Phenomenological Spectral Function for Multiband Systems
The Case of the Periodic Anderson Model (PAM)

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Outline:

- **Continued Fraction, Padé Approximant and Fermi Liquid Terminator**
- **Single Band versus Multiband Dyson Equation**
- **PAM as Doped Charge Transfer Insulator**
- **Hartree and Hubbard-1 approximations**
- **Obtaining higher sumrules**
- **Minimal scenario to capture singlet-triplet splitting**

Mathematical tools: $\langle n-1/n\rangle$, $\langle n-1/n\rangle_D$, $\{n/n+1\}_D$

Continued Fraction Expansion (CFE) ….. truncated

Iterative steps to obtain the CFE of a scalar Green function $G_0(k,\omega)$

First step: Determine center of gravity ω_1 and variance s_2 of $G_0(k,\omega)$

$$G_0^{-1} = \omega - \omega_1 - s_2^2 G_1(k,\omega)$$

Iterate: Determine C.o.G. ω_{2n-1} and variance s_{2n} of $G_{n-1}(k,\omega)$

$$G_{n-1}^{-1} = \omega - \omega_{2n-1} - s_{2n}^2 G_n(k,\omega)$$

Three kinds of truncation:

1) Set $s_{2n}^2 G_n(k,\omega)=0$ to obtain Padé approximant $\langle n-1/n\rangle$

2) Set $s_{2n}^2 G_n(k,\omega)=iD$ to obtain broadened Padé approximant $\langle n-1/n\rangle_D$

3) Set $\omega_{2n-1} + s_{2n}^2 G_n(k,\omega) = \underline{\omega}_{2n-1} + \underline{s}_{2n}^2/(\omega - \underline{\omega}_{2n+1})$ to obtain (n+1)-Pole approximant $\{n/n+1\}$ with Fermi Liquid terminator

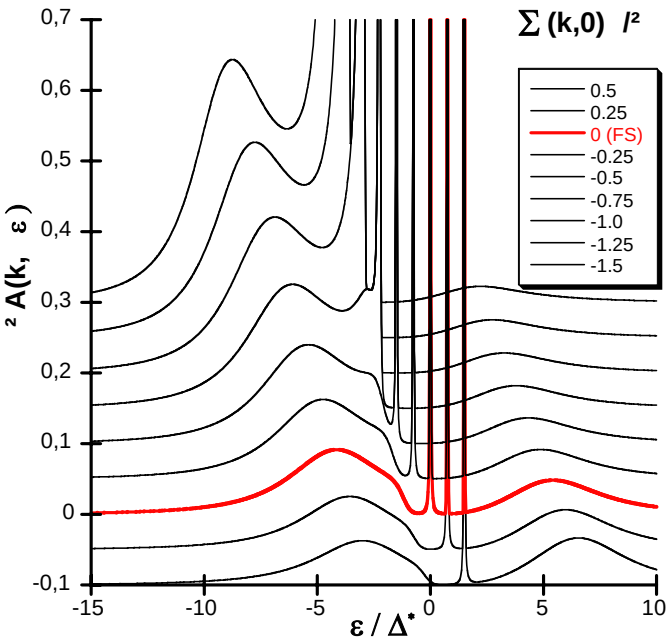
Algorithm: J. Electron Spectroscopy 117-118, 13 (2001)

Previous implementations with one band models

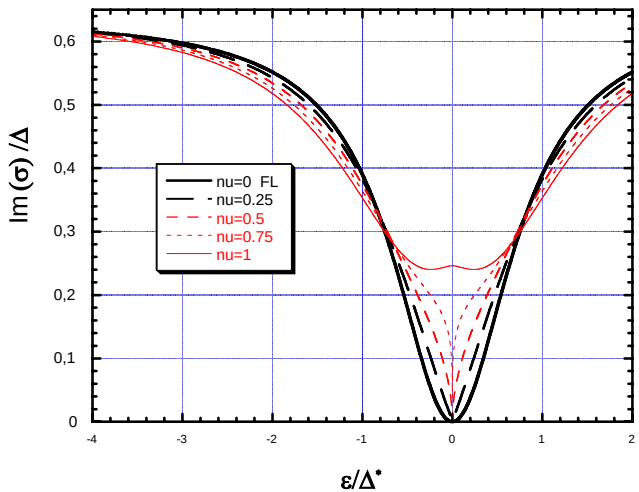
Momentum resolved spectra and phenomenological non-FL selfenergy (See review paper)

- **Approximation $\{1/2\}_D$ was used for TiTe2**
- **Approximation $\{2/3\}_D$ allows to model a QP band with strongly asymmetric background (see figure)**

