$

scaling equations

thus the Kondo Hamiltonian is modified as follows

$$\begin{aligned} \Gamma &\rightarrow \Gamma' = \Gamma + \delta\Gamma, \\ \frac{\delta\Gamma}{\delta \ln D} &= \frac{1}{2}\rho(\varepsilon_F)\Gamma^2 \end{aligned}$$

scaling equations

$$\Gamma' = \frac{\Gamma}{1 + \frac{1}{2}\rho(\varepsilon_F)\Gamma \ln \frac{D'}{D}}.$$

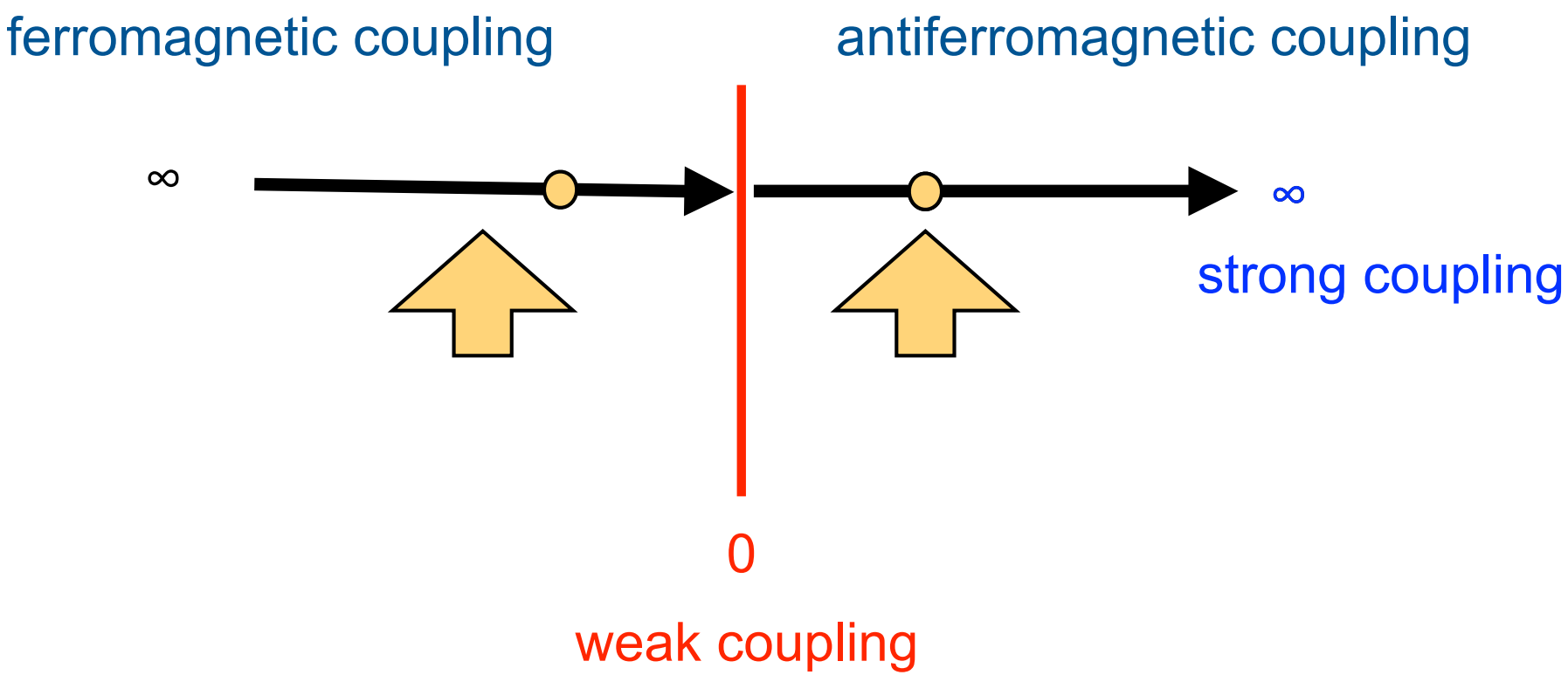
KONDO TEMPERATURE

$$T_k = De^{-2/\rho\Gamma}$$

scaling equations

$$\Gamma \rightarrow \Gamma' = \Gamma + \delta\Gamma,$$

$$\frac{\delta\Gamma}{\delta \ln D} = \frac{1}{2}\rho(\varepsilon_F)\Gamma^2$$



strong-coupling case

one electron screens local moment

spin zero system!

starting point for perturbation theory

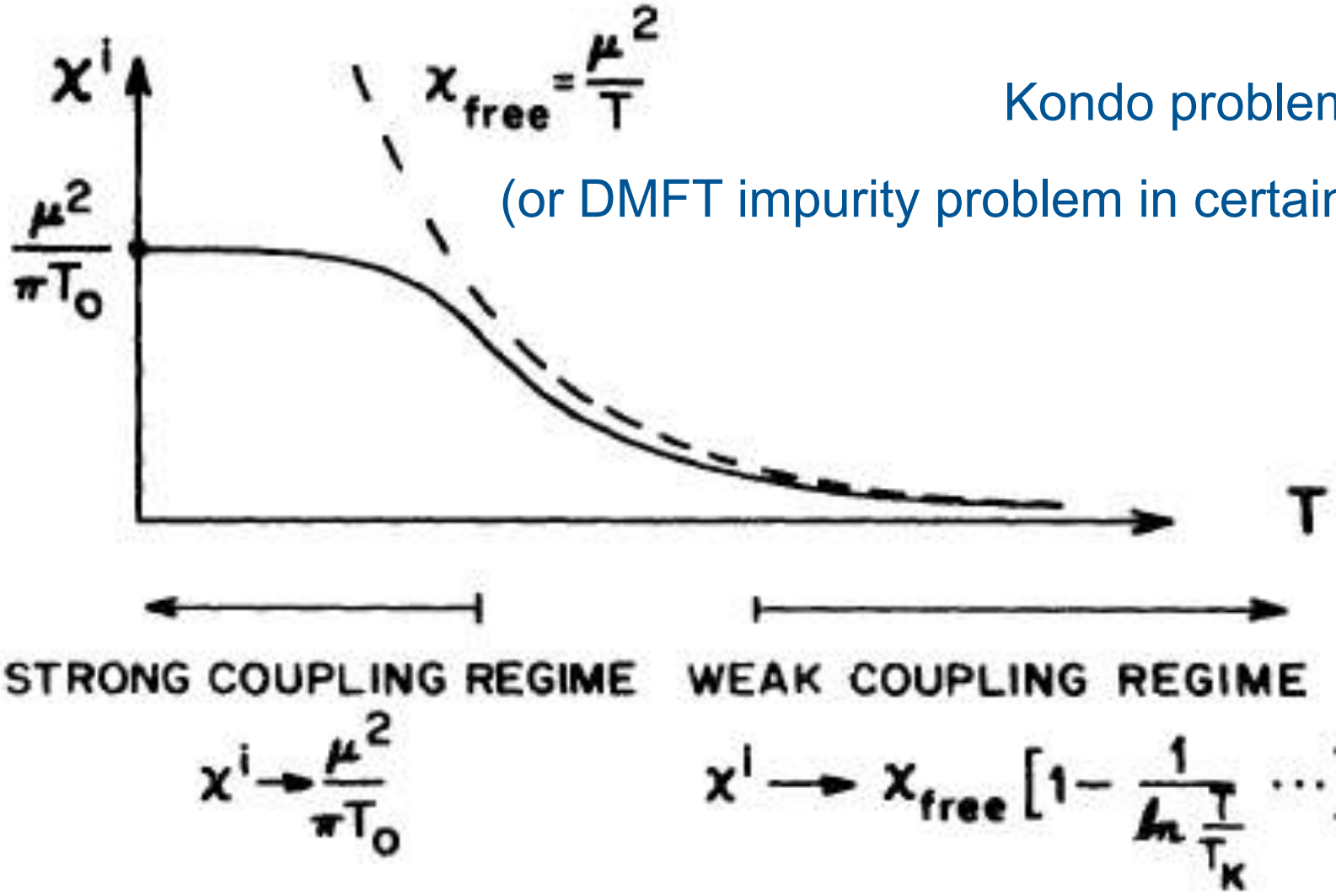
nearby electrons polarize moment via virtual excitations

effective repulsive on-site Coulomb interaction

Nozières Fermi liquid

screening of local moments

linear magnetic susceptibility



Kondo problem

(or DMFT impurity problem in certain regime)

similarities with Hubbard model

local moments vs Fermi-liquid (Curie vs Pauli paramagnetism)

Kondo problem non-perturbative

however with normal baths (flat DOS) metallic….

self-consistency loop

lattice model

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

impurity model (Anderson model)

