“w2dynamics”: operation and applications

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ERC Kick-off Meeting, 2.9.2013

Hackers

- Nico Parragh (Uni Wü)
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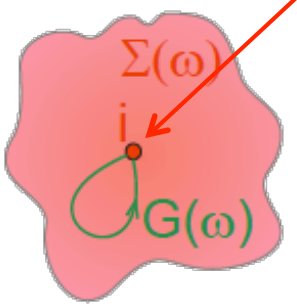
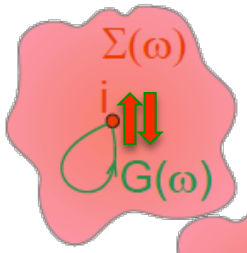
- Patrik Gunacker (TU)
- Andreas Hausoel (Uni Wü)

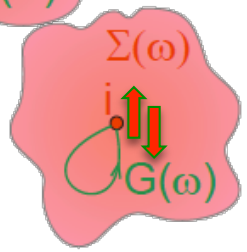
A solver for multi-orbital problems

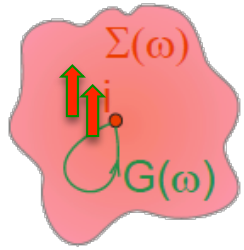
- For LDA+DMFT we need to solve an Anderson model containing one correlated impurity site, with typically several *d*-orbitals

$a = 1, \ldots, N_{orb}$









$$\mathcal{H}_{loc} = \sum_a U n_{a,\uparrow} n_{a,\downarrow}$$

$$+ \sum_{a>b,\sigma} \left[U' n_{a,\sigma} n_{b,-\sigma} + (U' - J) n_{a,\sigma} n_{b,\sigma} \right]$$

$$- \sum_{a \neq b} J (c^\dagger_{a,\downarrow} c^\dagger_{b,\uparrow} c_{b,\downarrow} c_{a,\uparrow} + c^\dagger_{b,\uparrow} c^\dagger_{b,\downarrow} c_{a,\uparrow} c_{a,\downarrow} + h.c.)$$

"spin-flip" "pair-hopping"

Hybridization-expansion

- the best continuous-time quantum Monte Carlo scheme to solve impurity models with complicated interactions (as e.g. the Kanamori Hamiltonian) is the hybridization-expansion ("CT-HYB")

terms leading to a bad sign problem in "BSS"/"Hirsch-Fye"-QMC

$$\mathcal{H}_{loc} = \sum_a U n_{a,\uparrow} n_{a,\downarrow} \qquad a = 1, ..., N_{orb}$$

$$+ \sum_{a>b,\sigma} \left[U' n_{a,\sigma} n_{b,-\sigma} + (U' - J) n_{a,\sigma} n_{b,\sigma} \right]$$

$$- \sum_{a \neq b} J (c^\dagger_{a,\downarrow} c^\dagger_{b,\uparrow} c_{b,\downarrow} c_{a,\uparrow} + c^\dagger_{b,\uparrow} c^\dagger_{b,\downarrow} c_{a,\uparrow} c_{a,\downarrow} + h.c.)$$

"spin-flip" "pair-hopping"

References

- hybridization expansion
  - P. Werner, *et al.*, Phys. Rev. Lett. **97**, 076405 (2006)
  - P. Werner and A. J. Millis, Phys. Rev. B **74**, 155107 (2006)
  - K. Haule, Phys. Rev B **75**, 155113 (2007)
  - E. Gull, *et al.*, Rev. Mod. Phys. **83**, 349 (2011)
  - N. Parragh, *et al.*, Phys. Rev. B **86**, 155158 (2012)
- hybridization expansion - Krylov
  - A. M. Laeuchli and P. Werner, Phys. Rev. B **76**, 035116 (2007)
  - T. J. Park and J. C. Light, J. Chem. Phys. **85**, 5870 (1986)
- Legendre representation
  - L. Boehnke, *et al.*, Phys. Rev. B **84**, 075145 (2011)

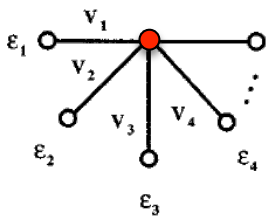
The impurity-model (AIM) to be solved

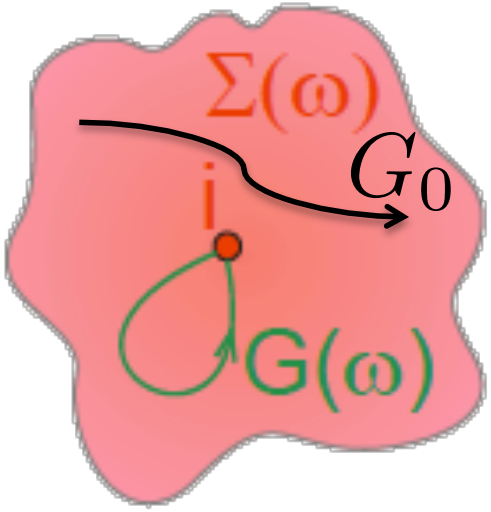
FROM SOMEWHERE → $F(\tau)$ or, equivalently $F(i\omega_n)$

$$G_0^{-1}(i\omega_n) = i\omega_n + \mu - F(i\omega_n)$$

In Exact Diagonalization :

$$F(i\omega_n) = \sum_l \frac{V_l^2}{i\omega_n - \varepsilon_l}$$



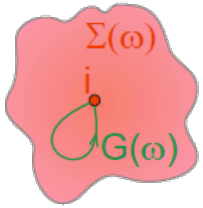


CT-HYB calculation → $F(\tau)$, $\mathcal{H}_{loc}$

Hybridization expansion

- Hamiltonian of the full Anderson model $\mathcal{H} = \mathcal{H}_{loc} + \mathcal{H}_{bath} + \mathcal{H}_{hyb}$

interaction picture



$$\mathcal{H}_{hyb} = \sum_{l} \left(V_l^{\alpha} c_{\alpha}^{\dagger} a_l + V_l^{\alpha *} a_l^{\dagger} c_{\alpha} \right)$$

"perturbation"

- expansion in the hybridization

$$Z = \sum_k \frac{1}{k!} \int_0^{\beta} d\tau_1 \cdots \int_0^{\beta} d\tau_k' \sum_{\alpha_1 \cdots \alpha_k} \sum_{\alpha_1' \cdots \alpha_k'} \sum_{l_1 \cdots l_k} \sum_{l_1' \cdots l_k'} V_{l_1}^{\alpha_1} V_{l_1'}^{\alpha_1' *} V_{l_k}^{\alpha_k} V_{l_k'}^{\alpha_k' *}$$

$$\times \mathrm{Tr}_c \left[e^{-\beta \mathcal{H}_{loc}} T c_{\alpha_k}(\tau_k) c_{\alpha_k'}^{\dagger}(\tau_k') \cdots c_{\alpha_1}(\tau_1) c_{\alpha_1'}^{\dagger}(\tau_1') \right]$$

"brute force"

$$\times \mathrm{Tr}_a \left[e^{-\beta \mathcal{H}_{bath}} T a_{l_k}^{\dagger}(\tau_k) a_{l_k'}(\tau_k') \cdots a_{l_1}^{\dagger}(\tau_1) a_{l_1'}(\tau_1') \right]$$

"analytically": *F(τ)*

Sampling the local trace

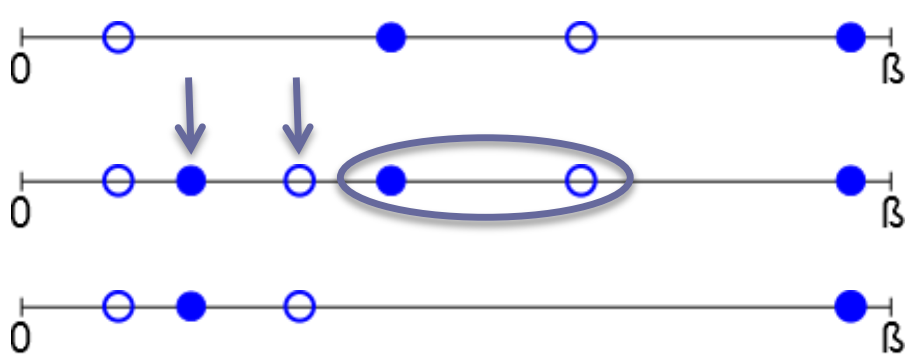
$$\mathcal{H}_{loc} = \sum_a U n_{a,\uparrow} n_{a,\downarrow} + \sum_{a>b,\sigma} \left[U' n_{a,\sigma} n_{b,-\sigma} + (U' - J) n_{a,\sigma} n_{b,\sigma} \right] - \sum_{a \neq b} J (c^\dagger_{a,\downarrow} c^\dagger_{b,\uparrow} c_{b,\downarrow} c_{a,\uparrow} + c^\dagger_{b,\uparrow} c^\dagger_{b,\downarrow} c_{a,\uparrow} c_{a,\downarrow} + h.c.)$$

$$\mathrm{Tr}_c \left[e^{-\beta \mathcal{H}_{loc}} T c_{\alpha_k}(\tau_k) c^\dagger_{\alpha'_k}(\tau'_k) \cdots c_{\alpha_1}(\tau_1) c^\dagger_{\alpha'_1}(\tau'_1) \right]$$