$\{1/2\}_D$ + non-FL Terminator was used for BISCO

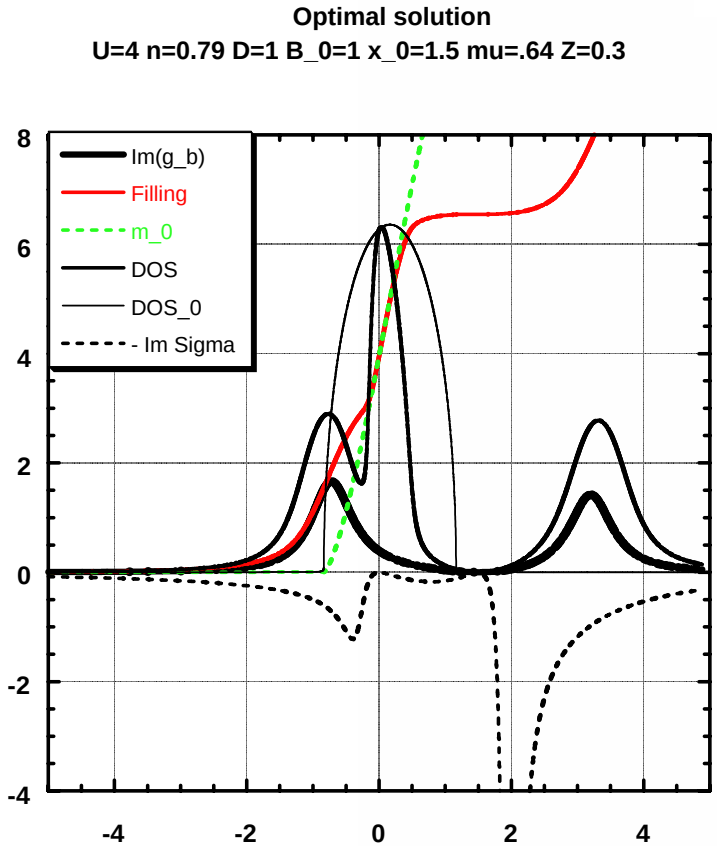


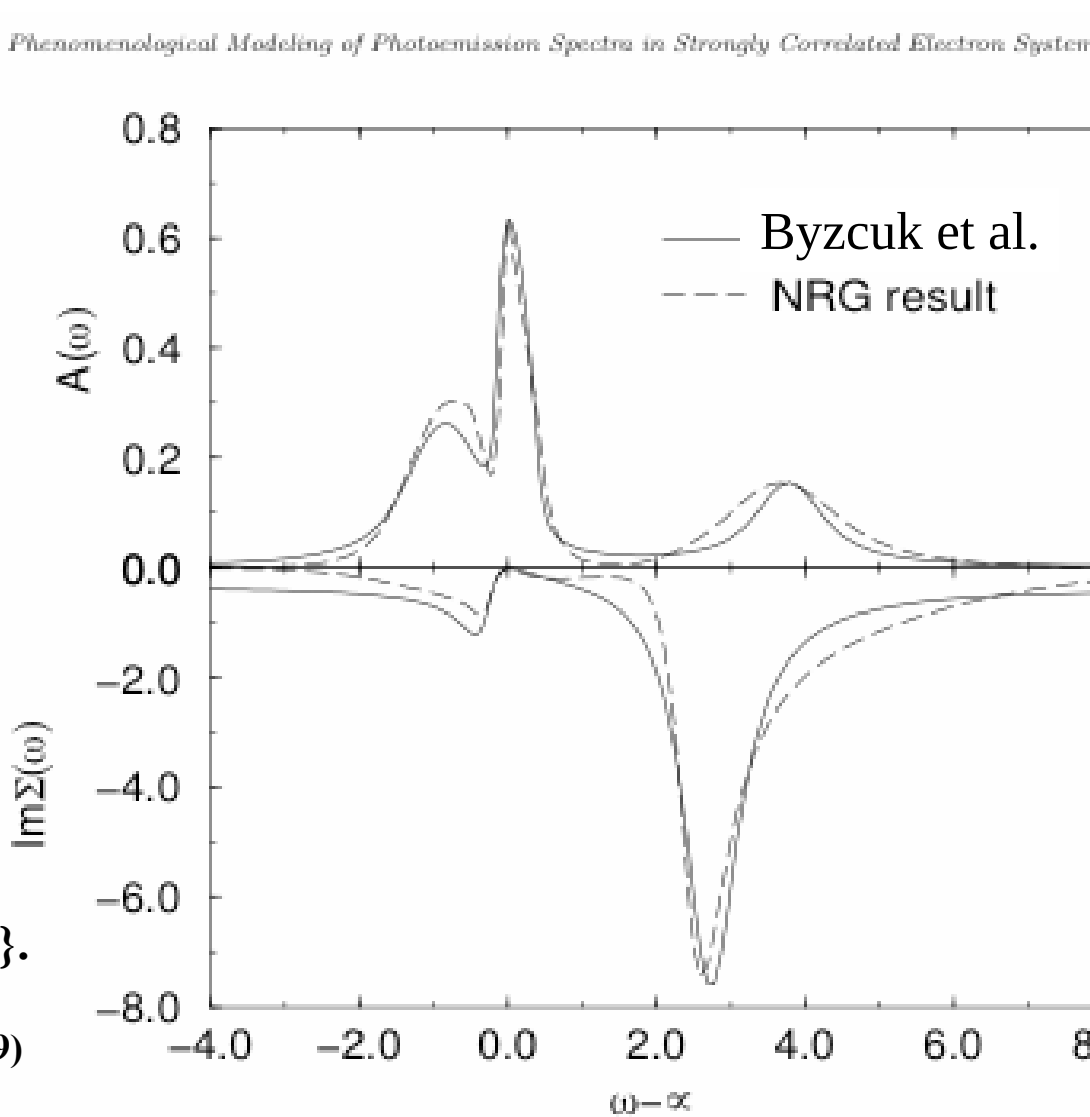
Phenomenological modeling of low energy Fermi Liquid behaviour in a hole-doped Hubbard model. Quasiparticle resonances and incoherent background. Fermi surface crossing defined by the vanishing of $\Sigma(k,0)$. The quasiparticle weight equals the ratio of energy scales Δ^*/Δ



Destruction of FL behaviour tuned by a power-law exponent nu. Vanishing residue, but finite resonance weight Δ^*/Δ distributed along branchcuts. For nuŠ0.25 => marginal FL. Scenario used to interprete lineshapes in Bi-2212. Andreas Müller, PhD Thesis, Shaker Verlag Aachen (2000). Computer programs for linefitting can be found there.

Phenomenological spectrum for Hubbard model (unpublished)