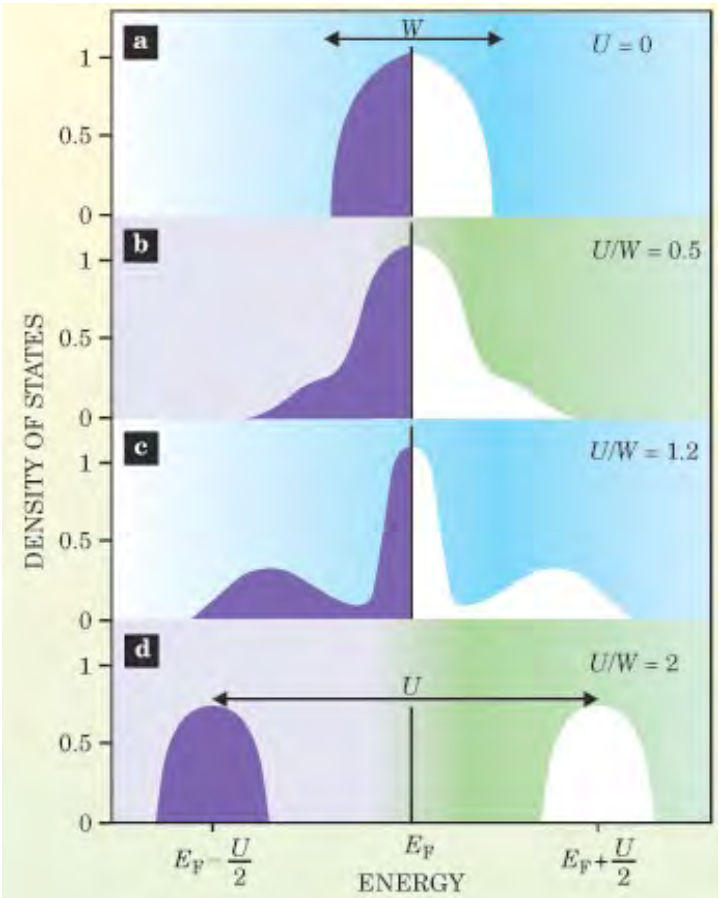
$$H_{\mathrm{A}} = \sum_\sigma \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_\sigma \varepsilon_f n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}$$

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

self-consistency loop

metal-insulator transition

Bethe lattice



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

metallic phase

$$\mathrm{Re}\Sigma(\omega + i0^+) = U/2 + (1 - 1/Z)\omega + O(\omega^3), \qquad (226)$$

$$\mathrm{Im}\Sigma(\omega + i0^+) = -B\omega^2 + O(\omega^4). \qquad (227)$$

The quasiparticle residue Z defines the renormalized Fermi energy of the problem:

$$\epsilon_F^* \equiv ZD \qquad (228)$$

This is also the Kondo temperature of the impurity model. Since the self-energy is momentum independent, Z directly yields the effective mass of quasiparticles (Müller-Hartmann, 1989c):

$$\frac{m^*}{m} = \frac{1}{Z} = 1 - \frac{\partial}{\partial\omega}\,\mathrm{Re}\Sigma(\omega + i0^+)\big|_{\omega=0}. \qquad (229)$$

insulating phase

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

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

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

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

Hartree-Fock vs DMFT

local-moment regime and HF

paramagnetic & ferromagnetic case

Bloch function

$$\Psi_{\boldsymbol{k}\sigma}(\boldsymbol{r}) = \frac{1}{\sqrt{N_s}} \sum_i e^{i\boldsymbol{k}\cdot\boldsymbol{T}_i}\ \Psi_{i\sigma}(\boldsymbol{r})$$

spin scattering function

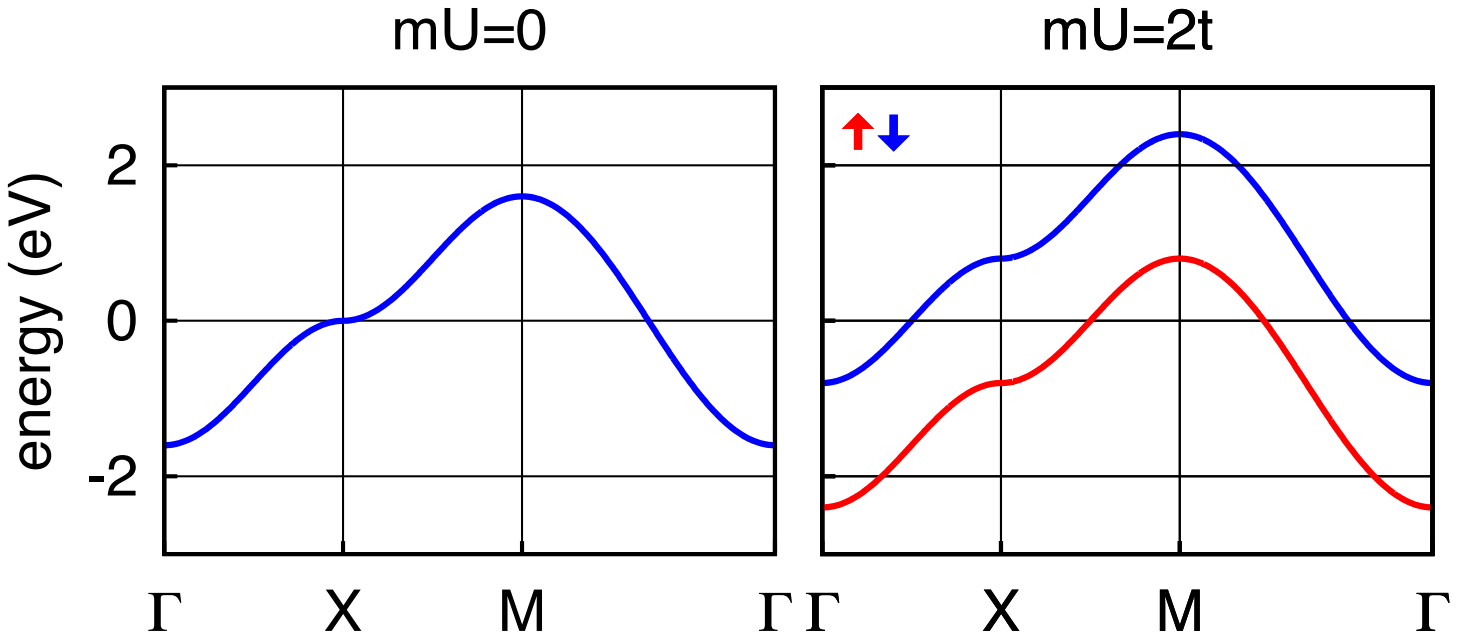
$$S_z(\boldsymbol{k},\boldsymbol{k}') = \frac{1}{N_s} \sum_i e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{T}_i}\ \underbrace{\frac{1}{2}\sum_\sigma \sigma c^\dagger_{i\sigma} c_{i\sigma}}_{S^i_z}$$

ferromagnetic case

Hartree-Fock Hamiltonian and bands

$$H = \sum_{\sigma} \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + U \sum_{\boldsymbol{k}} \left[-2m\, S_z(\boldsymbol{k}, \boldsymbol{k}) + m^2 + \frac{n^2}{4} \right]$$

diagonal in ***k***



Hartree-Fock bands

very large mU case, half filling

spin down band empty, m=1/2

total energy

$$E_{\mathrm{F}} = \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \left[\varepsilon_{\boldsymbol{k}\sigma} - \mu \right] = \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \left[\varepsilon_{\boldsymbol{k}} - \frac{1}{2} U \right] = -\frac{1}{2} U$$

no t^2/U term!

antiferromagnetic case

two sublattices with opposite magnetization +m and -m

$$H_U^{\mathrm{HF}} = \sum_{i\in A}\left[-2mS_z^i + m^2 + \frac{n^2}{4}\right] + \sum_{i\in B}\left[+2mS_z^i + m^2 + \frac{n^2}{4}\right]$$

Bloch function

original lattice

Bloch functions

two sublattices A and B

$$\Psi_{\boldsymbol{k}\sigma}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\left[\Psi^A_{\boldsymbol{k}\sigma}(\boldsymbol{r}) + \Psi^B_{\boldsymbol{k}\sigma}(\boldsymbol{r})\right]$$

$$\Psi^\alpha_{\boldsymbol{k}\sigma}(\boldsymbol{r}) = \frac{1}{\sqrt{N_{s_\alpha}}}\sum_{i_\alpha} e^{i\boldsymbol{T}_i^\alpha\cdot\boldsymbol{k}}\,\Psi_{i_\alpha\sigma}(\boldsymbol{r})$$

antiferromagnetic case

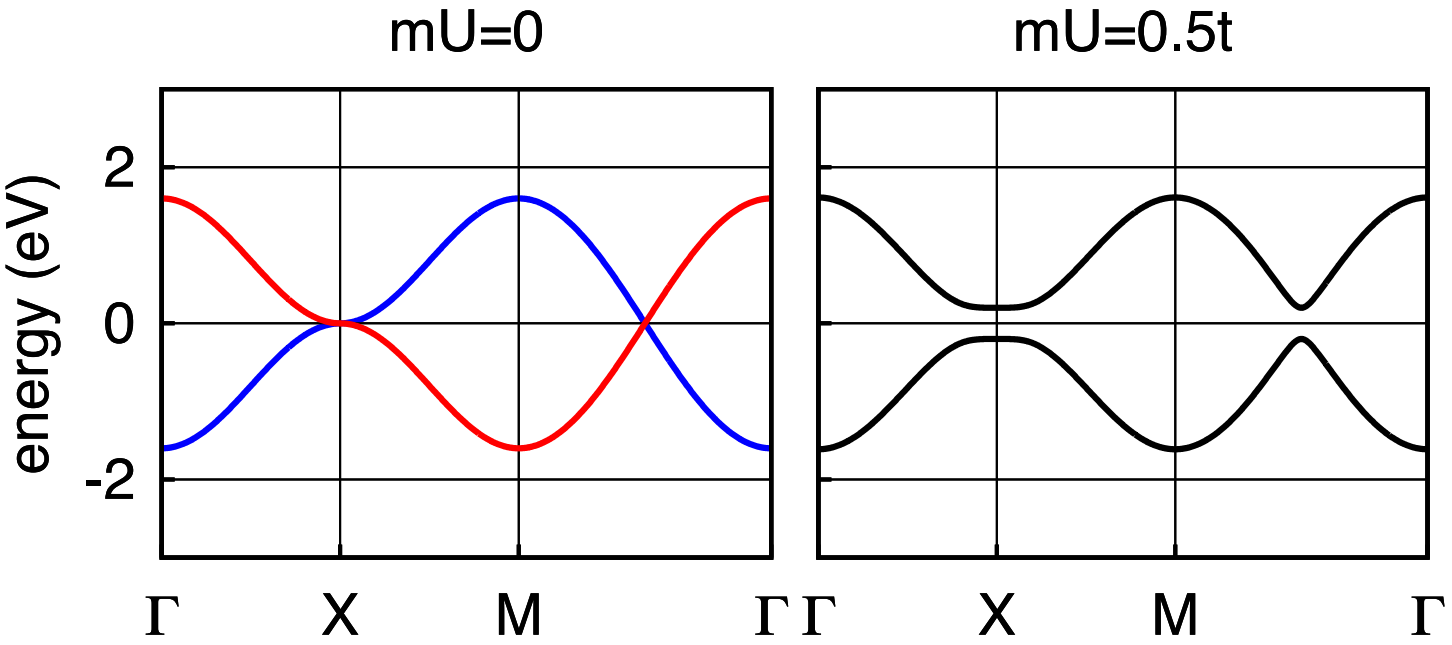
$$
\begin{aligned}
H &= \sum_{\boldsymbol{k}} \sum_{\sigma} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}} \sum_{\sigma} \varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2} n_{\boldsymbol{k}+\boldsymbol{Q}_2\sigma} \\
&+ U \sum_{\boldsymbol{k}} \left[-2m\, S_z(\boldsymbol{k}, \boldsymbol{k}+\boldsymbol{Q}_2) + 2m^2 + 2\frac{n^2}{4} \right]
\end{aligned}
$$