after warmup

insertion

removal

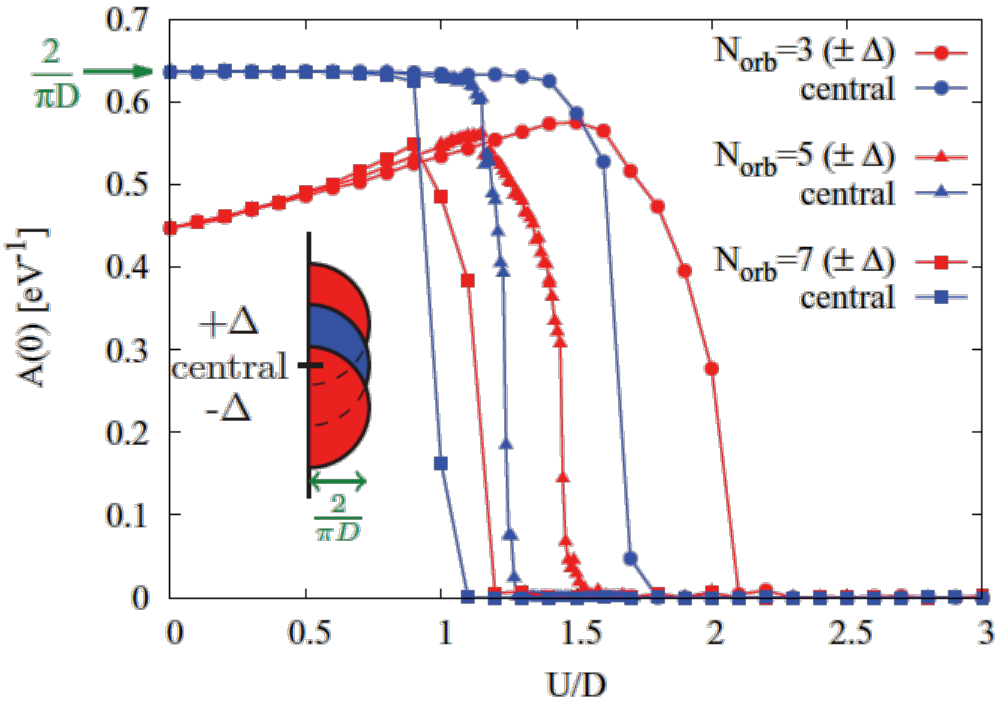


One flavor of creation/ annihilation operators

generalization to multiple flavors

Advantages of the Krylov scheme

- 7 orbitals with Kanamori interaction doable with Krylov!



N. Parragh, *et al.*,
PRB **86**, 155158 (2012)

- other CT-HYB scheme (so-called "matrix-matrix"):
  - cheap exact time evolution (basis is the eigenbasis of $\mathcal{H}_{loc}$)
  - matrix representation of annihilation/creation operators

Krylov implementation

- bottleneck:
  computation of the "local trace":

$$\mathrm{Tr}_c \left[\mathrm{e}^{-\beta \mathcal{H}_{loc}} c_{\alpha_k}(\tau_k) c^\dagger_{\alpha'_k}(\tau'_k) \cdots c_{\alpha_1}(\tau_1) c^\dagger_{\alpha'_1}(\tau'_1) \right]$$

β ... 0

- our basis: occupation numbers

eigenvectors of H_{loc}
example for 1 orbital

$\{ |0\rangle,\ |\uparrow\rangle,\ |\downarrow\rangle,\ |\uparrow\downarrow\rangle \}$

sparse matrix in our basis
eff. matrix-vector product

$$\cdots \quad \mathrm{e}^{\tau'_1 \mathcal{H}_{loc}} \quad c^\dagger_{\alpha'_1} \quad \mathrm{e}^{-\tau'_1 \mathcal{H}_{loc}} \quad |\phi_0\rangle$$

with Lanczos

$$\mathrm{e}^{-\tau \mathcal{H}_{loc}} |v\rangle \simeq \sum_{k=0}^{p-1} \frac{(-\tau)^k}{k!} \mathcal{H}^k_{loc} |v\rangle$$

- how many outer states are needed for the computation of the trace?
- how to keep the matrix-size as small as possible?

How many outer states?

$$\mathrm{Tr}_c\left[e^{-\beta\mathcal{H}_{loc}}Tc_{\alpha_k}(\tau_k)c^\dagger_{\alpha'_k}(\tau'_k)\cdots c_{\alpha_1}(\tau_1)c^\dagger_{\alpha'_1}(\tau'_1)\right] =$$

$$= \langle\phi_0|e^{-\beta E^{(0)}_{loc}}\ldots|\phi_0\rangle + \underbrace{e^{-\beta(E^{(1)}_{loc}-E^{(0)}_{loc})}} \cdot \langle\phi_1|e^{-\beta E^{(0)}_{loc}}\ldots|\phi_1\rangle + \ldots$$

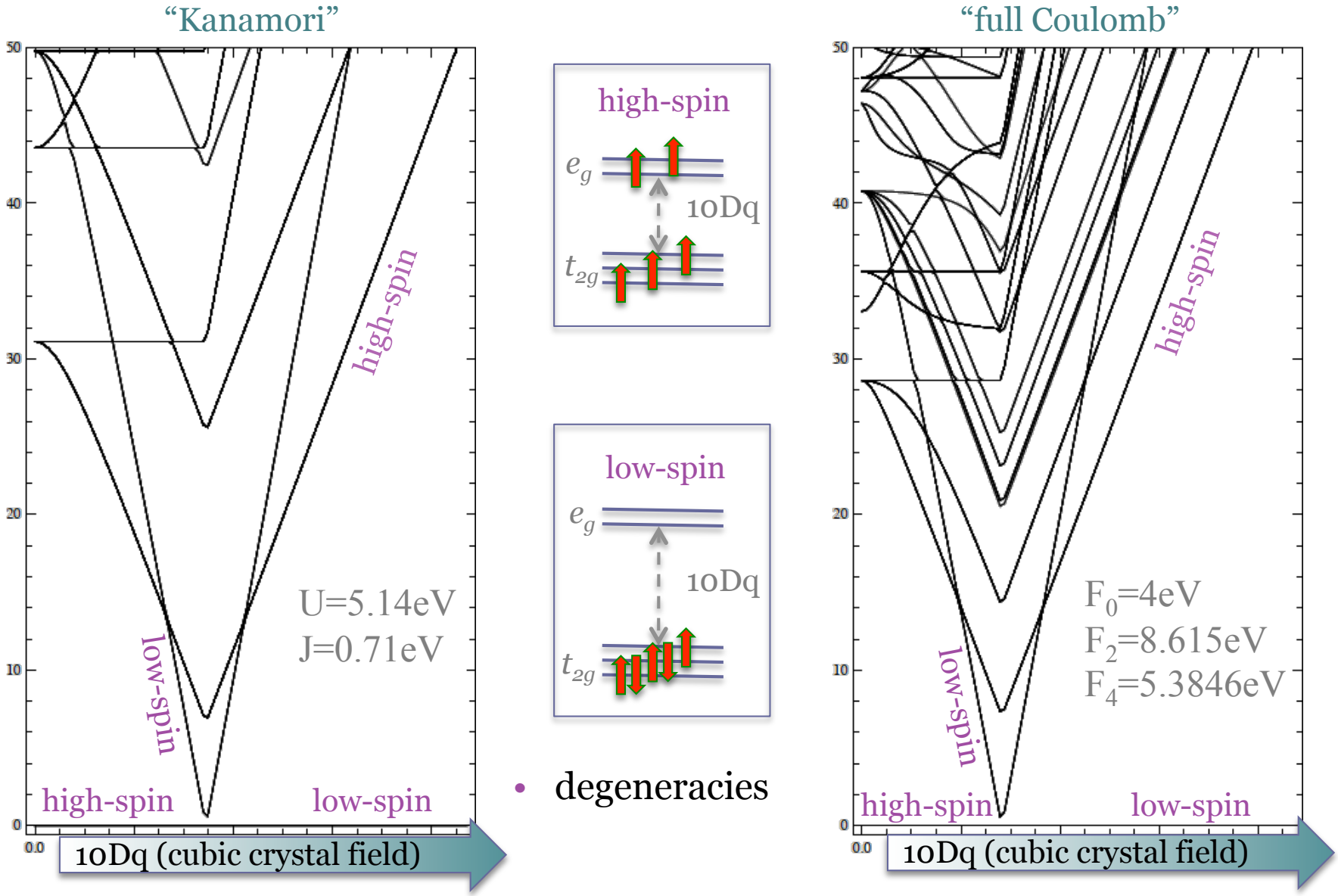
- at low-T: $\beta(E^{(1)}_{loc} - E^{(0)}_{loc}) \gg 1$ $\Rightarrow$ we "fix" the outer state(s)
- because of c/c^+ we can still "visit" an excited state for a short time inside the trace

$$\cancel{\sum_{i=0}}\ \langle\cancel{\phi_i}|e^{-\beta\mathcal{H}_{loc}}\ \ldots\ \ e^{\tau'_1\mathcal{H}_{loc}}\ \ c^\dagger_{\alpha'_1}\ \ e^{-\tau'_1\mathcal{H}_{loc}}\ \ |\cancel{\phi_i}\rangle$$

ϕ_0 ϕ_0

- at low-T the trace is long $\Rightarrow$ easy to accommodate enough "visits"
- very controllable and convenient "`truncation`" parameter of Krylov CT-HYB
- at very low T we can restrict ourselves to the lowest multiplet