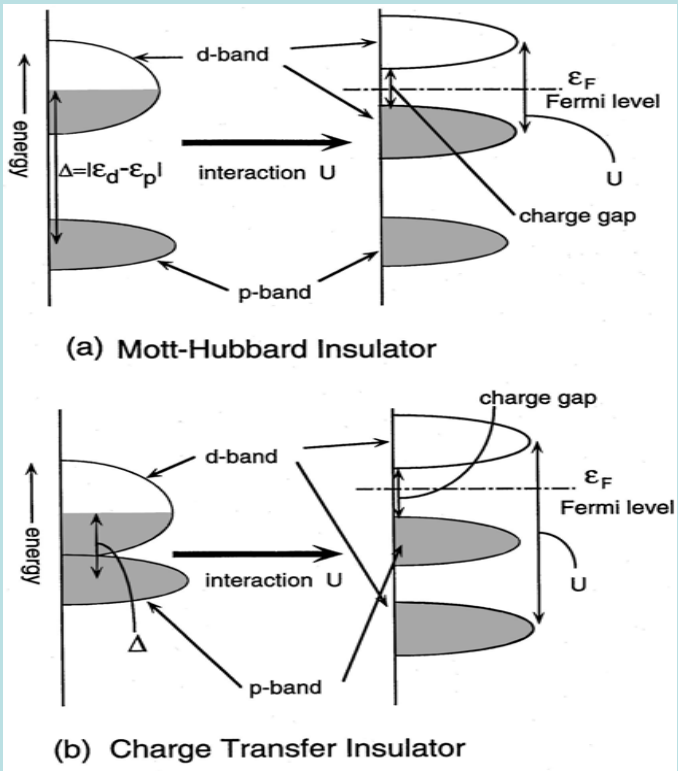


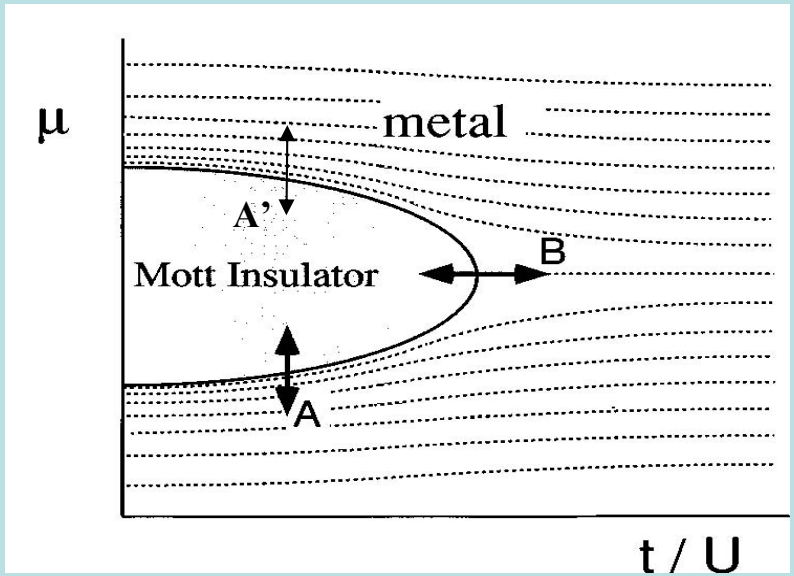
Selfenergy and integrated DOS of Hubbard model in approximation {3/4}.

Comparison to Augsburg phenomenology (Byzcuk et al. Int.J.Mod.Phys. B 16 (2002) 3759)

- **Check of Herglotz property and numerical (NRG) result both in favour of our ansatz**

Obtaining a Strongly Correlated Metal by doping the Charge Transfer Insulator





Six generic cases encountered in transition metal oxides

Minimal scenario for cases (a,A), (a,A') and (a,B): <u>One band Hubbard model</u>

Minimal scenario for cases (b,A), (b,A') and (b,B): <u>Two-band periodic Anderson model.</u>

<u>Aspect of charge transfer:</u> Strongly correlated orbital "d" is coupled via hopping or hybridisation with non-interacting ligand orbital "p". Cases (b,A) and (b,A'): Large U; doping relative to n=3 (1 hole/site), no symmetry n>3 n<3. Relevant for high T_c cuprates.

Dyson Equation

$$G^{-1} = \omega - \Sigma(k,\omega)$$

- **Dyson equation is a matrix, block diagonal in k, spanned by orbitals l (usually a finite set obtained from "downfolding")**
- **Hubbard U, local repulsion: Two-body interaction in one spin-degenerate local orbital l="d" (higher degeneracy also possible)**
- **Hopping: One-body hopping terms couple an arbitrary number of ligand orbitals l="p" to the correlated orbital. Direct hopping often much smaller than transfer through the ligands**
- **The PAM has a non-trivial zero bandwidth limit: a two orbital local molecule. But, in general, local hybridisation V not realistic.**
- **For indices (l,l')=(p,p'), (p,d) and (p',d), elements $(G^{-1})_{ll'}$, in this matrix are bare, unrenormalized one-body terms, except for a shift in the diagonal, due to the chemical potential μ**
- **Only the element $(G^{-1})_{dd} = \omega - \Sigma_{dd}(k,\omega)$ is renormalized.**

Fermi Surface determined by manybody eigenvalues at T=0

$\Sigma(k,0)$ is a hermitean matrix

- Diagonalisation yields Eigenvektors $u_{il}(k)$ and their Eigenvalues $\eta_i(k)$, forming bands.
- Labeling of quasiparticles in multiorbital case : Each vanishing eigenvalue defines one QP-band.
- Representation of the Dyson equation in the priviledged frame of the $u_{il}(k)$ (unitary transformation):
- $\mathbf{(G^{-1})_{ij} = (\omega - \eta_i(k))\delta_{ij} - u_{id}(k)\, \delta\Sigma_{dd}(k,\omega)\, u_{dj}(k)}$
- Twobandmodels i=±: Set $ep(k)-\Sigma_{dd}(k,0) = A\cos(2\theta)$
  $V = A\sin(2\theta)$
  then $u_{+p} = u_{-d} = \cos(\theta)$ and $u_{+d} = -u_{-p} = \sin(\theta)$ covers all possible cases. Angle θ characterises degree of hybridisation.
- PAM: Only one of the eigenvalues can cross zero.

Exact relations between Greenfunctions in the twoband case (including PAM):

$$G_{pp}=\omega - \varepsilon_p(k) - V_k^2/(\omega - \Sigma_{dd}(k,\omega))$$
$$G_{dd}=\omega - \Sigma_{dd}(k,\omega) - V_k^2/(\omega - \varepsilon_p(k))$$

To obtain the CFE expansion of G_{pp}, set:

- **$G_0 = G_{pp}$**
- **Sofar, in the spirit of DMFT, k-dependence other than $\varepsilon_p(k)$ was neglected**
- **$G_1 = 1/(\omega - \Sigma_{dd}(\omega))$ in the iterative process**

Input U, V, W, Δ, n

- **U = local interaction U_{dd} (repulsive)**
- **V = hybridisation V_{pd} (k-independent)**
- **W = 4t = halfwidth of bandstates $\{E_k\}$ on 2-dimensional lattice**
- **$E_p(k) = \Delta + E_k$ = bare p-band (V=0)**
- **$E_d = -\ \Delta$ = bare d-level (k-independent)**
- **n=3+X = filling per lattice site I X I <1**
- **$\{k_F\}$ = Fermi surface: k C $\{k_F\}$ when $E_k=\mu_0(n)$**

Output μ, m, ρ(ε) $A_{ij}(k,\varepsilon)$, $\rho_{ij}(\varepsilon)$,

Selfconsistent chemical potential

$\mu(n)$

Selfconsistent filling of d-level

$m(n) = \langle n_{d\sigma} \rangle$ (per spin)