scattering function couples $\boldsymbol{k}$ and $\boldsymbol{k}+\boldsymbol{Q}_2$

$$
\varepsilon_{\boldsymbol{k}\pm} - \mu = \frac{1}{2}(\varepsilon_{\boldsymbol{k}} + \varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2}) \pm \frac{1}{2}\sqrt{(\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2})^2 + 4(mU)^2}
$$

HF bands

antiferromagnetic case



gap: mU

$$\varepsilon_{\boldsymbol{k}\pm} - \mu = \frac{1}{2}(\varepsilon_{\boldsymbol{k}} + \varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2}) \pm \frac{1}{2}\sqrt{(\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2})^2 + 4(mU)^2}$$

HF bands

antiferromagnetic case

very large U case
half-filling, m=1/2

$$\varepsilon_{\boldsymbol{k}-} - \mu \sim -\frac{1}{2}U - \frac{\varepsilon_{\boldsymbol{k}}^2}{U} = -\frac{1}{2}U - \frac{4t^2}{U}\left(\frac{\varepsilon_{\boldsymbol{k}}}{2t}\right)^2$$

total energy

$$E_{\mathrm{AF}} = -\frac{1}{2}U - \frac{4t^2}{U}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}}\left(\frac{\varepsilon_{\boldsymbol{k}}}{2t}\right)^2 \sim -\frac{1}{2}U - \frac{4t^2}{U}$$

energy difference

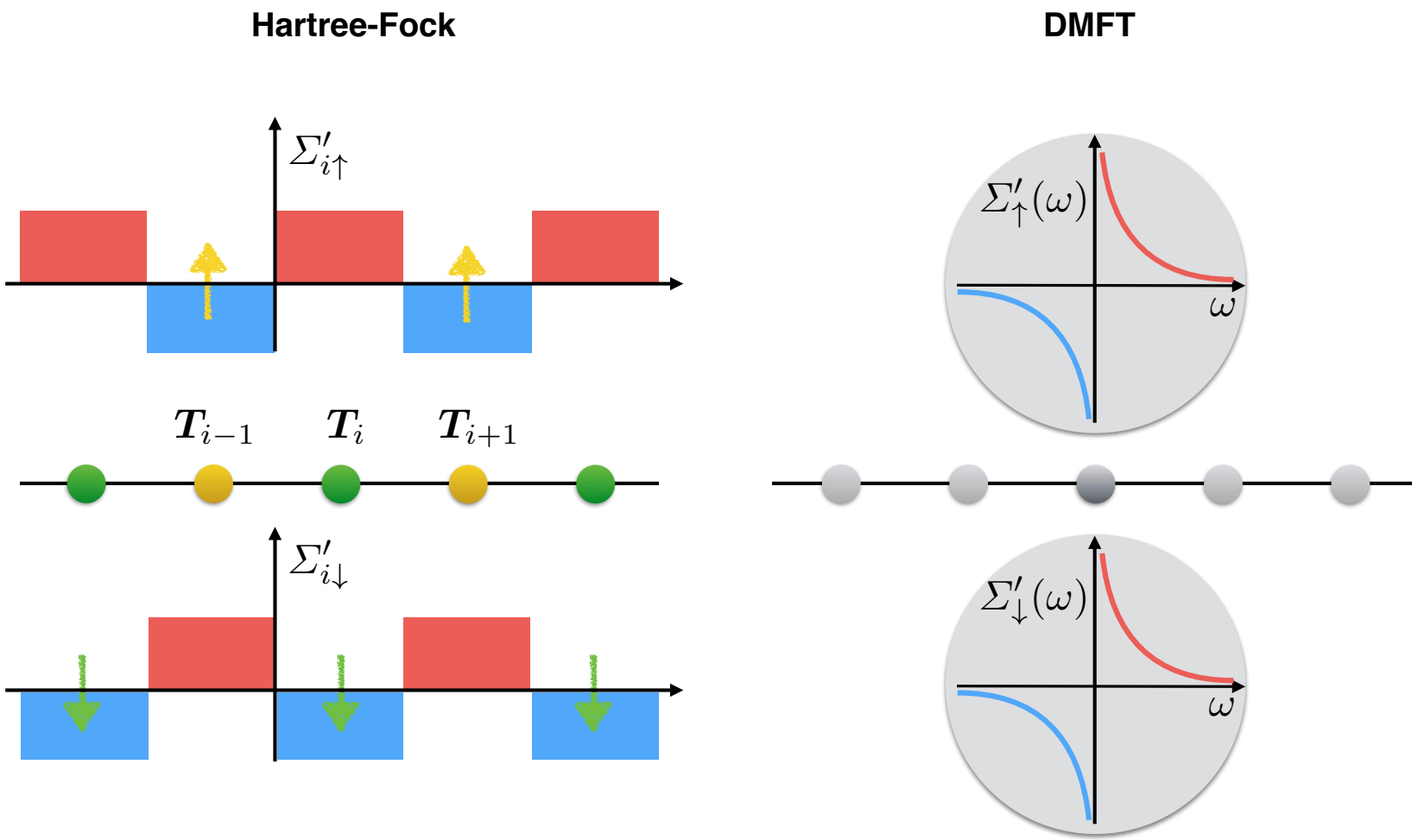
$$\Delta E^{\mathrm{HF}} = E^{\mathrm{HF}}_{\uparrow\uparrow} - E^{\mathrm{HF}}_{\uparrow\downarrow} = \frac{2}{n_{\langle ii' \rangle}} \left[E_{\mathrm{F}} - E_{\mathrm{AF}} \right] \sim \frac{1}{2} \frac{4t^2}{U} \sim \frac{1}{2} \Gamma$$

in this example for this quantity we obtain
the same result as in exact solution!

however, this is not the triplet-singlet splitting

$$\Delta E = E_{S=1} - E_{S=0} = \Gamma$$

Mott transition: HF vs DMFT



LDA+U

LDA+DMFT

DMFT: metallic Fermi-liquid phase

$$\Sigma(\omega) \sim \frac{1}{2}U + \left(1 - \frac{1}{Z}\right)\omega - \frac{i}{2\tau^{\mathrm{QP}}},$$

enhanced m*/m

$$\frac{m^*}{m} \sim \frac{1}{Z} = 1 - \left.\frac{d\Sigma'(\omega)}{d\omega}\right|_{\omega\to 0}$$

note: in HF no such mass enhancement

quasi-particle lifetime

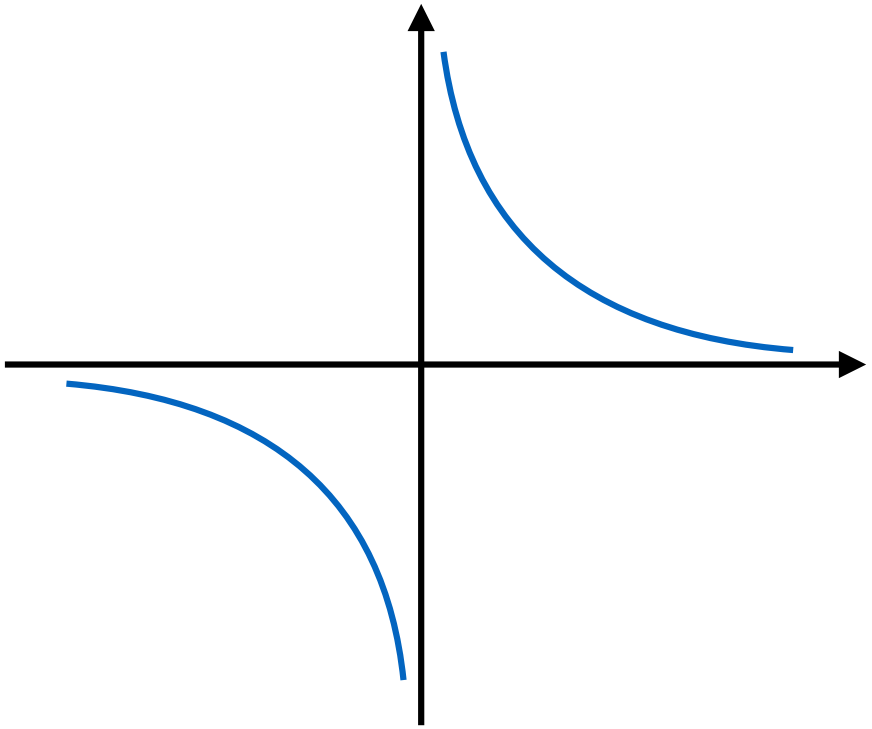
$$\frac{1}{\tau^{\mathrm{QP}}} \sim -2Z\Sigma''(0) \propto (\pi k_B T)^2 + \omega^2.$$