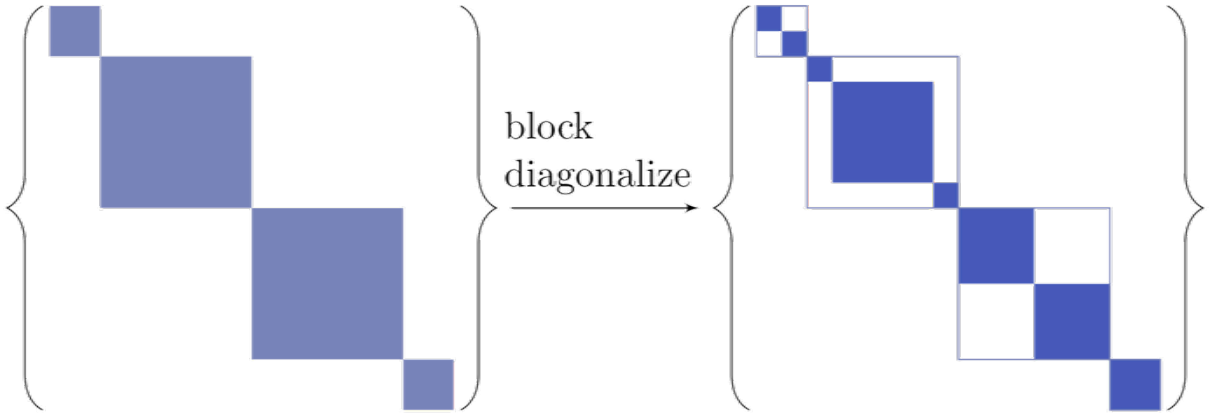
Tanabe-Sugano diagram for d^5



- degeneracies

Exploiting conserved quantities

- good quantum numbers of $\mathcal{H}_{loc}$ ⇒ maximum "block-diagonalization"



eigenvectors of H_{loc}
example for 1 orbital

$$\{\ |0\rangle,\ |\uparrow\rangle,\ |\downarrow\rangle,\ |\uparrow\downarrow\rangle\ \}$$

$$\cdots\ \ \mathrm{e}^{\tau_1' \mathcal{H}_{loc}}\ c^{\dagger}_{\alpha_1'}\ \mathrm{e}^{-\tau_1' \mathcal{H}_{loc}}\ |\phi_0\rangle$$

with Lanczos $\mathrm{e}^{-\tau \mathcal{H}_{loc}}\,|v\rangle \simeq \sum_{k=0}^{p-1} \frac{(-\tau)^k}{k!} \mathcal{H}_{loc}^k |v\rangle$

Example for two orbitals

- eigenbasis of the "Kanamori" Hamiltonian

$$\mathcal{H}_{loc} = \sum_a U n_{a,\uparrow} n_{a,\downarrow} + \sum_{a>b,\sigma} \left[U' n_{a,\sigma} n_{b,-\sigma} + (U' - J) n_{a,\sigma} n_{b,\sigma} \right] - \sum_{a \neq b} J (c^\dagger_{a,\downarrow} c^\dagger_{b,\uparrow} c_{b,\downarrow} c_{a,\uparrow} + c^\dagger_{b,\uparrow} c^\dagger_{b,\downarrow} c_{a,\uparrow} c_{a,\downarrow} + h.c.)$$

TABLE II. Eigenstates and eigenenergies for the local part of the two-orbital model. The first entry corresponds to orbital 1 and the second entry to orbital 2.

Eigenstates	Energy	Eigenstates	Energy
$\|1\rangle = \|0,0\rangle$	0	$\|9\rangle = 1/\sqrt{2}(\|\uparrow,\downarrow\rangle - \|\downarrow,\uparrow\rangle)$	$U-J-2\mu$
$\|2\rangle = \|\uparrow,0\rangle$	$-\mu$	$\|10\rangle = 1/\sqrt{2}(\|\uparrow\downarrow,0\rangle - \|0,\uparrow\downarrow\rangle)$	$U-J-2\mu$
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$\|6\rangle = \|\uparrow,\uparrow\rangle$	$U-3J-2\mu$	$\|14\rangle = \|\uparrow,\uparrow\downarrow\rangle$	$3U-5J-3\mu$
$\|7\rangle = 1/\sqrt{2}(\|\uparrow,\downarrow\rangle + \|\downarrow,\uparrow\rangle)$	$U-3J-2\mu$	$\|15\rangle = \|\downarrow,\uparrow\downarrow\rangle$	$3U-5J-3\mu$
$\|8\rangle = \|\downarrow,\downarrow\rangle$	$U-3J-2\mu$	$\|16\rangle = \|\uparrow\downarrow,\uparrow\downarrow\rangle$	$6U-10J-4\mu$

N_{tot}	$(Sz)_{tot}$	S^2_{tot}
1	+½	½

P. Werner and A. J. Millis, PRB **74**, 155107 (2006)

Example for two orbitals

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N_{tot}	$(Sz)_{tot}$	S^2_{tot}
1	-½	½

Example for two orbitals

- eigenbasis of the "Kanamori" Hamiltonian

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2		1

Example for two orbitals

- eigenbasis of the "Kanamori" Hamiltonian

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N_{tot}	$(Sz)_{tot}$	S^2_{tot}
2	+1	1

Example for two orbitals

- eigenbasis of the "Kanamori" Hamiltonian

$$\mathcal{H}_{loc} = \sum_a U n_{a,\uparrow} n_{a,\downarrow} + \sum_{a>b,\sigma} \left[U' n_{a,\sigma} n_{b,-\sigma} + (U' - J) n_{a,\sigma} n_{b,\sigma} \right] - \sum_{a \neq b} J (c^\dagger_{a,\downarrow} c^\dagger_{b,\uparrow} c_{b,\downarrow} c_{a,\uparrow} + c^\dagger_{b,\uparrow} c^\dagger_{b,\downarrow} c_{a,\uparrow} c_{a,\downarrow} + h.c.)$$

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$\|7\rangle = 1/\sqrt{2}(\|\uparrow,\downarrow\rangle + \|\downarrow,\uparrow\rangle)$	$U-3J-2\mu$	$\|15\rangle = \|\downarrow,\uparrow\downarrow\rangle$	$3U-5J-3\mu$
$\|8\rangle = \|\downarrow,\downarrow\rangle$	$U-3J-2\mu$	$\|16\rangle = \|\uparrow\downarrow,\uparrow\downarrow\rangle$	$6U-10J-4\mu$

N_{tot}	$(Sz)_{tot}$	S^2_{tot}
2	-1	1

Example for two orbitals

- eigenbasis of the "Kanamori" Hamiltonian

$$\mathcal{H}_{loc} = \sum_a U n_{a,\uparrow} n_{a,\downarrow} + \sum_{a>b,\sigma} \left[U' n_{a,\sigma} n_{b,-\sigma} + (U' - J) n_{a,\sigma} n_{b,\sigma} \right] - \sum_{a \neq b} J (c^\dagger_{a,\downarrow} c^\dagger_{b,\uparrow} c_{b,\downarrow} c_{a,\uparrow} + c^\dagger_{b,\uparrow} c^\dagger_{b,\downarrow} c_{a,\uparrow} c_{a,\downarrow} + h.c.)$$

TABLE II. Eigenstates and eigenenergies for the local part of the two-orbital model. The first entry corresponds to orbital 1 and the second entry to orbital 2.

Eigenstates	Energy	Eigenstates	Energy
$\|1\rangle = \|0,0\rangle$	0	$\|9\rangle = 1/\sqrt{2}(\|\uparrow,\downarrow\rangle - \|\downarrow,\uparrow\rangle)$	$U-J-2\mu$
$\|2\rangle = \|\uparrow,0\rangle$	$-\mu$	$\|10\rangle = 1/\sqrt{2}(\|\uparrow\downarrow,0\rangle - \|0,\uparrow\downarrow\rangle)$	$U-J-2\mu$
$\|3\rangle = \|\downarrow,0\rangle$	$-\mu$	$\|11\rangle = 1/\sqrt{2}(\|\uparrow\downarrow,0\rangle + \|0,\uparrow\downarrow\rangle)$	$U+J-2\mu$
$\|4\rangle = \|0,\uparrow\rangle$	$-\mu$	$\|12\rangle = \|\uparrow\downarrow,\uparrow\rangle$	$3U-5J-3\mu$
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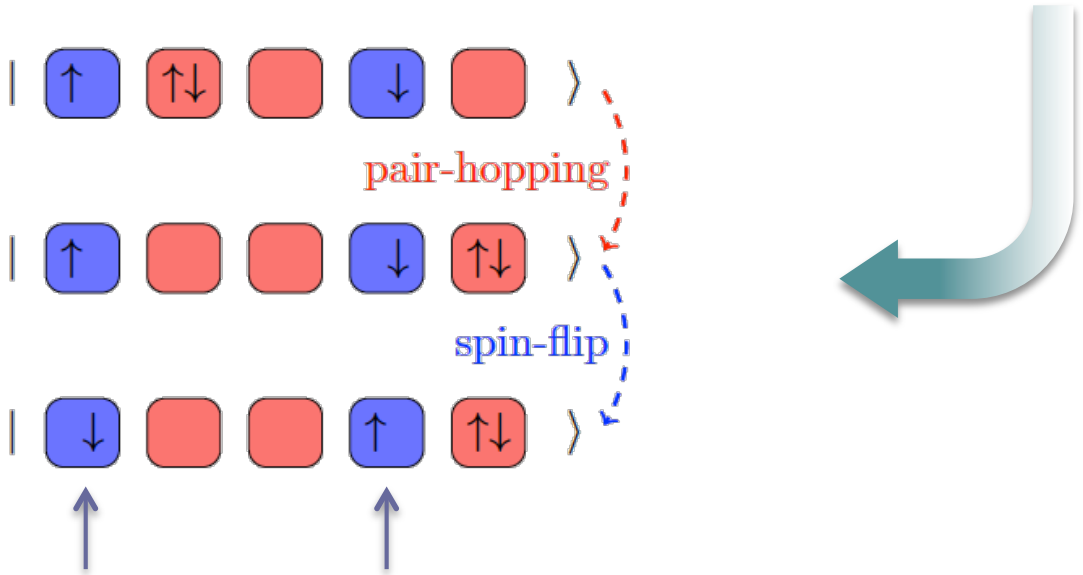
$\|8\rangle = \|\downarrow,\downarrow\rangle$	$U-3J-2\mu$	$\|16\rangle = \|\uparrow\downarrow,\uparrow\downarrow\rangle$	$6U-10J-4\mu$