Density of states $\rho(\varepsilon)$

Partial k-resolved spectra

$A_{ij}(k,\varepsilon)$

Partial densities $\rho_{ij}(\varepsilon)$

Relevant regime is $2\Delta < U < 4\Delta$

Charge transfer gap roughly determined by $\Delta_{CT} = U-2\Delta$

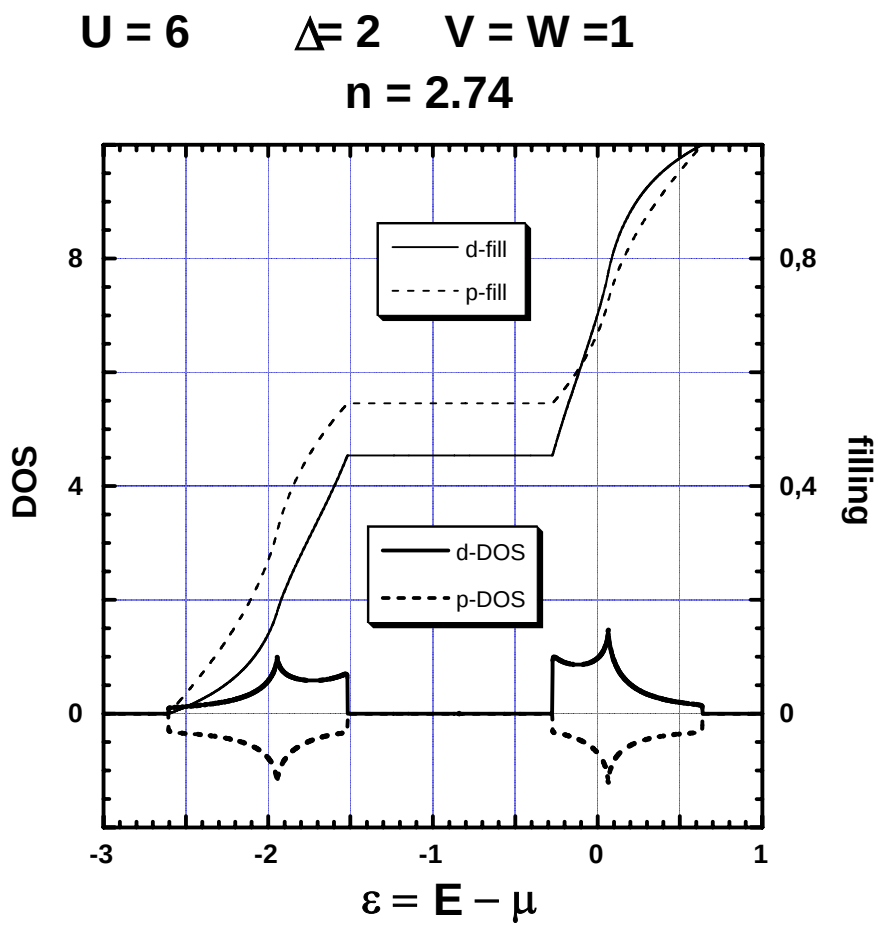
Hartree approximation as uncorrelated reference system: Padé <1/2>

- Exact sumrule: $\omega_3 = mU - \Delta - \mu$
- Hartree is obtained by setting $G_2 = 0$
- Although selfconsistently determined, values of m and μ are incorrect

Typical selfconsistent Hartree

Accentuates hybridisation

Fulfills Luttinger sumrule



Hubbard-I: Padé <2/3> is first systematic approximation showing correlations

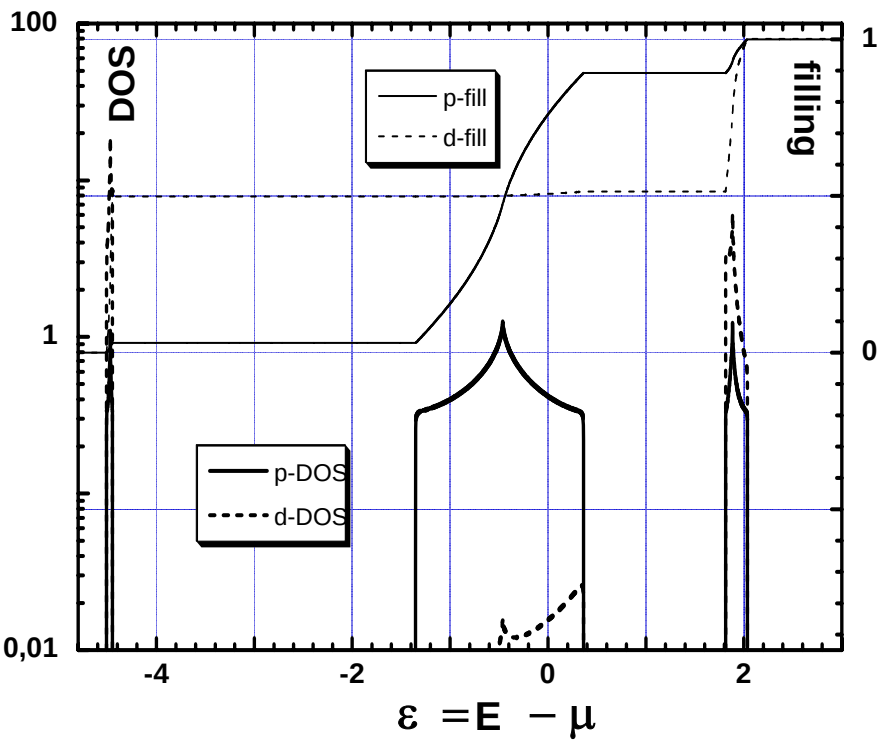
- Next exact sumrule: $s_4^2 = m\,(1-m)\,U^2$
- Approximate sumrule (a kinetic energy term neglected): $\omega_5 = (1-m)\,U - \mu$
- Then, setting $G_3 = 0$, a Hubbard-I type solution is obtained