note: in HF life-time is infinite

DMFT: insulating phase

divergence at low frequency

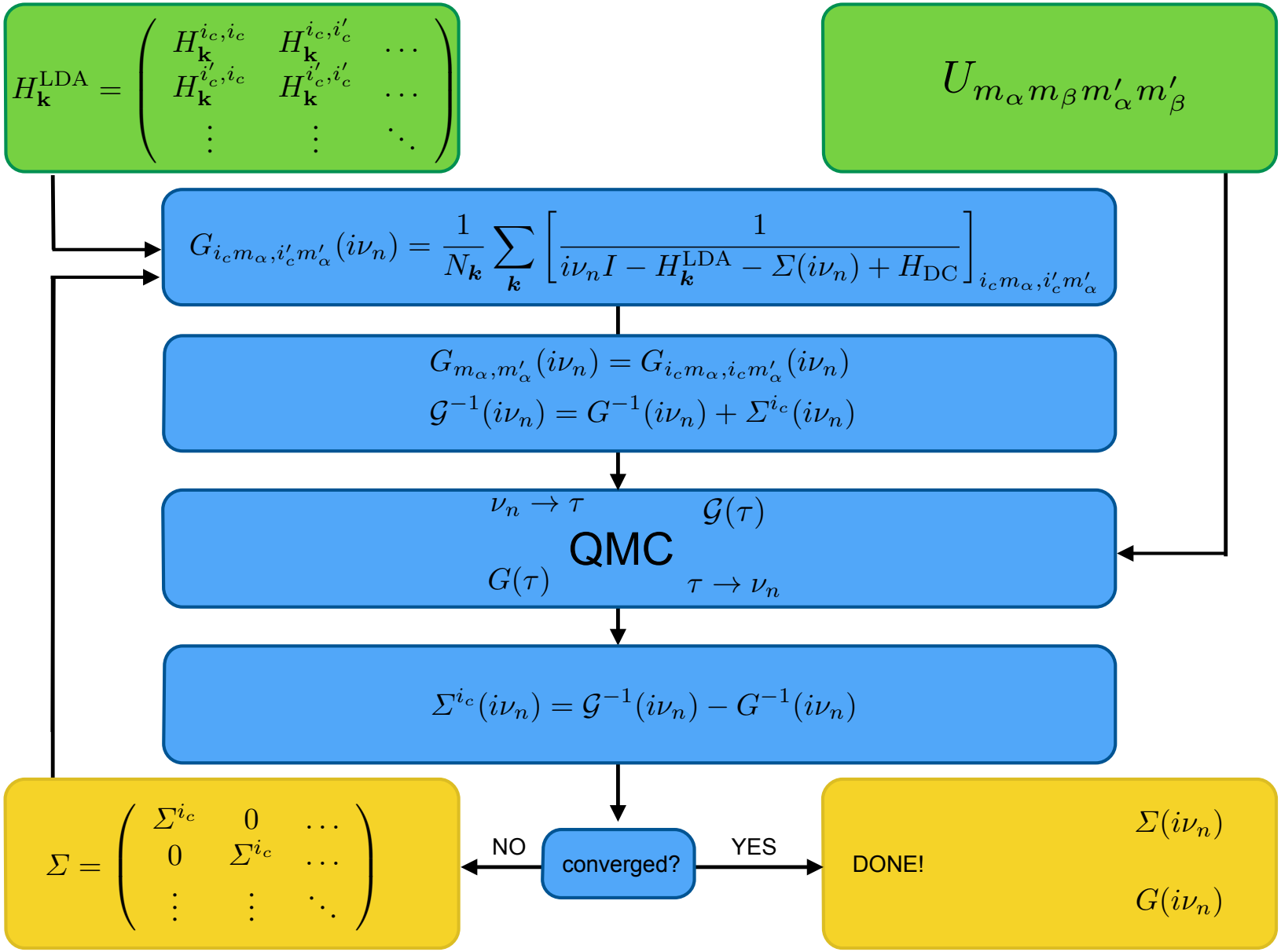
$$\Sigma(\omega) \sim \frac{rU^2}{4}\left[\frac{1}{\omega} - i\pi\delta(\omega) - i f_U(\omega)\right],$$



no such behavior in HF

DFT+DMFT

DFT+DMFT


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

the issue of model building

chosen one electron basis

$$\hat{H}_e = \hat{H}_0 + \hat{H}_U .$$

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

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

$$t^{i,i'}_{n,n'} = -\int d\mathbf{r}\, \overline{\psi_{in\sigma}}(\boldsymbol{r}) \left[-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r}) \right] \psi_{i'n'\sigma}(\boldsymbol{r}),$$

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

the issue of the basis

why Wannier functions ?

can be constructed site-centered

span exactly the one-electron Hamiltonian

they are orthogonal

natural basis for local Coulomb term

flexible, can be used with or without massive downfolding

the issue of the basis

why DFT Wannier functions ?

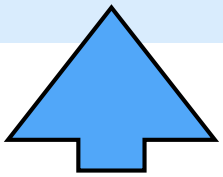
“best” Wannier basis

very good for weakly correlated systems

average and long-range Coulomb effects

information on lattice and chemistry

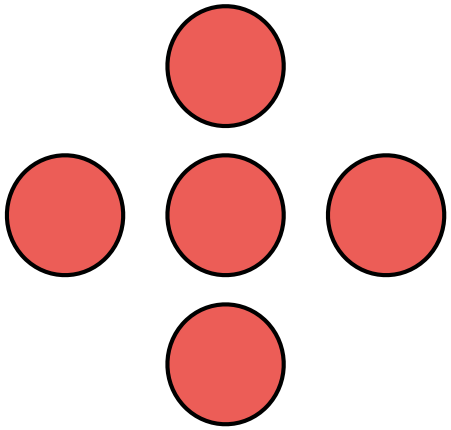
$$\hat{H}_e = \hat{H}_0 + \hat{H}_U \longrightarrow \hat{H}^{\mathrm{LDA}} + \hat{H}_U - \hat{H}_{dc}$$



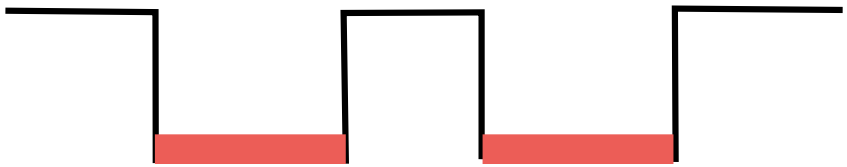
if long range Hartree and mean-field exchange-correlation already are well described by LDA (GGA,..) local

approximated basis

method based on space tiling



easier to embed in DFT codes but inconsistent

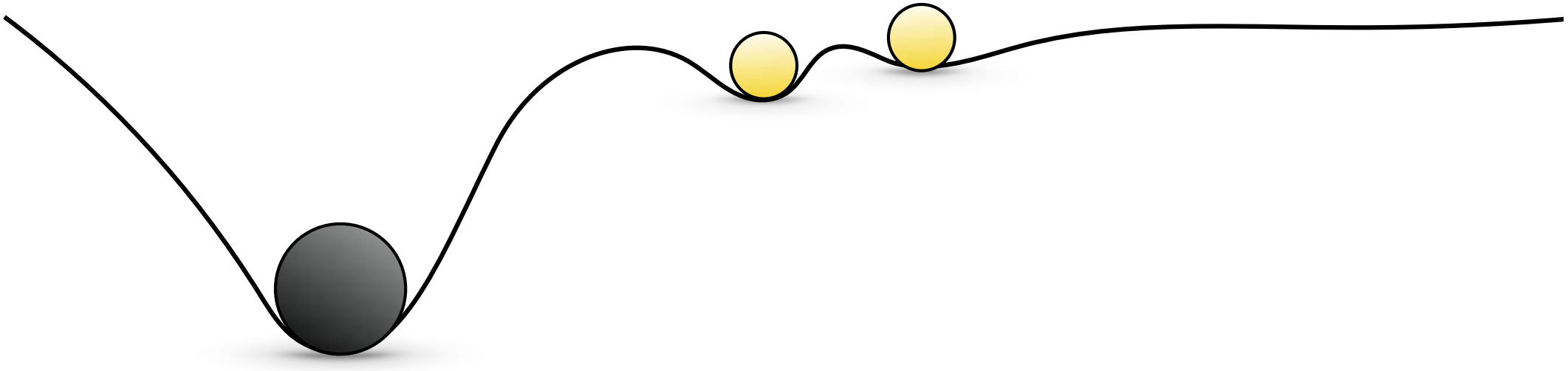


- non-local Coulomb weak ?