N_{tot}	$(Sz)_{tot}$	
2	0	

Example for two orbitals

- eigenbasis of the "Kanamori" Hamiltonian

$$\mathcal{H}_{loc} = \underbrace{\sum_a U n_{a,\uparrow} n_{a,\downarrow} + \sum_{a>b,\sigma} \left[U' n_{a,\sigma} n_{b,-\sigma} + (U' - J) n_{a,\sigma} n_{b,\sigma} \right]}_{\text{diagonal in the occupation-number basis}} - \underbrace{\sum_{a \neq b} J (c^\dagger_{a,\downarrow} c^\dagger_{b,\uparrow} c_{b,\downarrow} c_{a,\uparrow} + c^\dagger_{b,\uparrow} c^\dagger_{b,\downarrow} c_{a,\uparrow} c_{a,\downarrow} + h.c.)}_{\text{off-diagonal}}$$



the pattern of singly-occupied orbitals is conserved! ⇒ "PS"-number

N. Parragh, *et al.*, PRB **86**, 155158 (2012)

Example for two orbitals

- eigenbasis of the "Kanamori" Hamiltonian

$$\mathcal{H}_{loc} = \sum_a U n_{a,\uparrow} n_{a,\downarrow} + \sum_{a>b,\sigma} \left[U' n_{a,\sigma} n_{b,-\sigma} + (U' - J) n_{a,\sigma} n_{b,\sigma} \right] - \sum_{a \neq b} J (c^\dagger_{a,\downarrow} c^\dagger_{b,\uparrow} c_{b,\downarrow} c_{a,\uparrow} + c^\dagger_{b,\uparrow} c^\dagger_{b,\downarrow} c_{a,\uparrow} c_{a,\downarrow} + h.c.)$$

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$\|8\rangle = \|\downarrow,\downarrow\rangle$	$U - 3J - 2\mu$	$\|16\rangle = \|\uparrow\downarrow,\uparrow\downarrow\rangle$	$6U - 10J - 4\mu$

N_{tot}	$(Sz)_{tot}$	
1	+½	

Example for two orbitals

- eigenbasis of the "Kanamori" Hamiltonian

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N_{tot}	$(Sz)_{tot}$	PS
1	+½	1

$$PS = \sum_{a=0}^{N_{orb}-1} 2^a (n_{a,\uparrow} - n_{a,\downarrow})^2$$

Example for two orbitals

- eigenbasis of the "Kanamori" Hamiltonian

$$\mathcal{H}_{loc} = \sum_a U n_{a,\uparrow} n_{a,\downarrow} + \sum_{a>b,\sigma} \left[U' n_{a,\sigma} n_{b,-\sigma} + (U' - J) n_{a,\sigma} n_{b,\sigma} \right] - \sum_{a \neq b} J (c^\dagger_{a,\downarrow} c^\dagger_{b,\uparrow} c_{b,\downarrow} c_{a,\uparrow} + c^\dagger_{b,\uparrow} c^\dagger_{b,\downarrow} c_{a,\uparrow} c_{a,\downarrow} + h.c.)$$

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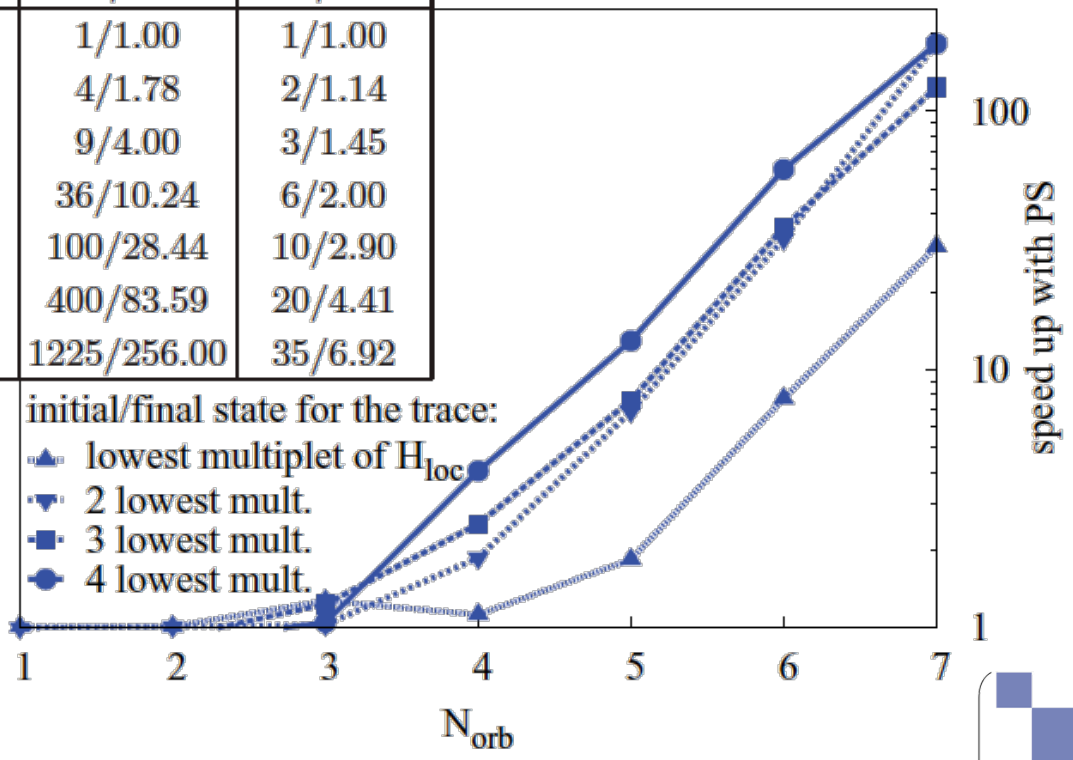
N_{tot}	$(Sz)_{tot}$	PS
1	+½	2

$$PS = \sum_{a=0}^{N_{orb}-1} 2^a (n_{a,\uparrow} - n_{a,\downarrow})^2$$

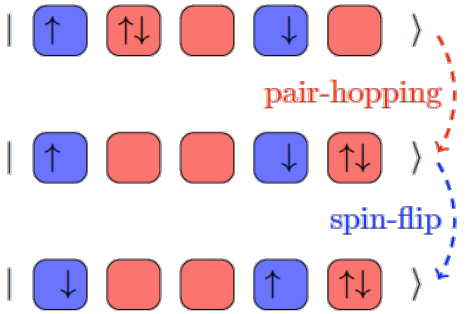
Advantages of the “PS”-number

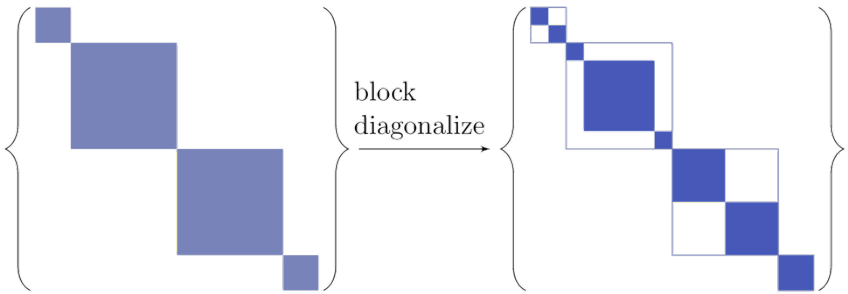
N_{orb}	$N\ S_z$ max/mean	$N\ S_z$ PS max/mean
1	1/1.00	1/1.00
2	4/1.78	2/1.14
3	9/4.00	3/1.45
4	36/10.24	6/2.00
5	100/28.44	10/2.90
6	400/83.59	20/4.41
7	1225/256.00	35/6.92



$$PS = \sum_{a=0}^{N_{orb}-1} 2^a (n_{a,\uparrow} - n_{a,\downarrow})^2$$

N. Parragh, *et al.*,
PRB **86**, 155158 (2012)





Where do the operators go?