Typical selfconsistent Hubbard-1

Exaggerates charge transfer

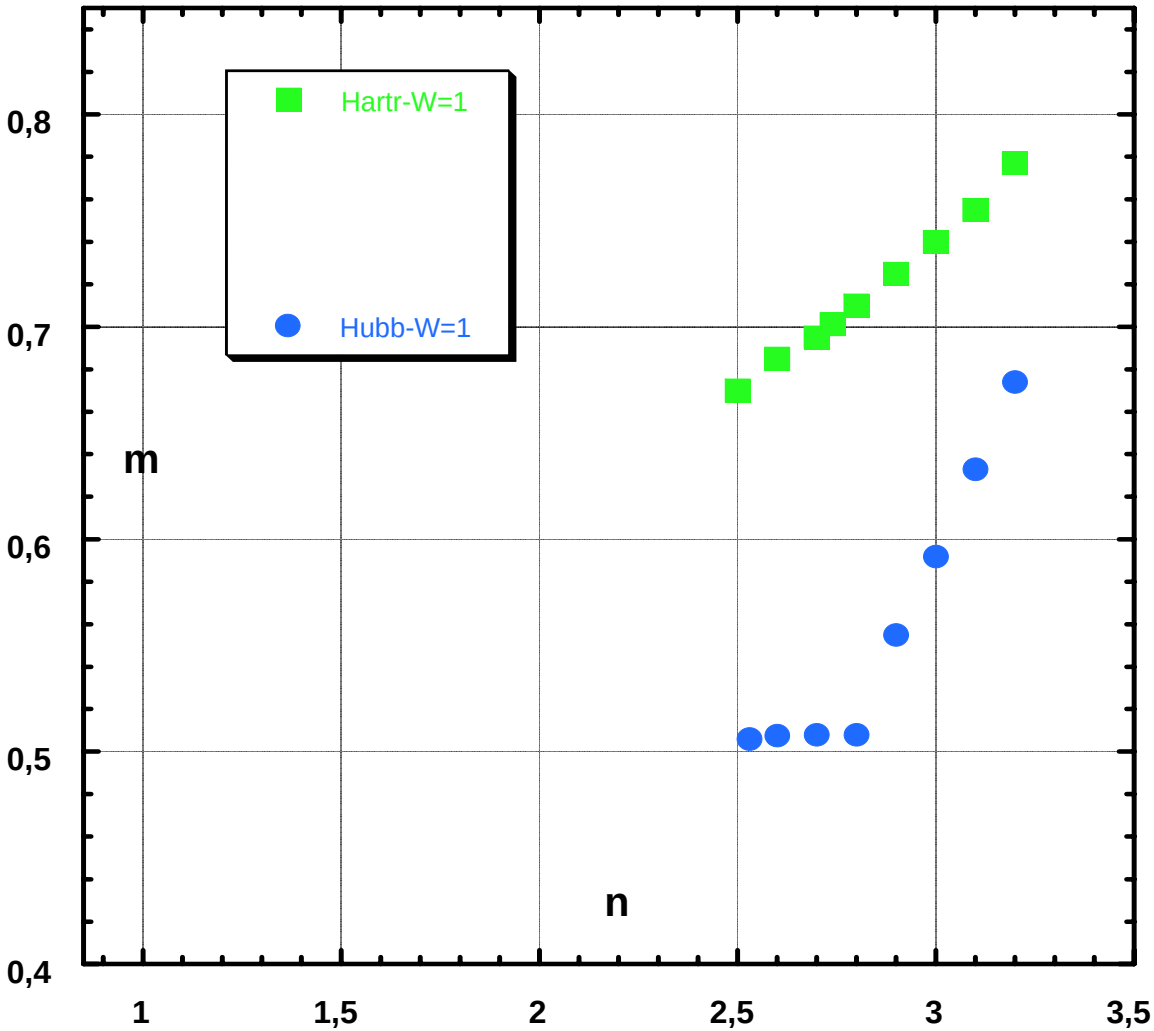
Suppresses hybridisation

Violates Luttinger sumrule



Partial filling m: A revealing problem

"Selfconsistency is necessary but not sufficient"



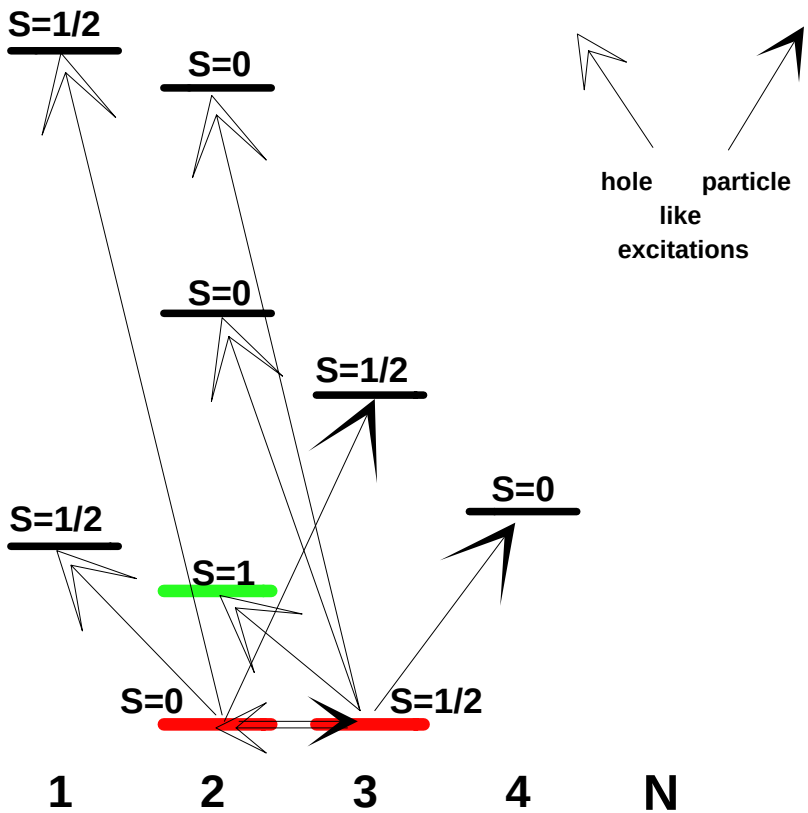
For further understanding: Go to the zero bandwidth limit, where Hartree and Hubbard-1 can be compared to exact solution

Level scheme at crossover N=2 <---> N=3

Groundstate probabilities P $P_2=1-v$ $P_3=v$

Mixed valence n=r+v r=[n]=2 0<v<1

Particle removal and particle addition: All possible transitions in the zero bandwidth limit



Gapless transition rate: $R_o = R_{o<}(n) + R_{o>}(n)$

alias "zero bias conductance peak"

Zero bandwidth limit

Average <n>=2.8

A "zero bias peak" at ε=0 characterises the configurational crossover between n=2 and n=3.