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

$$t^{i,i'}_{n,n'} = -\int d\mathbf{r}\, \overline{\psi_{in\sigma}}(\boldsymbol{r}) \left[-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r})\right] \psi_{i'n'\sigma}(\boldsymbol{r}),$$

heavy electrons, light electrons



light electrons → DFT (LDA, GGA,…)

heavy electrons → U correction, DMFT

Hamiltonian after the separation

l shell

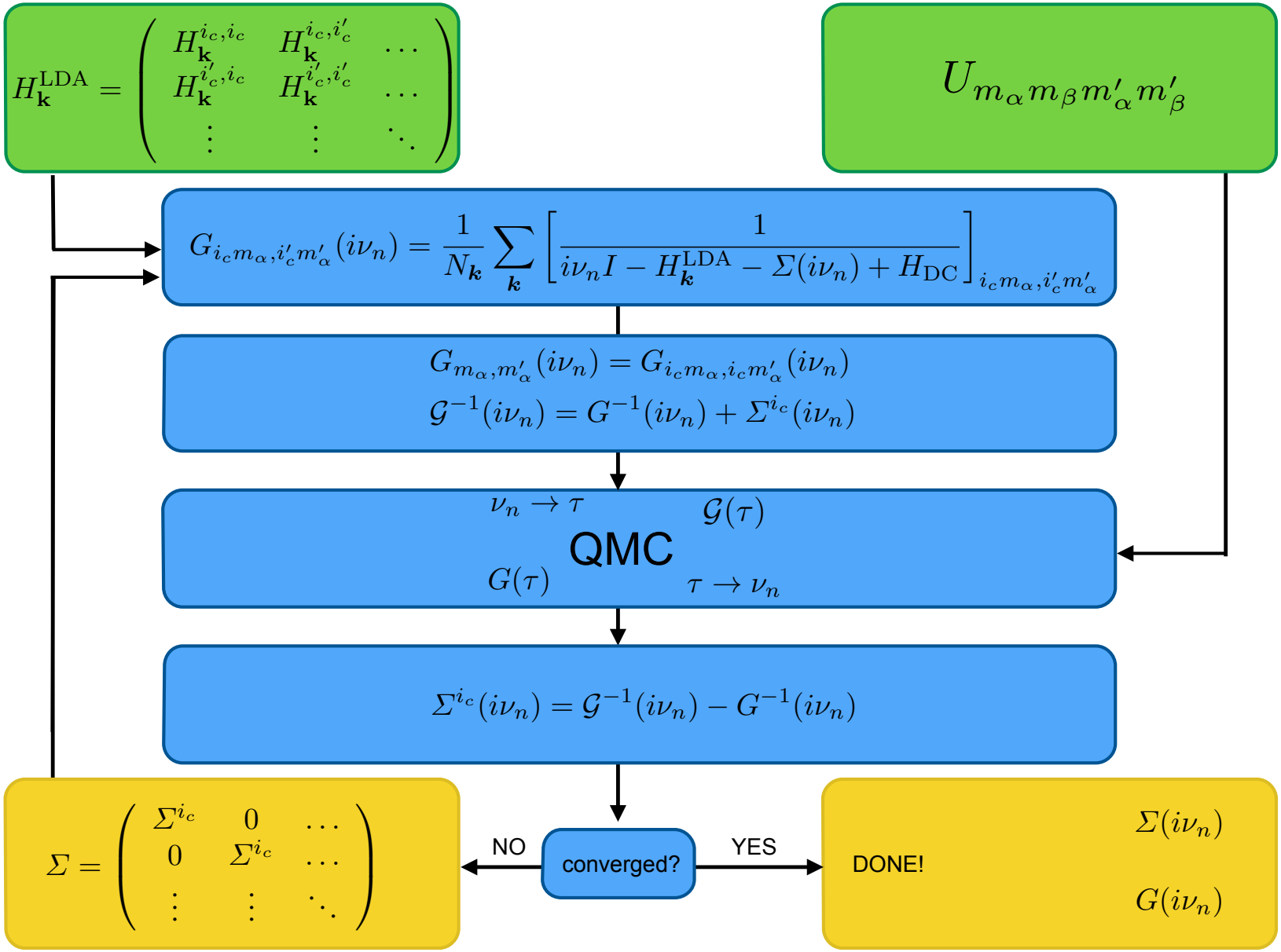
$$\hat{H}_e = \hat{H}^{\mathrm{LDA}} + \hat{H}^l_U - \hat{H}^l_{\mathrm{DC}}.$$

$$\hat{H}^{\mathrm{LDA}} = -\sum_{ii'}\sum_{\sigma}\sum_{m_\alpha m'_\alpha} t^{i,i'}_{m_\alpha,m'_\alpha} c^\dagger_{im_\alpha\sigma} c_{i'm'_\alpha\sigma} = \sum_{\boldsymbol{k}}\sum_{\sigma}\sum_{m_\alpha m'_\alpha} \left[H^{\mathrm{LDA}}_{\boldsymbol{k}}\right]_{m_\alpha,m'_\alpha} c^\dagger_{\boldsymbol{k}m_\alpha\sigma} c_{\boldsymbol{k}m'_\alpha\sigma},$$

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

screening? cRPA, cLDA ?

DFT+DMFT


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

early successes: details matter

mechanism of Mott transition in the series explained

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

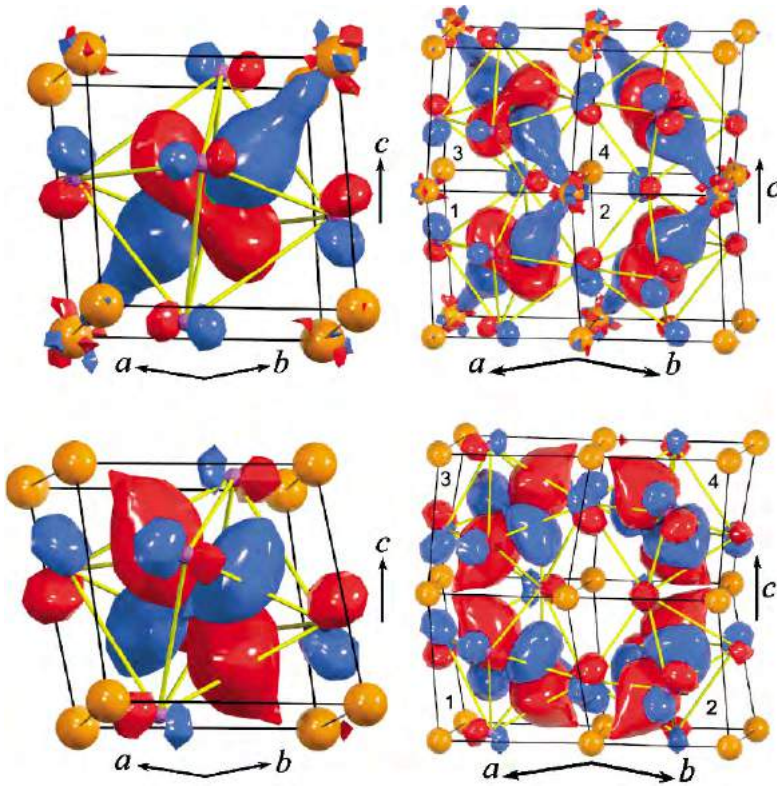
Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites

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

t_{2g}^1

Δ=200-300 meV

LDA+DMFT 770 K



a small crystal field plays a key role

spectral functions

(one-electron Green function)

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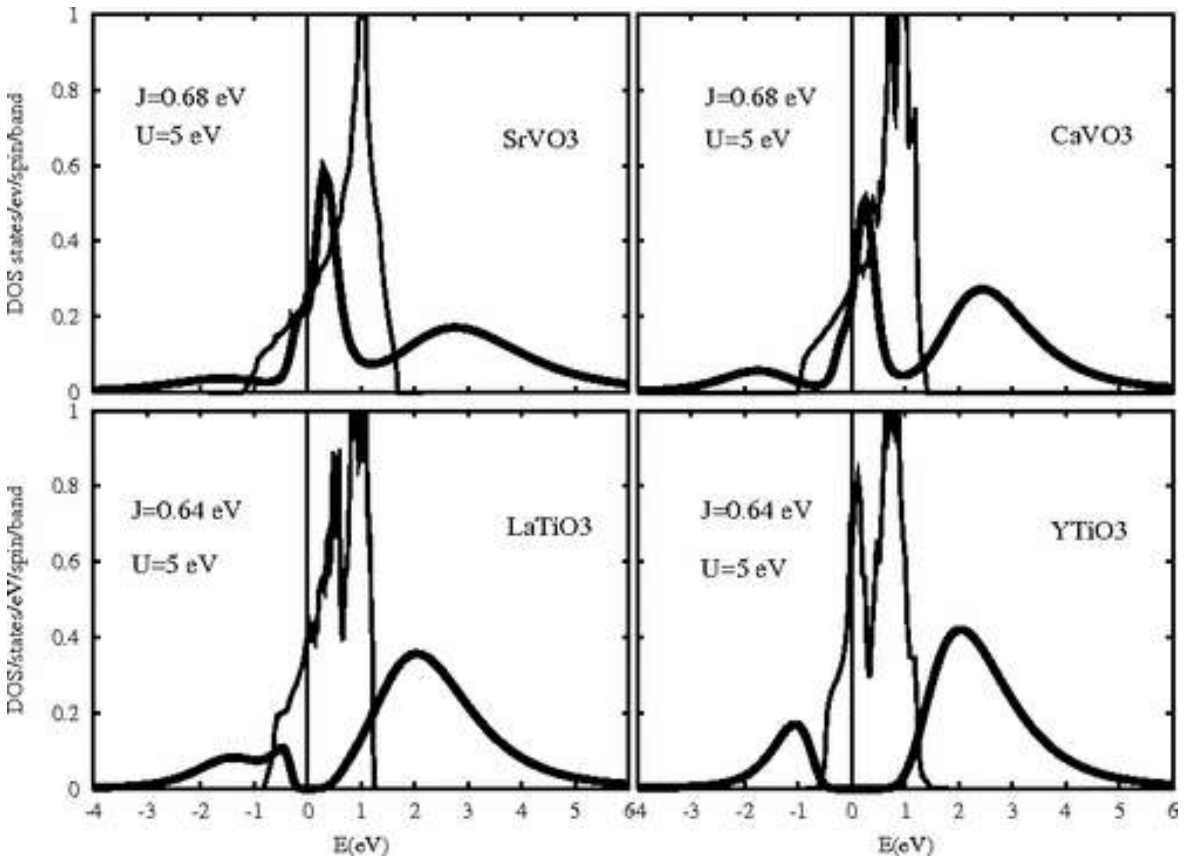