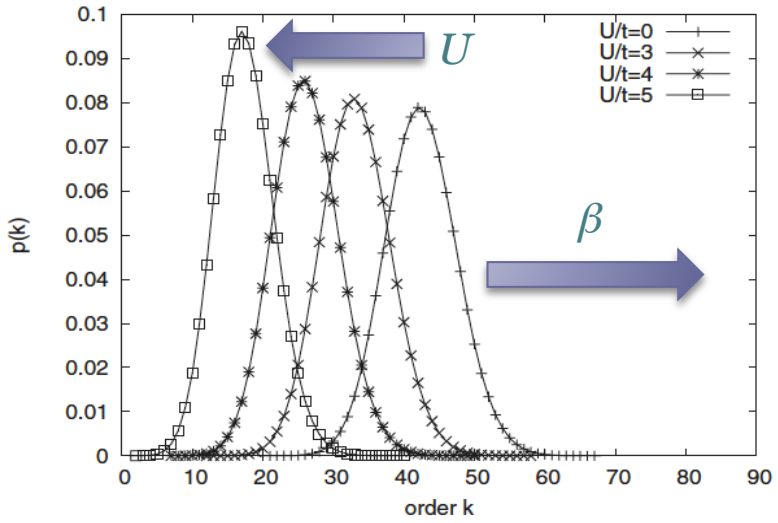
- We sample partition-function configurations

$$Z = \sum_k \frac{1}{k!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau'_k \sum_{\alpha_1 \cdots \alpha_k} \sum_{\alpha'_1 \cdots \alpha'_k} \sum_{l_1 \cdots l_k} \sum_{l'_1 \cdots l'_k} V_{l_1}^{\alpha_1} V_{l'_1}^{\alpha'_1 *} V_{l_k}^{\alpha_k} V_{l'_k}^{\alpha'_k *}$$

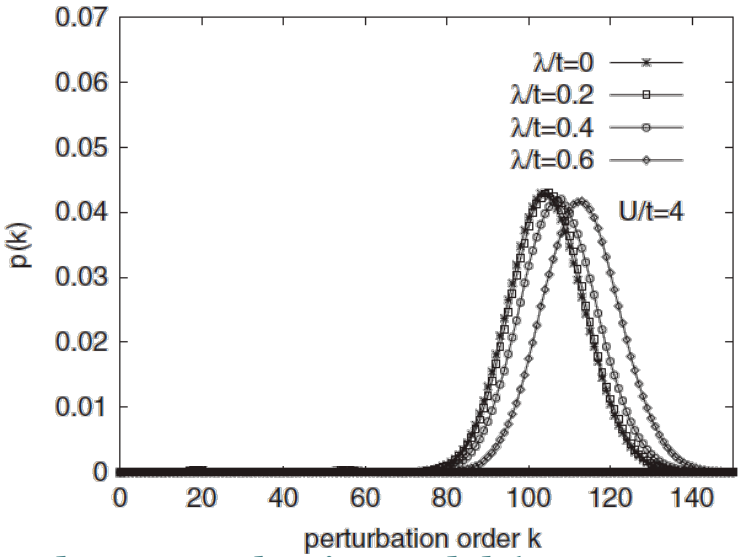
$$\times \mathrm{Tr}_c \left[e^{-\beta \mathcal{H}_{loc}} T c_{\alpha_k}(\tau_k) c^\dagger_{\alpha'_k}(\tau'_k) \cdots c_{\alpha_1}(\tau_1) c^\dagger_{\alpha'_1}(\tau'_1) \right]$$

$$\times \mathrm{Tr}_a \left[e^{-\beta \mathcal{H}_{bath}} T a^\dagger_{l_k}(\tau_k) a_{l'_k}(\tau'_k) \cdots a^\dagger_{l_1}(\tau_1) a_{l'_1}(\tau'_1) \right]$$

p(k):
distribution of the "*c*" operators



Anderson model (βt=100)
P. Werner, *et al.*, PRL **97**, 076405 (2006)



Anderson-Holstein model (βt=400, ω_0=0.2t)
E. Gull, *et al.*, RMP **83**, 349 (2006)

Where do the operators go?

- We sample partition-function configurations

$$Z = \sum_k \frac{1}{k!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau'_k \sum_{\alpha_1 \cdots \alpha_k} \sum_{\alpha'_1 \cdots \alpha'_k} \sum_{l_1 \cdots l_k} \sum_{l'_1 \cdots l'_k} V_{l_1}^{\alpha_1} V_{l'_1}^{\alpha'_1 *} V_{l_k}^{\alpha_k} V_{l'_k}^{\alpha'_k *}$$

$$\times \mathrm{Tr}_c \left[e^{-\beta \mathcal{H}_{loc}} T c_{\alpha_k}(\tau_k) c^\dagger_{\alpha'_k}(\tau'_k) \cdots c_{\alpha_1}(\tau_1) c^\dagger_{\alpha'_1}(\tau'_1) \right]$$

$$\times \mathrm{Tr}_a \left[e^{-\beta \mathcal{H}_{bath}} T a^\dagger_{l_k}(\tau_k) a_{l'_k}(\tau'_k) \cdots a^\dagger_{l_1}(\tau_1) a_{l'_1}(\tau'_1) \right]$$

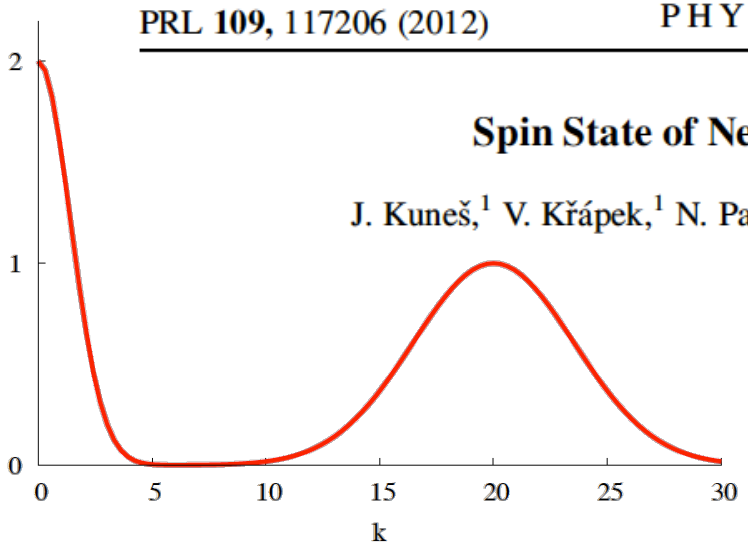
p(k):
distribution of the "*c*" operators

- but we have encountered situations with more complicated p(k):

PRL **109,** 117206 (2012) PHYSICAL REVIEW LETTERS week ending 14 SEPTEMBER 2012

Spin State of Negative Charge-Transfer Material $SrCoO_3$

J. Kuneš,[1] V. Křápek,[1] N. Parragh,[2] G. Sangiovanni,[2] A. Toschi,[3] and A. V. Kozhevnikov[4]



DOUBLE-PEAKED HISTOGRAM???

Where does the AIM come from?

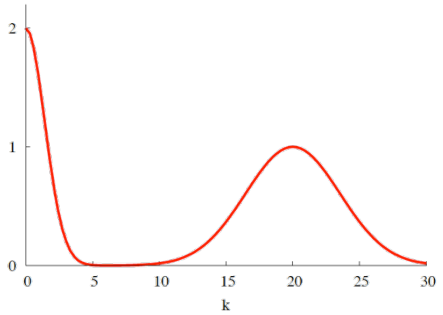
FROM SOMEWHERE → $F(\tau)$ or, equivalently $F(i\omega_n)$

$$G_0^{-1}(i\omega_n) = i\omega_n + \mu - F(i\omega_n)$$

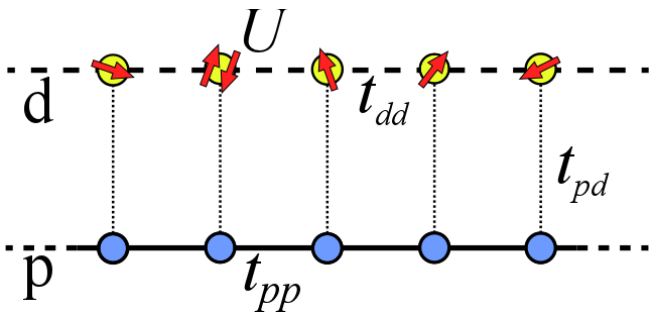
- "plain vanilla" DMFT
- LDA+DMFT – *H(k)* in `wannier90`-format
- long-range ordered magnetic solutions
- enlarged basis ("PAM"/*dp*-models) and DMFT+Hartree
- various flavors of non-equivalent atoms/layers/…
- real-space schemes ("*nano*DMFT" and "*nano*DΓA")

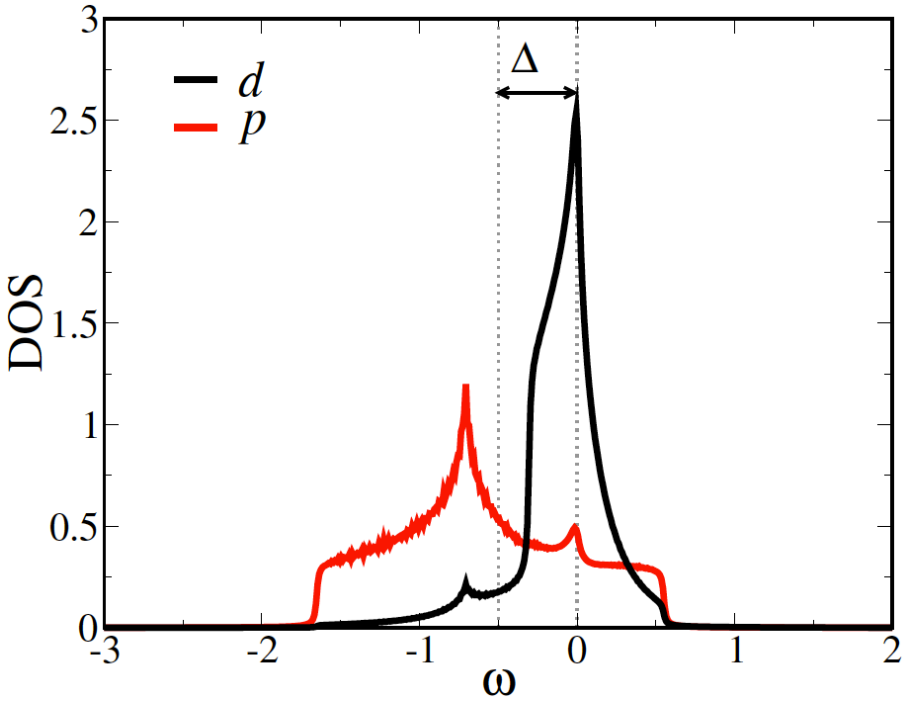
flexible and user-defined Python classes in w2dynamics