The exact partial Green functions

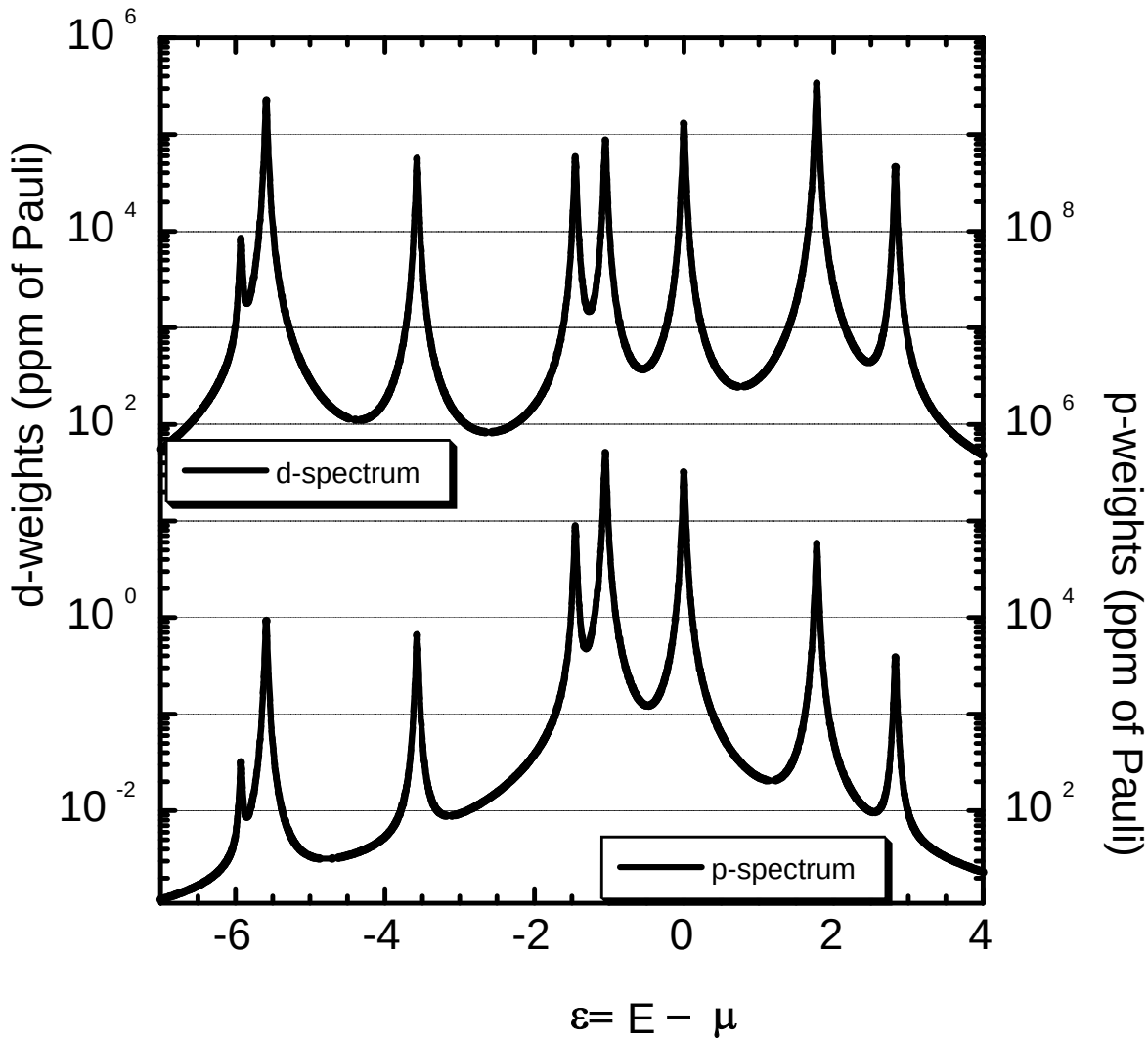
$G_{dd}(\omega)$ **and** $G_{pp}(\omega)$

are Padés of order

<7/8>

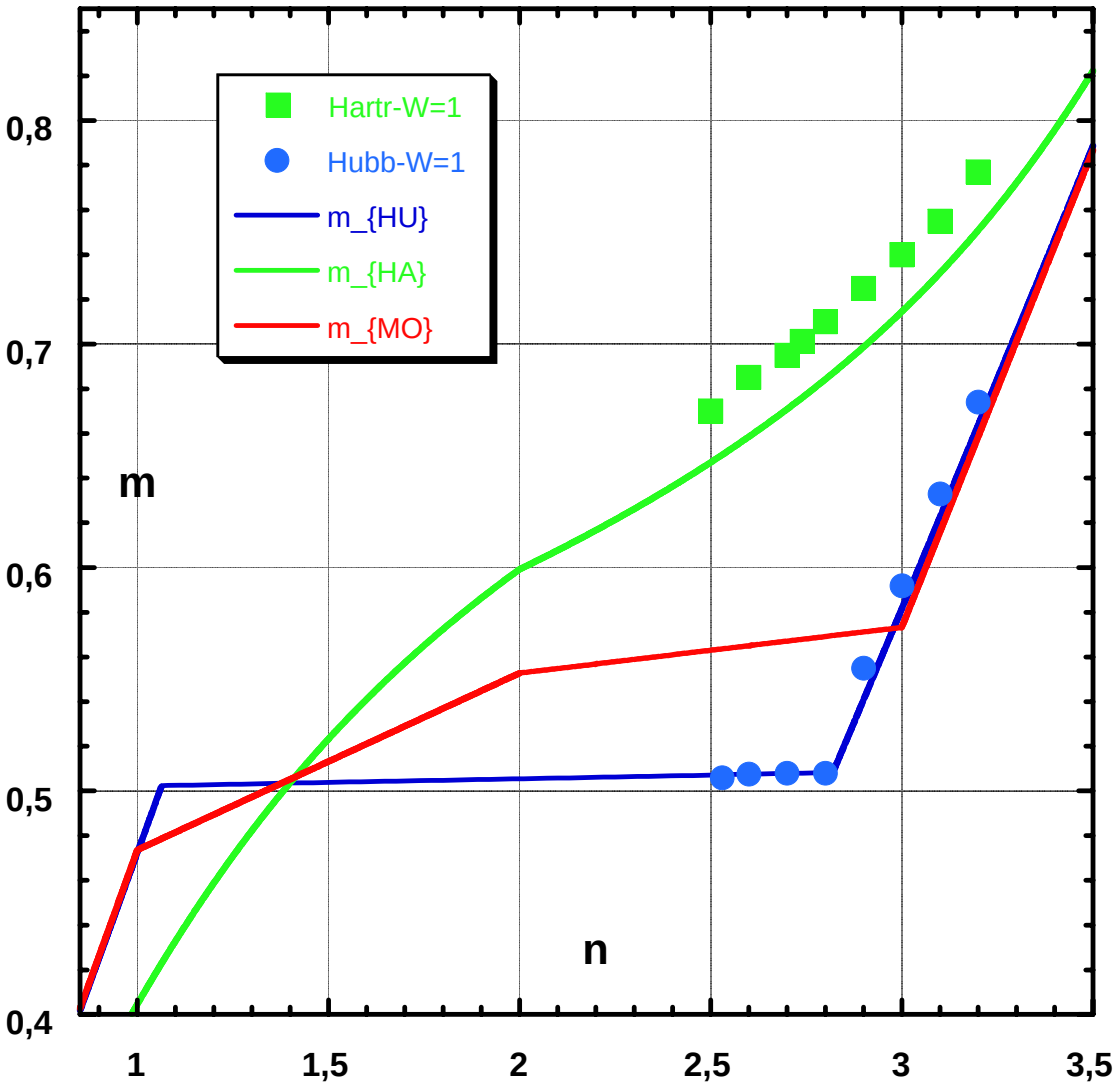
Molecule at configurational crossover

Exact spectra of G_{dd} and G_{pp}



Partial filling m: A revealing problem

Exact solution in the zero bandwidth limit



How many sumrules from the

Zero bandwidth limit

is it useful to keep ?