LDA+DMFT with Wannier functions

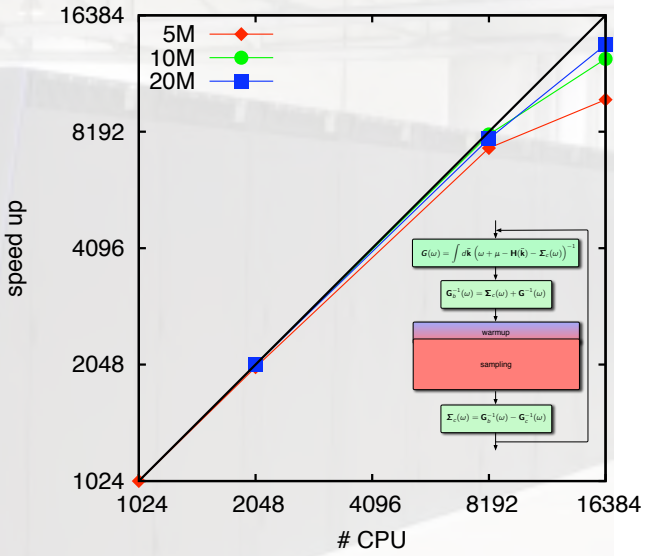
$$
\begin{aligned}
H = & - \sum_{ii'} \sum_{mm'} \sum_{\sigma} t^{ii'}_{mm'} c^{\dagger}_{im\sigma} c_{i'm'\sigma} \\
& + U \sum_{im} n_{im\uparrow} n_{im\downarrow} \\
& + \frac{1}{2} \sum_{im \neq m' \sigma\sigma'} (U - 2J - J\delta_{\sigma\sigma'}) n_{im\sigma} n_{im'\sigma'} \\
& - J \sum_{m \neq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

self-energy matrix spin-orbital space

DMFT and cDMFT

quantum impurity solvers:

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

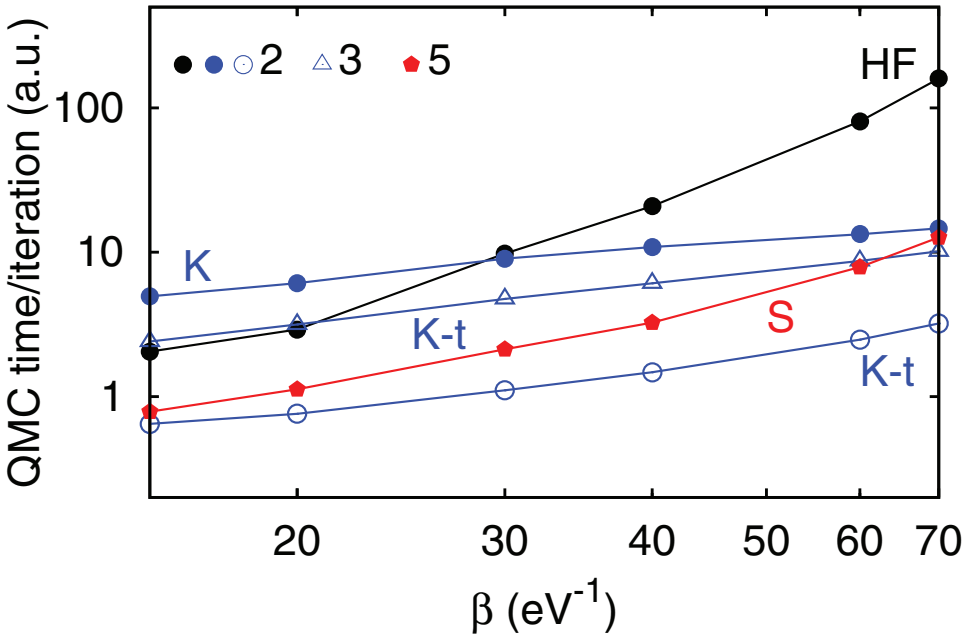


- A. Flesch, E. Gorelov, E. Koch and E. Pavarini
  Multiplet effects in orbital and spin ordering phenomena: A hybridization-expansion quantum impurity solver study
  Phys. Rev. B **87**, 195141 (2013)

JÜLICH
FORSCHUNGSZENTRUM

CT-QMC solver

(performance of our general code on BlueGene)



can include:

full self-energy matrix in spin-orbital space

full Coulomb matrix

spin-orbit

Phys. Rev. B **87**, 195141

t_{2g} full self-energy matrix

full Coulomb matrix

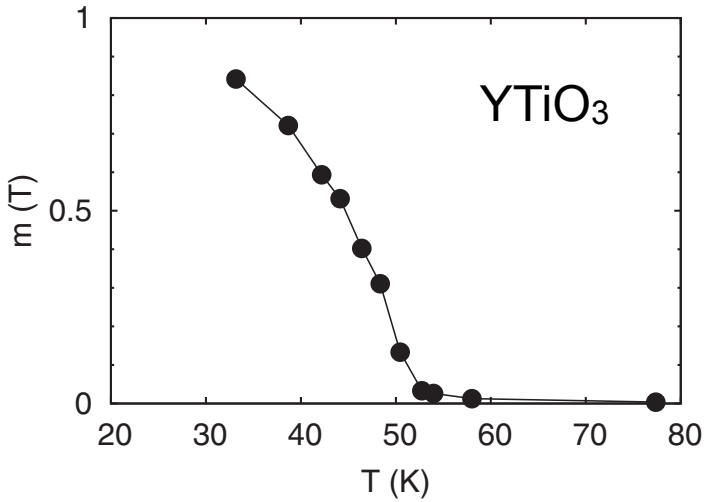


FIG. 3. Ferromagnetic spin polarization as a function of temperature in $YTiO_3$. The plot shows a transition at the critical temperature $T_C \sim 50$ K, slightly overestimating the experimental value $T_C \sim 30$ K, as one might expect from a mean-field calculations.

DFT+U vs DFT+ DMFT

DFT+U

HF, but embedded in DFT

$$\hat{H}^{\mathrm{LDA}} + \hat{U}^{l} - \hat{H}^{l}_{\mathrm{DC}} = \hat{H}^{\mathrm{LDA}} + \frac{1}{2}U \sum_{i} \sum_{m\sigma \neq m'\sigma'} \hat{n}_{im\sigma}\hat{n}_{im'\sigma'} - \frac{1}{2}U \sum_{i} \sum_{m\sigma \neq m'\sigma'} \langle \hat{n}_{im\sigma} \rangle \langle \hat{n}_{im'\sigma'} \rangle$$

HF mean field energy

HF Hamiltonian

$$\hat{H} = \hat{H}^{\mathrm{LDA}} + \sum_{im\sigma} t^{\sigma}_{m} \hat{n}_{im\sigma}, \quad \text{with} \quad t^{\sigma}_{m} = U \left(\frac{1}{2} - \langle \hat{n}_{im\sigma} \rangle \right).$$

what could be the functional?

let us guess the functional

$$E_{\mathrm{LDA+U}}[n] = E_{\mathrm{LDA}}[n] + \sum_i \left[\frac{1}{2} U \sum_{m\sigma \neq m'\sigma'} \langle \hat{n}_{im\sigma} \rangle \langle \hat{n}_{im'\sigma'} \rangle - E_{\mathrm{DC}} \right]$$

$$E_{\mathrm{DC}} = \frac{1}{2} U N^l (N^l - 1)$$

$$\varepsilon_{im\sigma}^{\mathrm{LDA+U}} = \frac{\partial E_{\mathrm{LDA+U}}}{\partial \langle \hat{n}_{im\sigma} \rangle} = \varepsilon_{im\sigma}^{\mathrm{LDA}} + U \left(\frac{1}{2} - \langle \hat{n}_{im\sigma} \rangle \right) = \varepsilon_{im\sigma}^{\mathrm{LDA}} + t_m^{\sigma}.$$

generalization

$$E_{\mathrm{LDA+U}}[n] = E_{\mathrm{LDA}}[n] + \frac{1}{2}\sum_{i\sigma}\sum_{mm'm''m'''} U_{mm''m'm'''}\langle\hat{n}^{\sigma}_{imm'}\rangle\langle\hat{n}^{-\sigma}_{im''m'''}\rangle$$