- "plain vanilla" DMFT
- LDA+DMFT – *H(k)* in `wannier90`-format
- long-range ordered magnetic solutions
- enlarged basis ("PAM"/*dp*-models) and DMFT+Hartree
- various flavors of non-equivalent atoms/layers/…
- real-space schemes ("*nano*DMFT" and "*nano*DΓA")



Periodic Anderson Model ("t_{dd}-PAM")



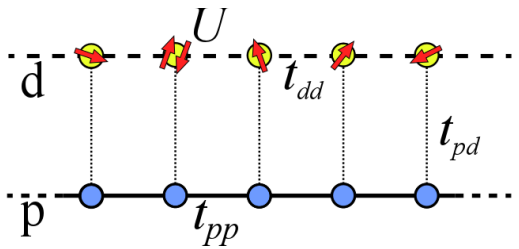


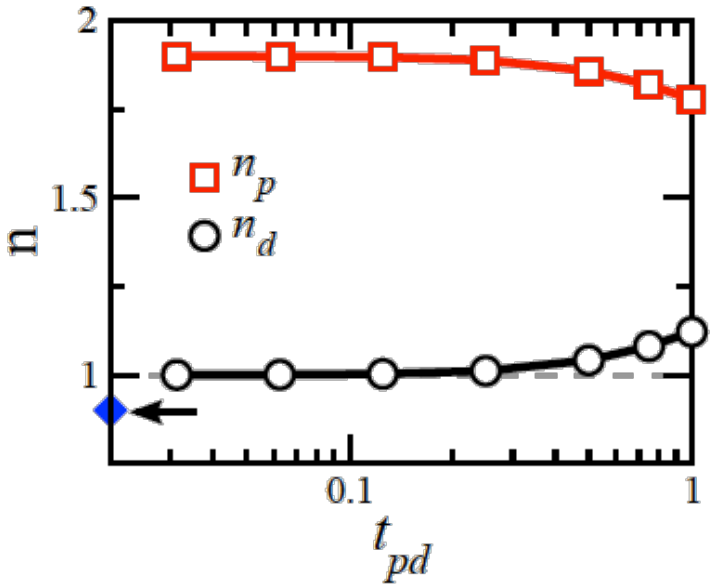
$$H = \sum_{\mathbf{k}\sigma} \varepsilon_p(\mathbf{k}) p^+_{\mathbf{k}\sigma} p_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \varepsilon_d(\mathbf{k}) d^+_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma} +$$

$$t_{pd} \sum_{i\sigma} \left(d^+_{i\sigma} p_{i\sigma} + p^+_{i\sigma} d_{i\sigma} \right) + U \sum_i d^+_{i\uparrow} d^+_{i\downarrow} d_{i\uparrow} d_{i\downarrow}$$

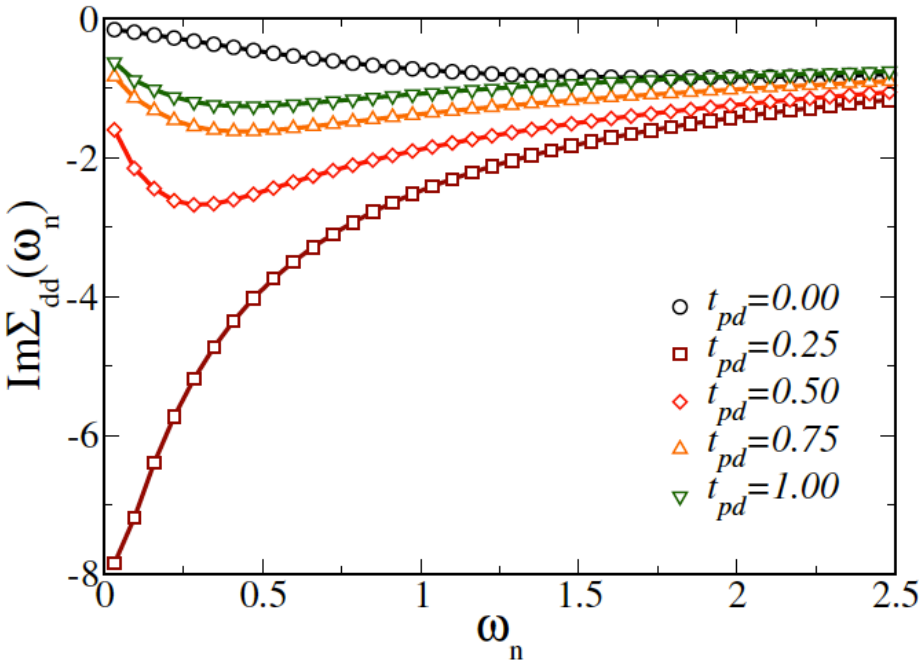
Hole-doped Mott insulator

- 10% doping with $t_{pd}=0 \Rightarrow \boldsymbol{n_d=0.9}$
- 10% doping with $t_{pd}\neq 0 \Rightarrow \boldsymbol{n_{tot}=n_d+n_p=2.9}$



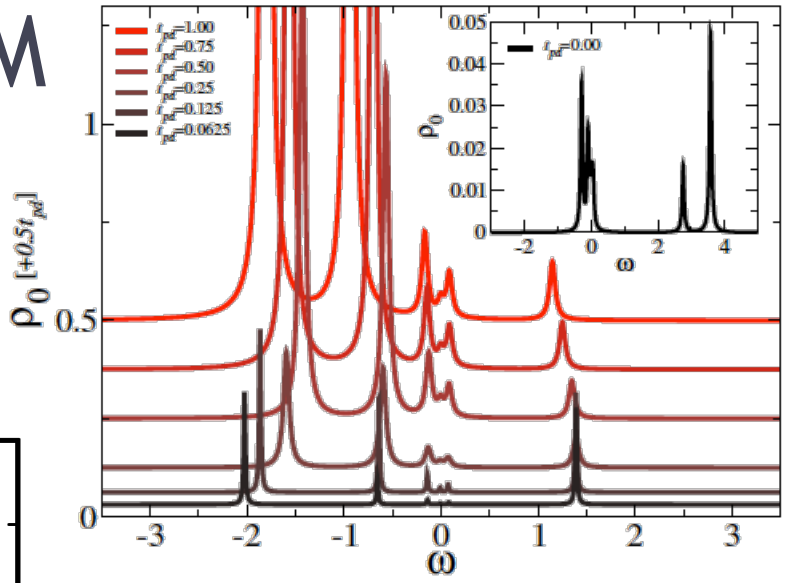


- all energies in units of t_{pp}
- $t_{dd}=1/4$

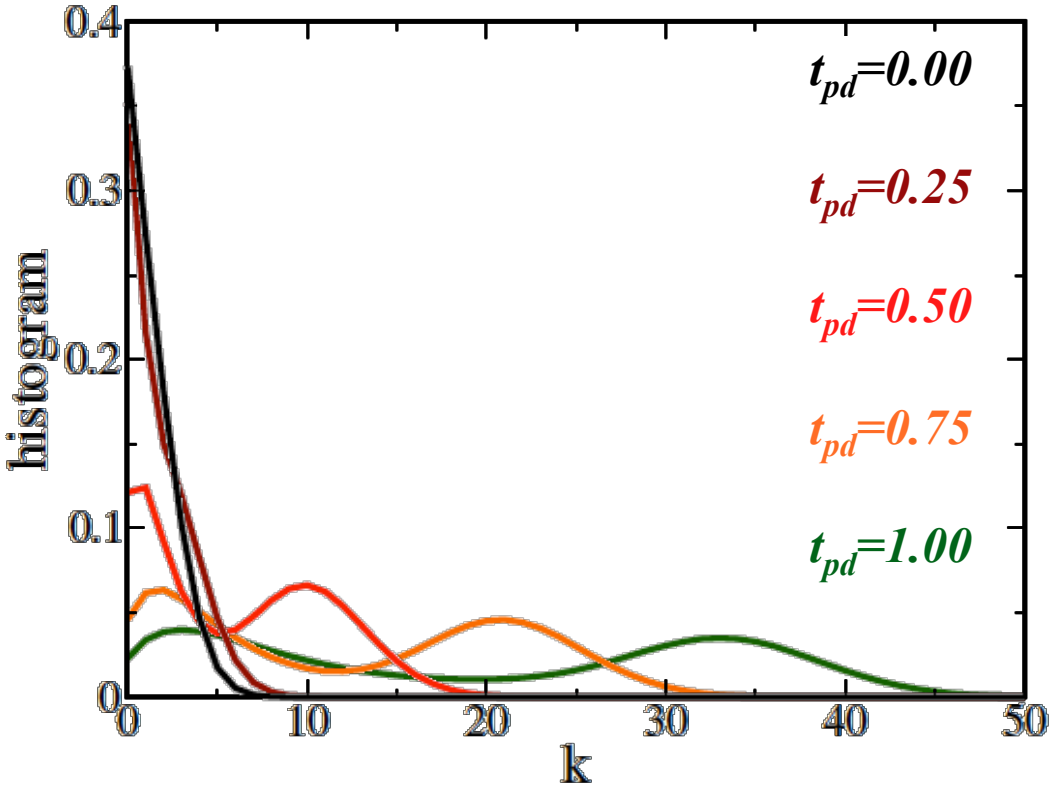


Histogram in the t_{dd}-PAM

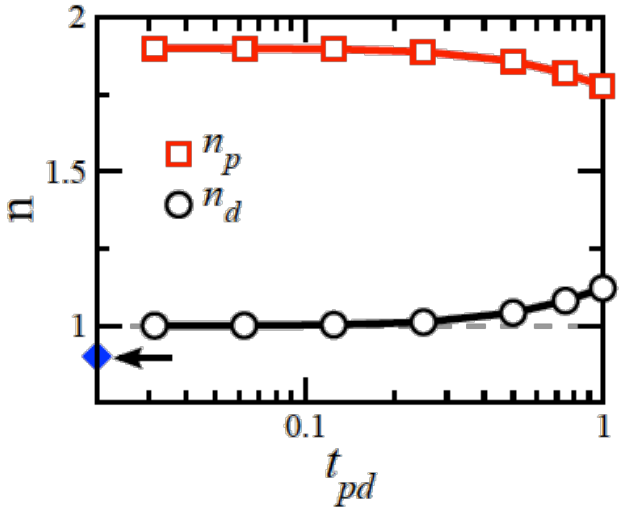
- spectral representation of the hyb. function



- CT-HYB histogram



expansion order



How can we label the histogram peaks?