Compare Padé approximants

<2/3> Hubbard-1 :

No "zero bias peak". Reason for violation of Luttinger SR !

No singlet-triplet splitting

<3/4> : Adopted approx.

Produces the correct "zero bias peak" and singlet-triplet splitting

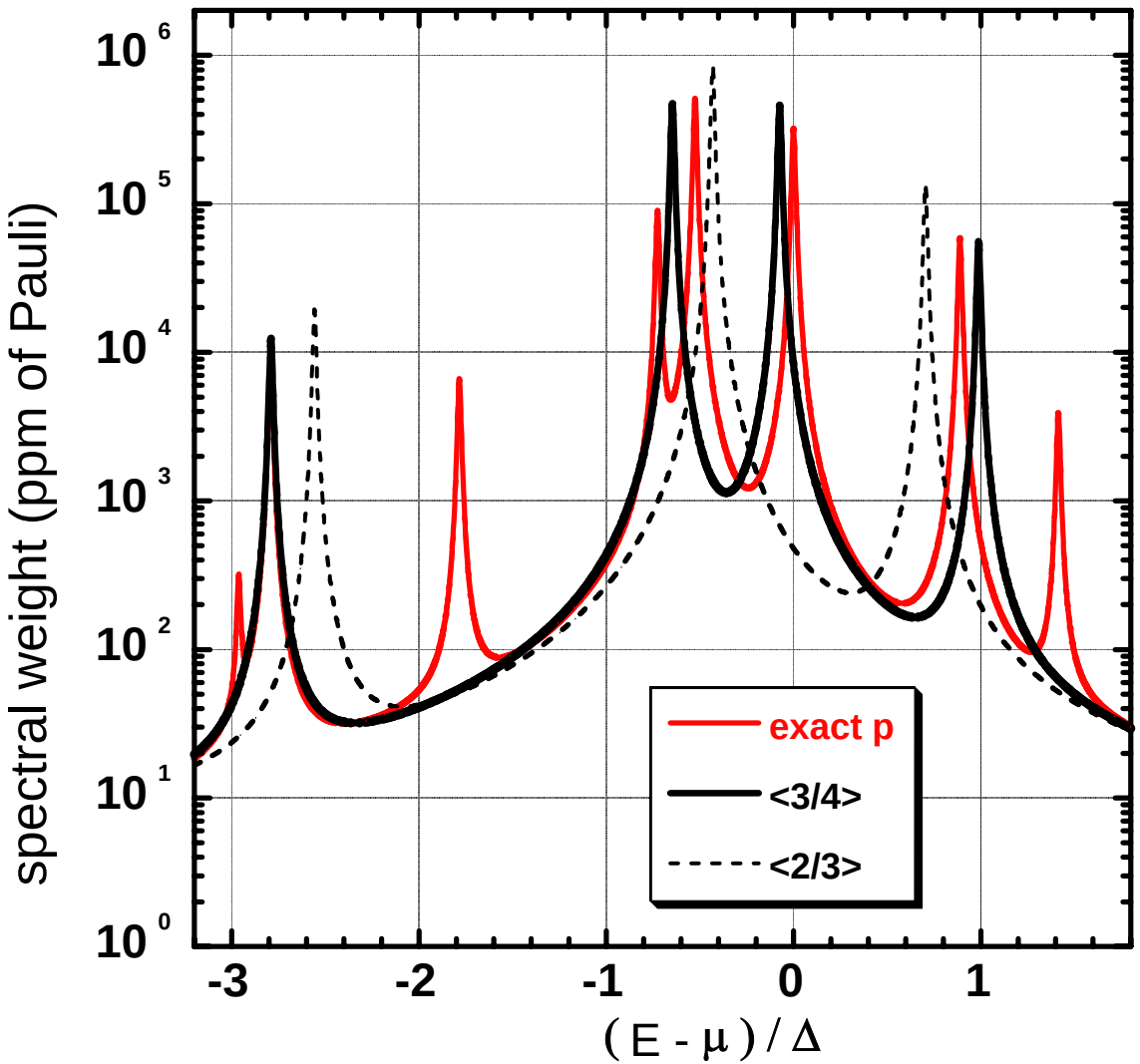
<7/8> : Exact

But: local finestructure does not survive hopping (finite W)