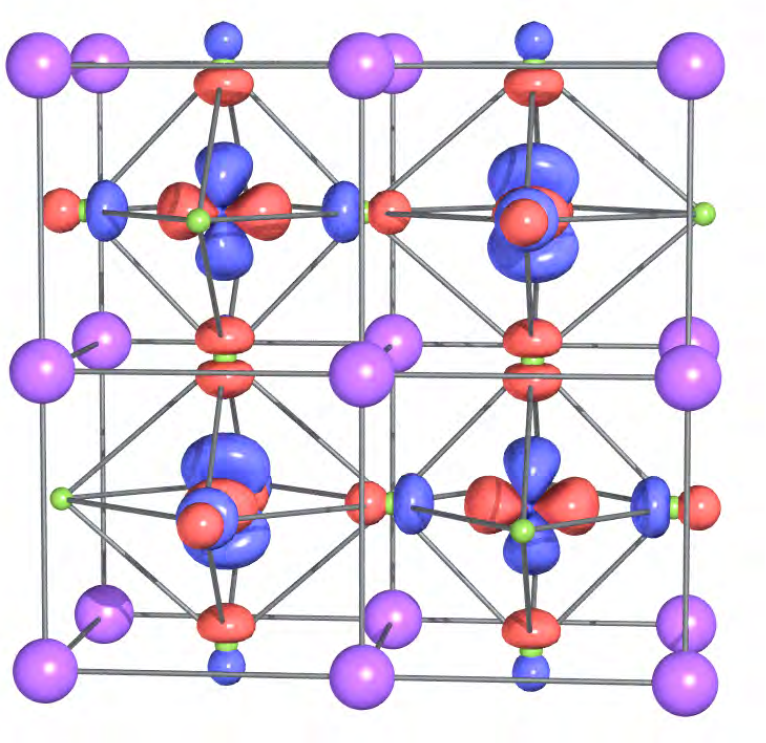
$$+\frac{1}{2}\sum_{i\sigma}\sum_{mm'm''m'''}\left[U_{mm''m'm'''} - U_{mm''m'''m'}\right]\langle\hat{n}^{\sigma}_{imm'}\rangle\langle\hat{n}^{\sigma}_{im''m'''}\rangle - E_{\mathrm{DC}}$$

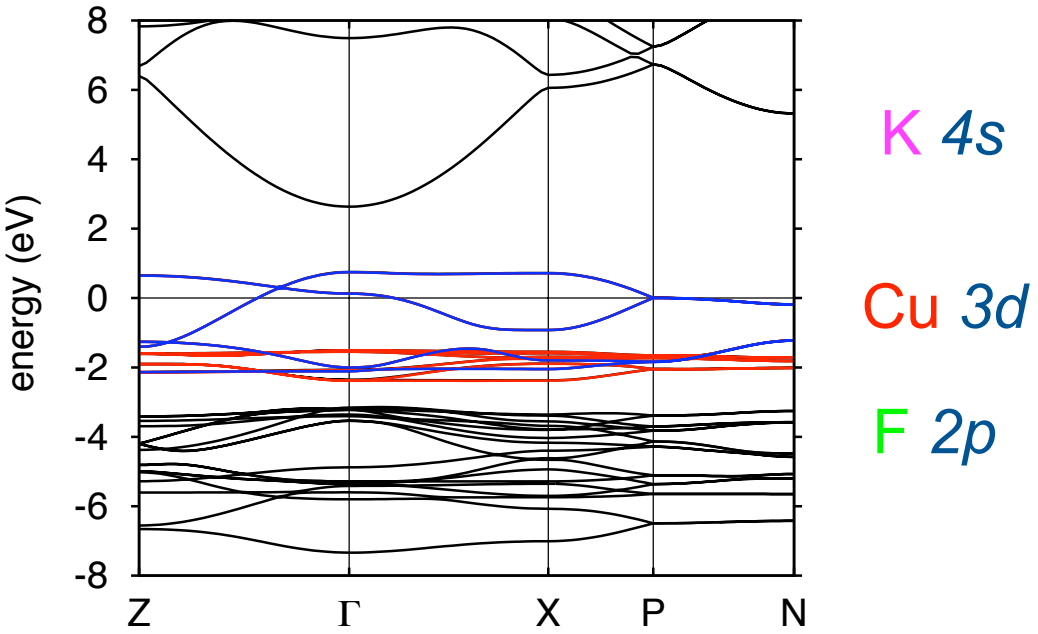
for DC correction several approx

$$E_{\mathrm{DC}} = \frac{1}{2}U_{\mathrm{avg}}N^{l}(N^{l}-1) - \frac{1}{2}J_{\mathrm{avg}}\sum_{\sigma}N^{l}_{\sigma}(N^{l}_{\sigma}-1),$$