- Hubbard model (t_{pd}=0) below half-filling

$\sigma = \uparrow$

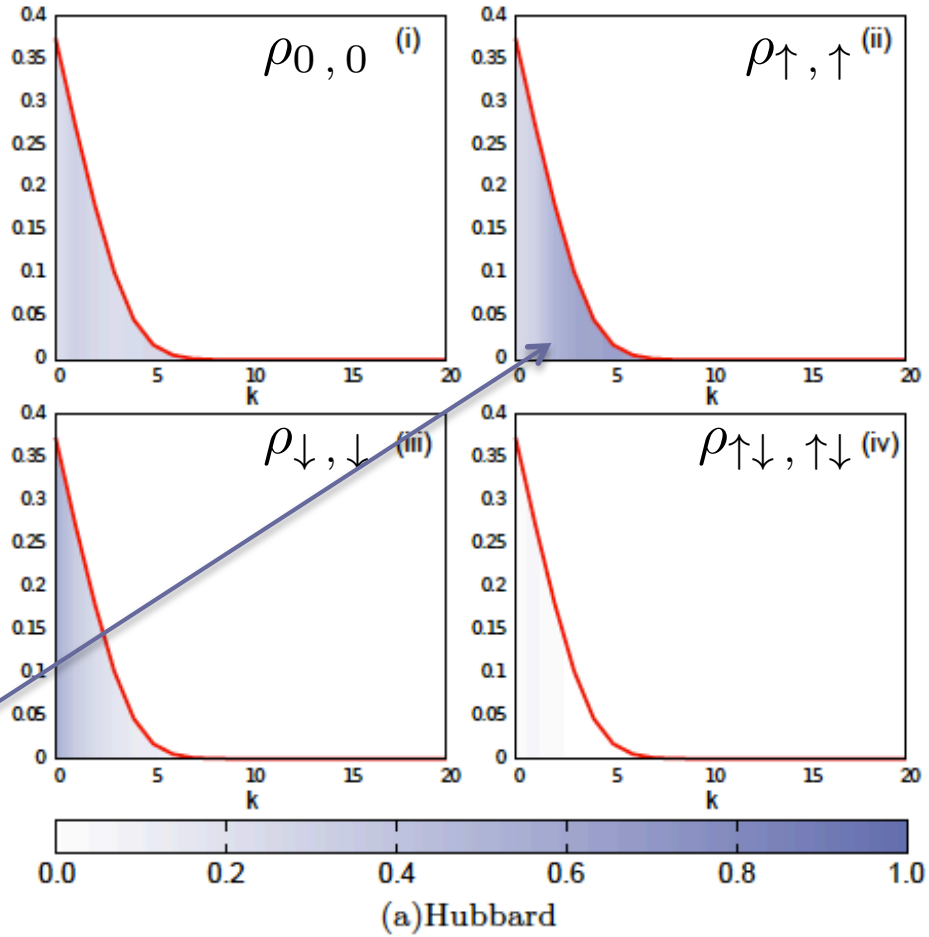
- one possible way:
  order-resolved density-matrix
  (in Fock space)

$$\forall k \quad \forall \sigma \quad \forall m \quad \rho_{\alpha\,,\,\alpha} = |\alpha\rangle\langle\alpha|$$

$$|\alpha\rangle = |0\rangle,\ |\uparrow\rangle,\ |\downarrow\rangle,\ |\uparrow\downarrow\rangle$$

$$\sum_{i=0} \langle\phi_i| e^{-\beta \mathcal{H}_{loc}} \ldots |\uparrow\rangle\langle\uparrow| \ldots c^{\dagger}_{\alpha'_1}(\tau'_1)|\phi_i\rangle$$

a bit more of hybridization
events with many spin up
in order to "empty" the impurity



How can we label the histogram peaks?

- t_{dd}-PAM (t_{pd}=0.75)

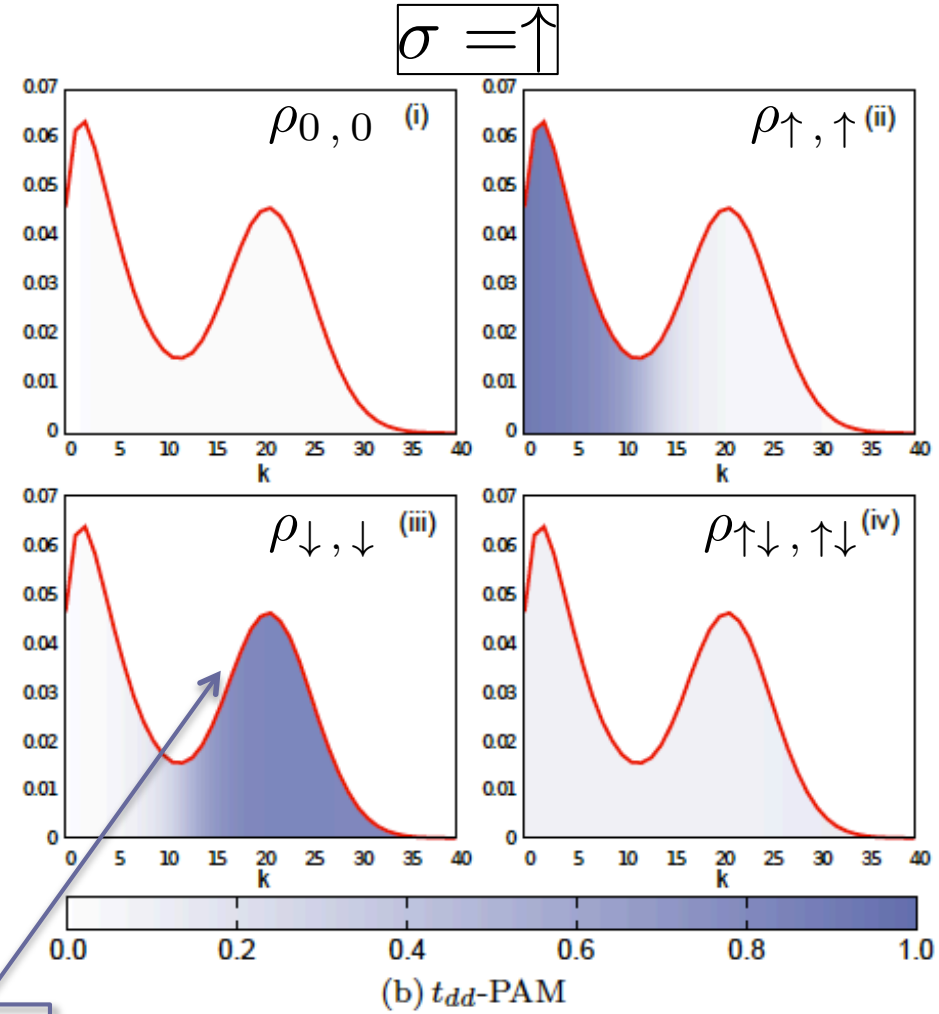
  10% hole doping

- order-resolved density-matrix:

$$\forall k \quad \forall \sigma \quad \forall m \quad \rho_{\alpha\,,\,\alpha} = |\alpha\rangle\langle\alpha|$$

- now diagrams "making" the impurity doubly occupied belong almost fully to the second peak
- in our case the *p*-band is almost full, it can only "give" electrons