an example: $KCuF_3$

nature: e_g^3 insulator, paramagnetic above 40 K, orbitally ordered





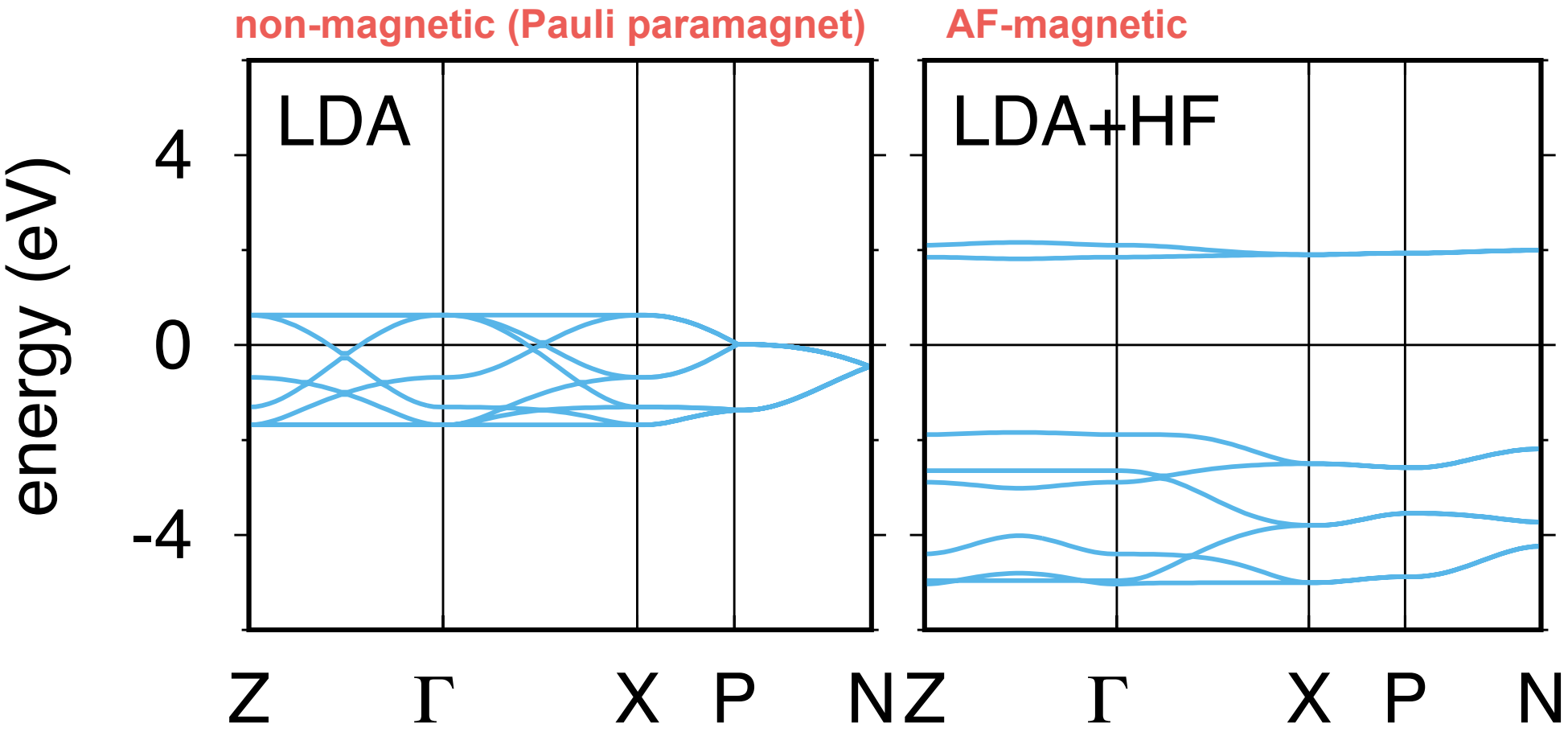
LDA: metallic, no orbital order

$KCuF_3$

shown e_g bands only

LDA+HF: insulator BUT only with orbital AND spin order

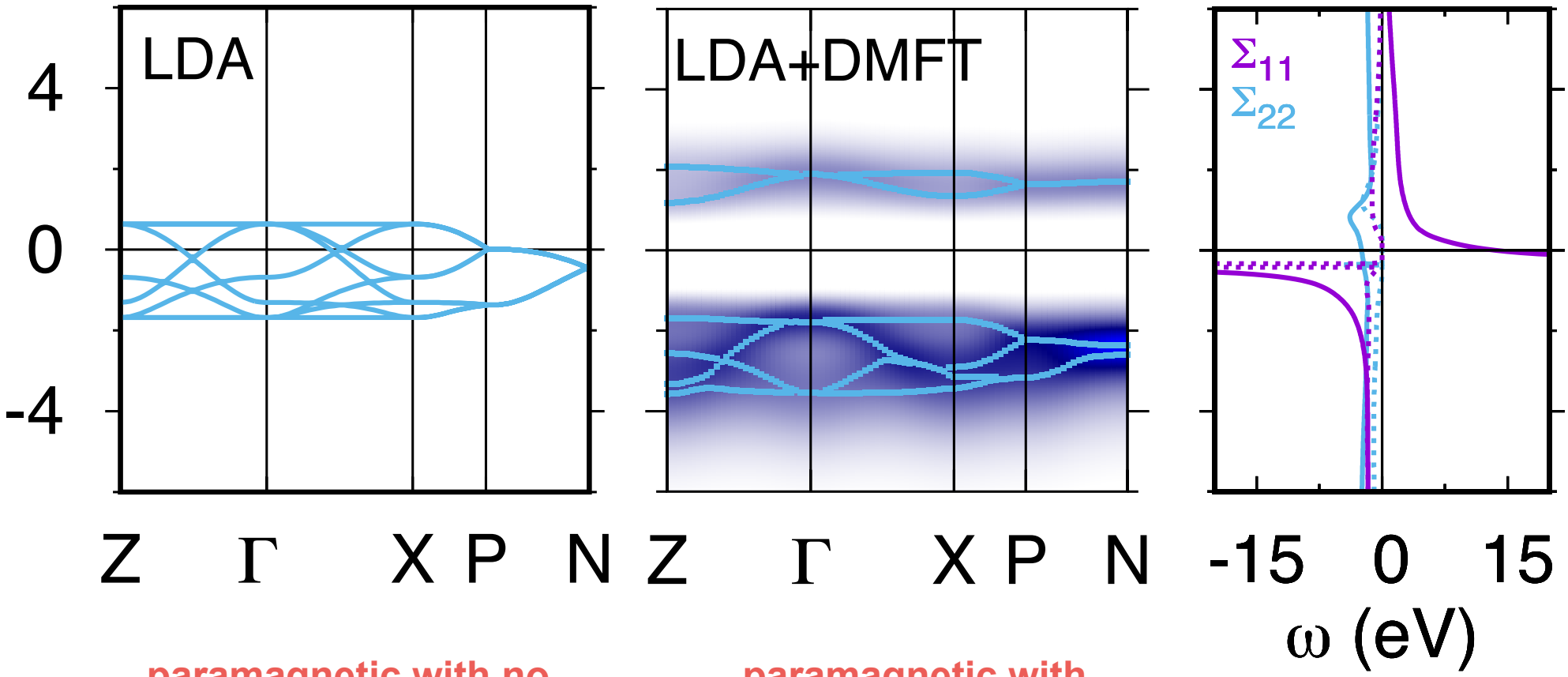
$T_N = T_{OO} = T_{MIT}$



$KCuF_3$

LDA+DMFT: orbital and spin order not needed

$T_N < T_{OO} < T_{MIT}$

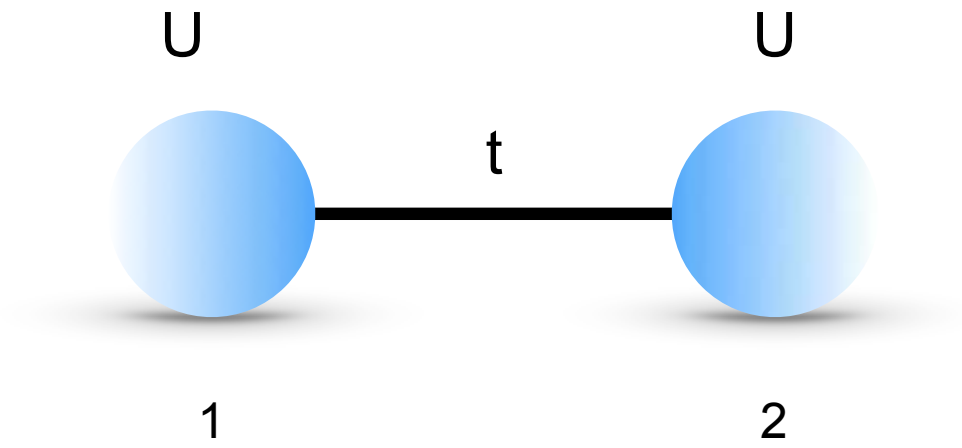


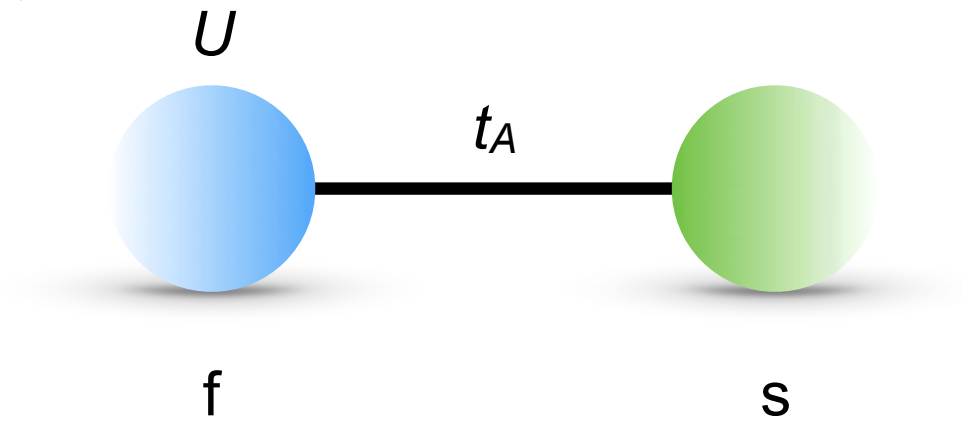
paramagnetic with no local moments

paramagnetic with local moments

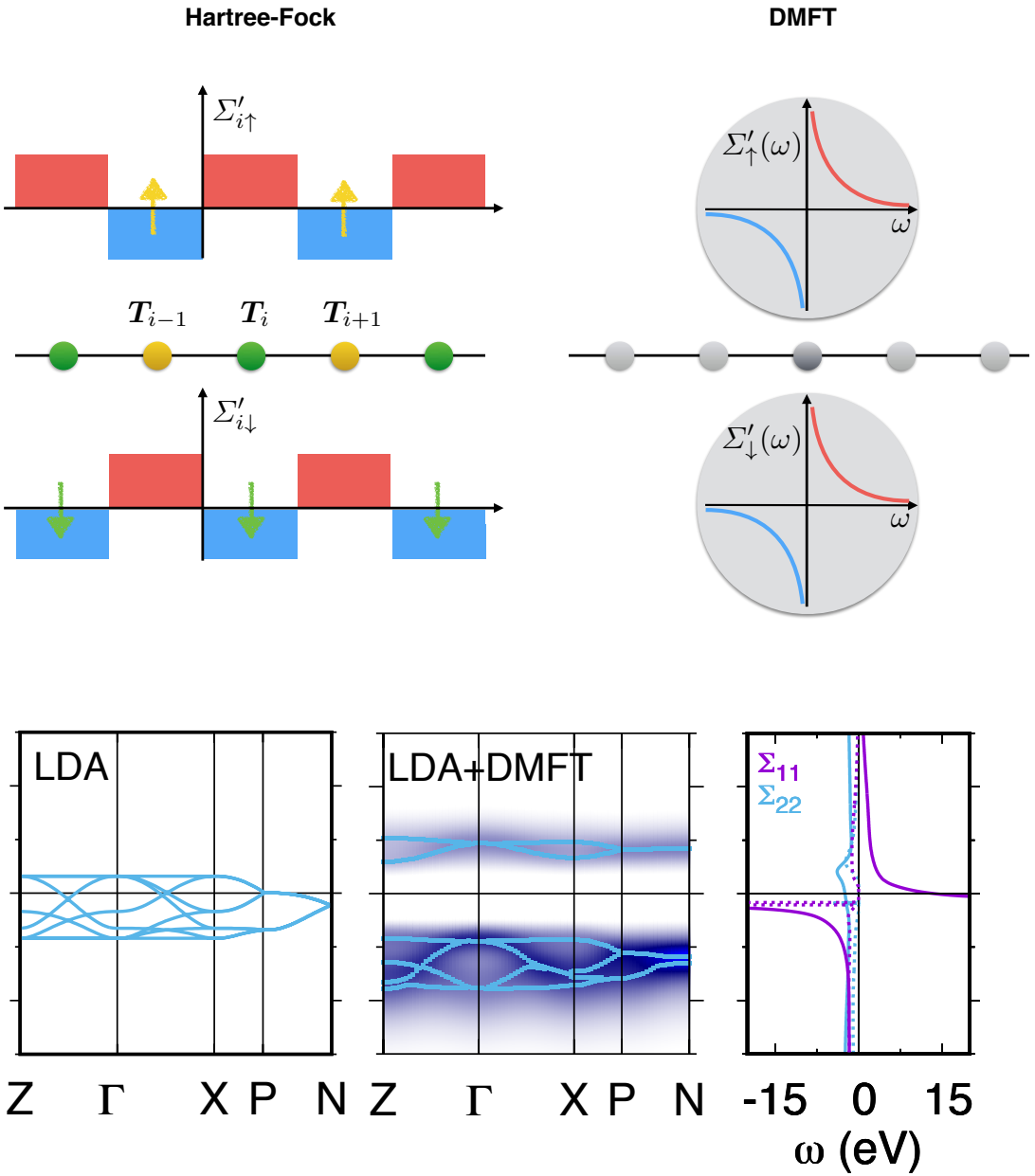
conclusions

- simple models
  - Hubbard dimer (HD)
  - Anderson molecule (AM)
- conclusions
  - self-energy HD non local
  - non-local Coulomb reduce correlations
  - local G similar for HD and AM
  - Hartree-Fock: static approximation
  - self-consistent AM as dynamical approx?





- models
  - Hubbard model
  - Anderson model
- methods
  - DMFT and DFT+DMFT
  - Hartree-Fock and DFT+U
- metal-insulator transition
  - Hartree-Fock vs DMFT
  - DFT+U vs DFT+DMFT



predictive power?

emergent behavior

The effectiveness of this message may be indicated by the fact that I heard it quoted recently by a leader in the field of materials science, who urged the participants at a meeting dedicated to "fundamental problems in condensed matter physics" to accept that there were few or no such problems and that nothing was left but extensive science, which he seemed to equate with device engineering.

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

4 August 1972, Volume 177, Number 4047

Philp Warren Anderson

Nobel Prize in Physics 1977

SCIENCE

http://www.emergentuniverse.org/

thank you!