⇒ **second peak has "*p* character"**



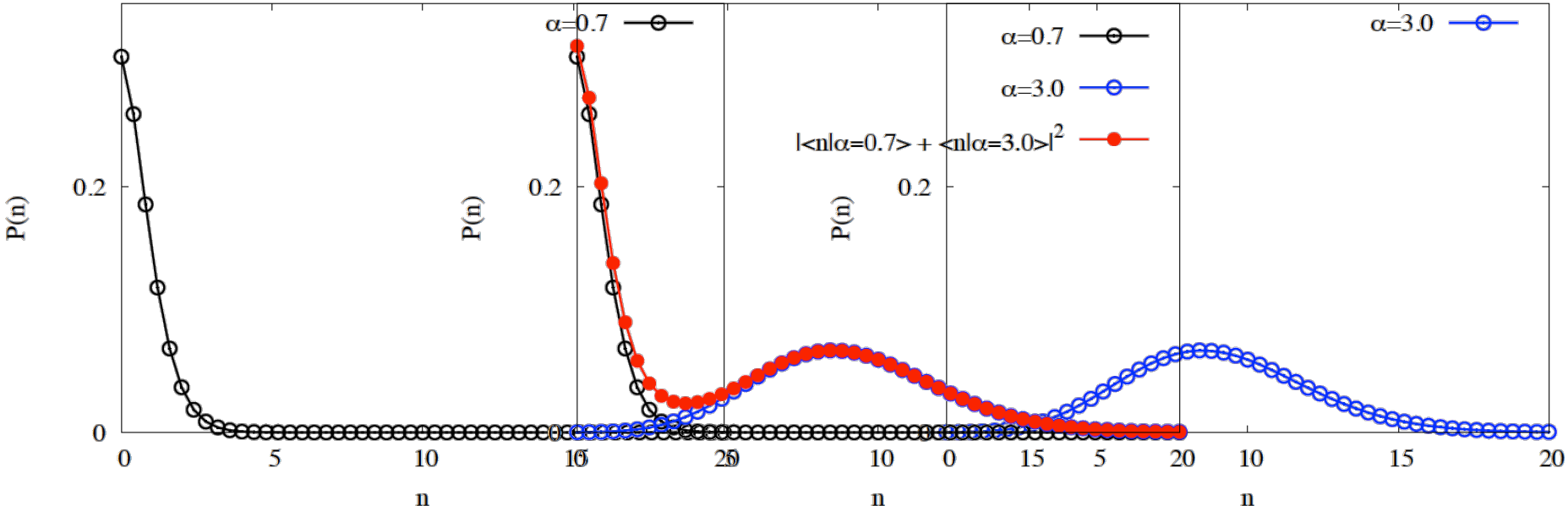
hybridization events "filling" the impurity

$$\sum_{i=0} \langle\phi_i| e^{-\beta\mathcal{H}_{loc}} \ldots |\downarrow\rangle\langle\downarrow| \ldots c^{\dagger}_{\alpha'_1}(\tau'_1)|\phi_i\rangle$$

Simple way of getting two peaks?

question (and answer) by Sergio Ciuchi on the bus

- coherent state of the harmonic oscillator $a|\alpha\rangle = \alpha|\alpha\rangle \qquad |\alpha\rangle = \mathrm{e}^{-\alpha^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$
- which n contribute? $P(n) = |\langle n|\alpha\rangle|^2 = \frac{\mathrm{e}^{-\alpha^2}}{n!}\alpha^{2n}$



- two components with different strength of the hybridization

Kinetic energy argument

$$E_{kin} = \sum_k \epsilon_k c_k^\dagger c_k = \mathrm{Tr}\left[\epsilon_k G_k\right]$$

$$G_k = \frac{1}{\omega_n + \mu - \epsilon_k - \Sigma} = \frac{1}{\zeta - \epsilon_k} \qquad \zeta = \omega_n + \mu - \Sigma$$

$$F = \omega_n + \bar{\mu} - \mathcal{G}_0^{-1}$$

"impurity μ"

$$\omega_n + \mu - \mathcal{G}_0^{-1} = F + \mu - \bar{\mu}$$

$$\epsilon_k G_k = \frac{\epsilon_k}{\zeta - \epsilon_k} = -1 + \frac{\zeta}{\zeta - \epsilon_k} = -1 + \left(\omega_n + \mu - \Sigma\right) G_k$$

$\Sigma = \mathcal{G}_0^{-1} - G_{loc}^{-1}$

$$= -1 + \left(\underbrace{\omega_n + \mu - \mathcal{G}_0^{-1}}_{F + \mu - \bar{\mu}} + G_{loc}^{-1}\right) G_k$$

$$\epsilon_k G_k = -1 + F G_k + (\mu - \bar{\mu}) G_k + G_{loc}^{-1} G_k$$

$$\sum_k \epsilon_k G_k = -1 + F \cdot G_{loc} + (\mu - \bar{\mu}) n + 1$$

$$\Rightarrow E_{kin} = \mathrm{Tr}\, F \cdot G_{loc} + \mathrm{Tr}\left[(\mu - \bar{\mu}) n\right]$$

Kinetic energy argument

- In CT-HYB the kinetic energy can be calculated from the average exp. order

$$Z = \sum_k \int \mathcal{D}[\psi^\dagger \psi] e^{-S_0} \frac{(-1)^k}{k!} (\Delta S)^k \qquad \Delta S = \text{hybridization part of the action}$$

$$\langle k \rangle = \frac{1}{Z} \int \mathcal{D}[\psi^\dagger \psi] e^{-S_0} \sum_k k \frac{(-1)^k}{k!} (\Delta S)^k = -\frac{1}{Z} \int \mathcal{D}[\psi^\dagger \psi] e^{-S_0} \sum_k \frac{(-1)^{k-1}}{(k-1)!} (\Delta S)^{k-1} \Delta S = -\langle \Delta S \rangle$$

$$\Delta S = \int_0^\beta d\tau \sum_{l,\sigma} \left[a^\dagger_{l\sigma} \left(\frac{\partial}{\partial \tau} - \mu + \varepsilon_l \right) a_{l\sigma} + V_l c^\dagger_\sigma a_{l\sigma} + V_l a^\dagger_{l\sigma} c_\sigma \right]$$

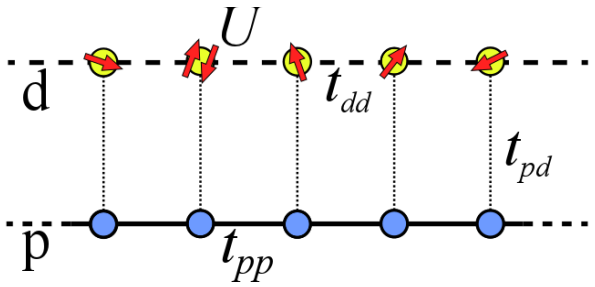
integrating out the bath fermions

$$\Delta S = \int_0^\beta \int_0^\beta d\tau d\tau' \sum_\sigma c^\dagger_\sigma(\tau) F(\tau - \tau') c_\sigma(\tau')$$

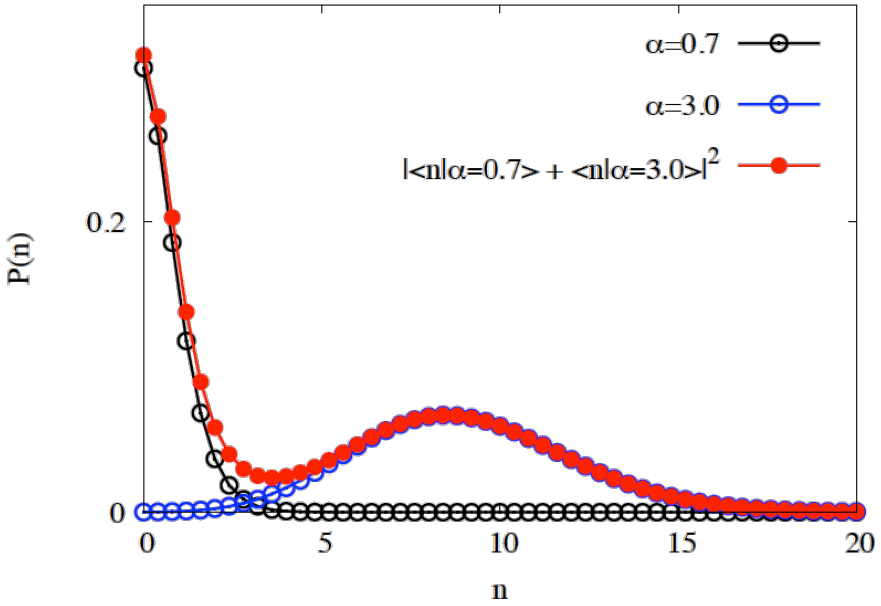
$$\langle \Delta S \rangle = \mathrm{Tr}[F \cdot G] \quad \Leftarrow \quad \langle k \rangle = \frac{1}{T} |E_{kin}|$$

Kinetic energy argument

- Two components with different mobility?



$$\langle k \rangle = \frac{1}{T} |E_{kin}|$$



- two different “screening” channels?

⇒ ongoing study of the spin susceptibility

Second moment

- What does the second moment of the distribution correspond to?

$$Z = \sum_k \int \mathcal{D}[\psi^\dagger \psi] e^{-S_0} \frac{(-1)^k}{k!} (\Delta S)^k \qquad \Delta S = \text{hybridization part of the action}$$

$$\langle k^2 \rangle = \frac{1}{Z} \int \mathcal{D}[\psi^\dagger \psi] e^{-S_0} \sum_k k^2 \frac{(-1)^k}{k!} (\Delta S)^k = \frac{1}{Z} \int \mathcal{D}[\psi^\dagger \psi] e^{-S_0} \sum_k \frac{k}{k-1} \frac{(-1)^{k-2}}{(k-2)!} (\Delta S)^{k-2} (\Delta S)^2 \longrightarrow \langle (\Delta S)^2 \rangle$$

- connected to a four-point T-product

⇒ does a susceptibility get large when the distribution becomes bi-modal?

- see also yesterday's talk by Sergio Ciuchi
- ongoing project with AG Held supervised by M. Wallerberger and A. Toschi

Conclusions

- "plain vanilla" DMFT
- LDA+DMFT – *H(k)* in `wannier90`-format
- long-range ordered magnetic solutions
- enlarged basis ("PAM"/*dp*-models) and DMFT+Hartree
- various flavors of non-equivalent atoms/layers/…
- real-space schemes ("*nano*DMFT" and "*nano*DΓA")

"w2dynamics"

talk by Nico about future developments
and
talk by Markus about two-particle results