Exact spectrum of G_{pp} compared

to Padé approximants <2/3> and <3/4>

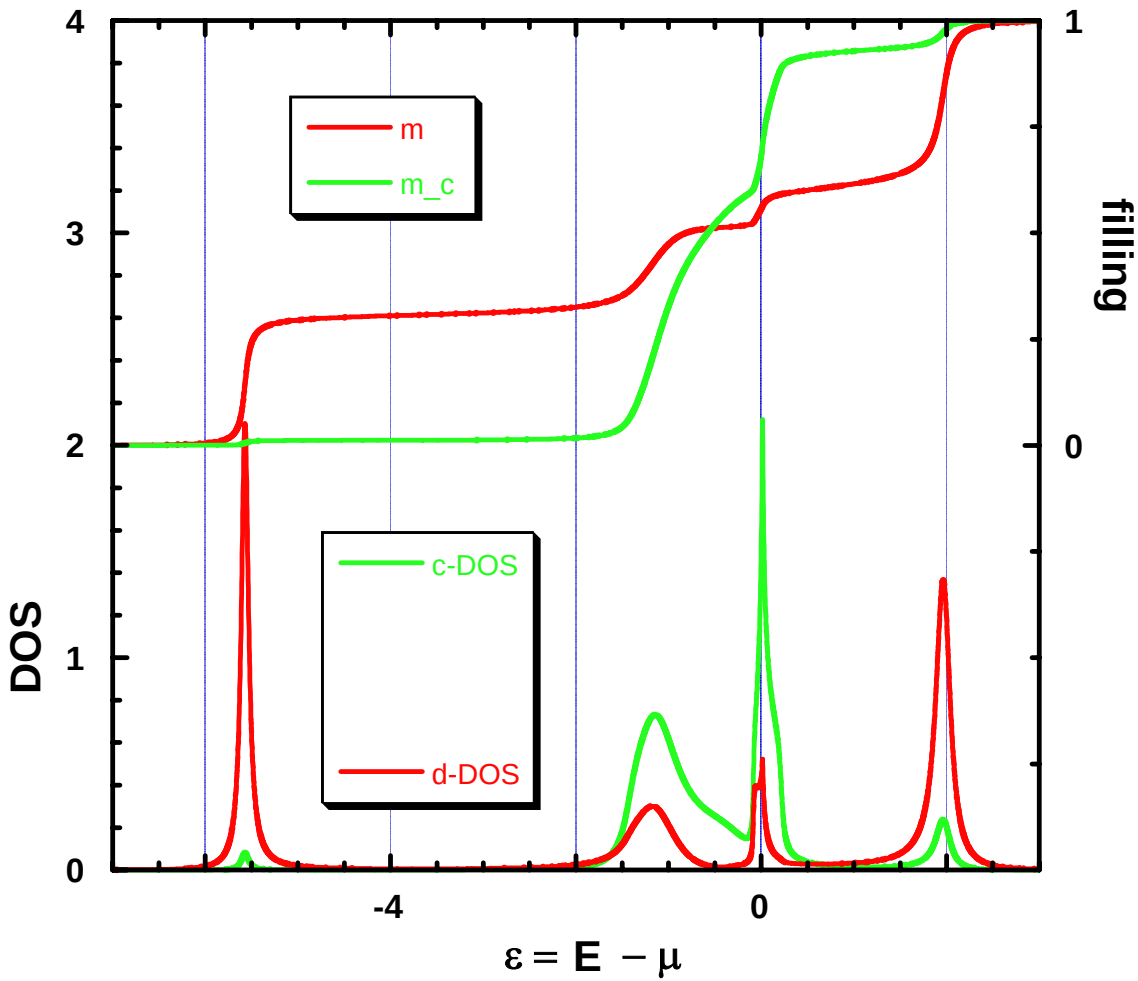
U/Delta = 3.0 V/Delta = 0.5 n=2.8



Use local sumrules from Padé <3/4> at W=0 to obtain solution for PAM with finite bandwidth at approximation level $\{4/\square 5\}_D$

Because of correct zero bias peak, a tiny shift of μ is enough to reach selfconsistency

Hubbard satellites, predominantly of d-character. Valence states, predominantly of c-character (label c was previously p). CT-gap around ε≈+1. QP band with singlet character around ε ≈0, valence band with triplet character around ε≈-1, separated by a quasigap

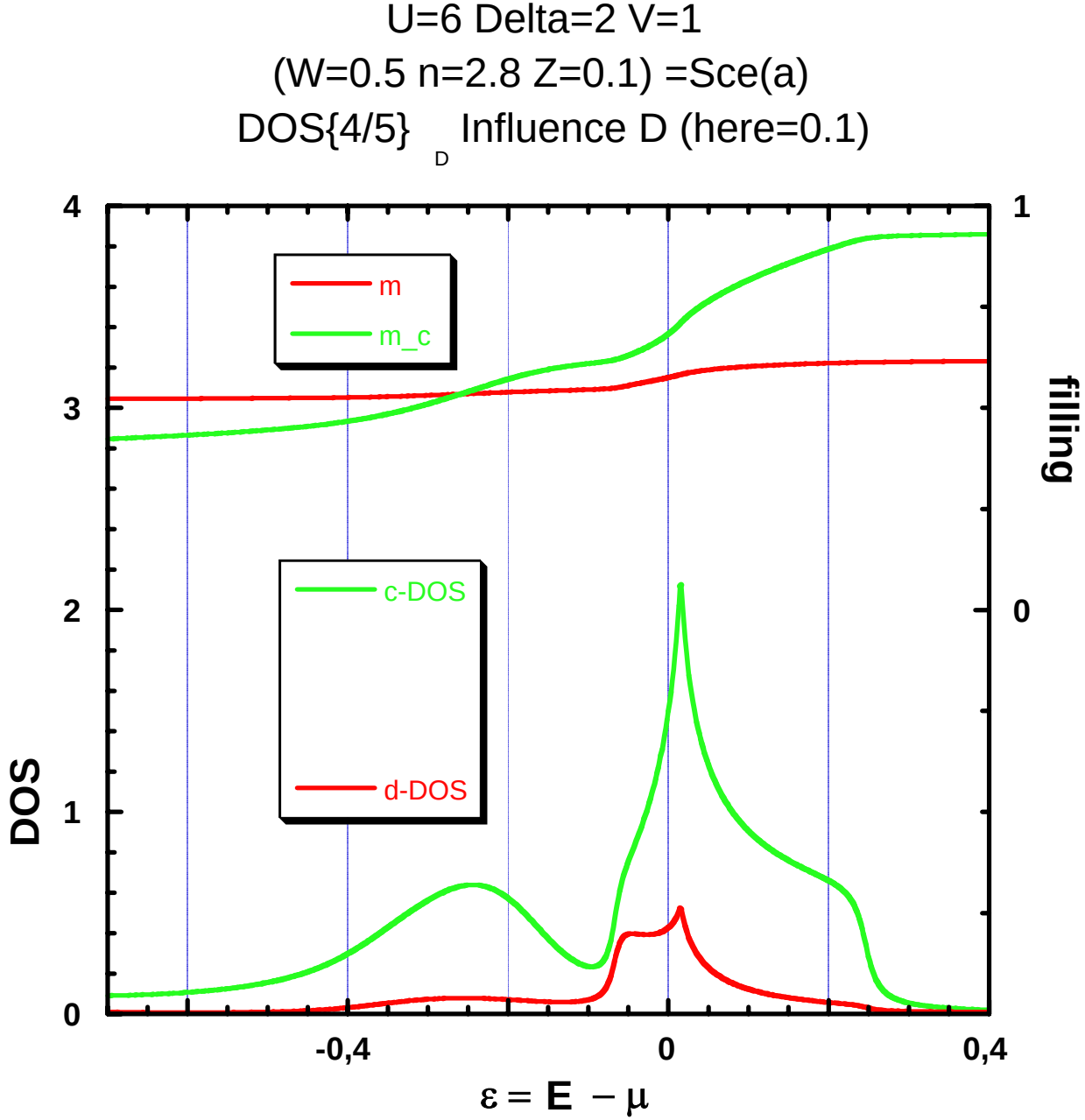


Conclusions I
Zoom on DOS in the valence region

n=2.8 : Hole doping relative to a parent CT-insulator with one hole per site.
Position of Van Hove singularity in the center of the QP-band in agreement with the Luttinger sumrule.

Momentum resolved spectra (also with k-dependent V_k) can be modeled.

Contact me for eventual applications and collaborations.



Conclusions II

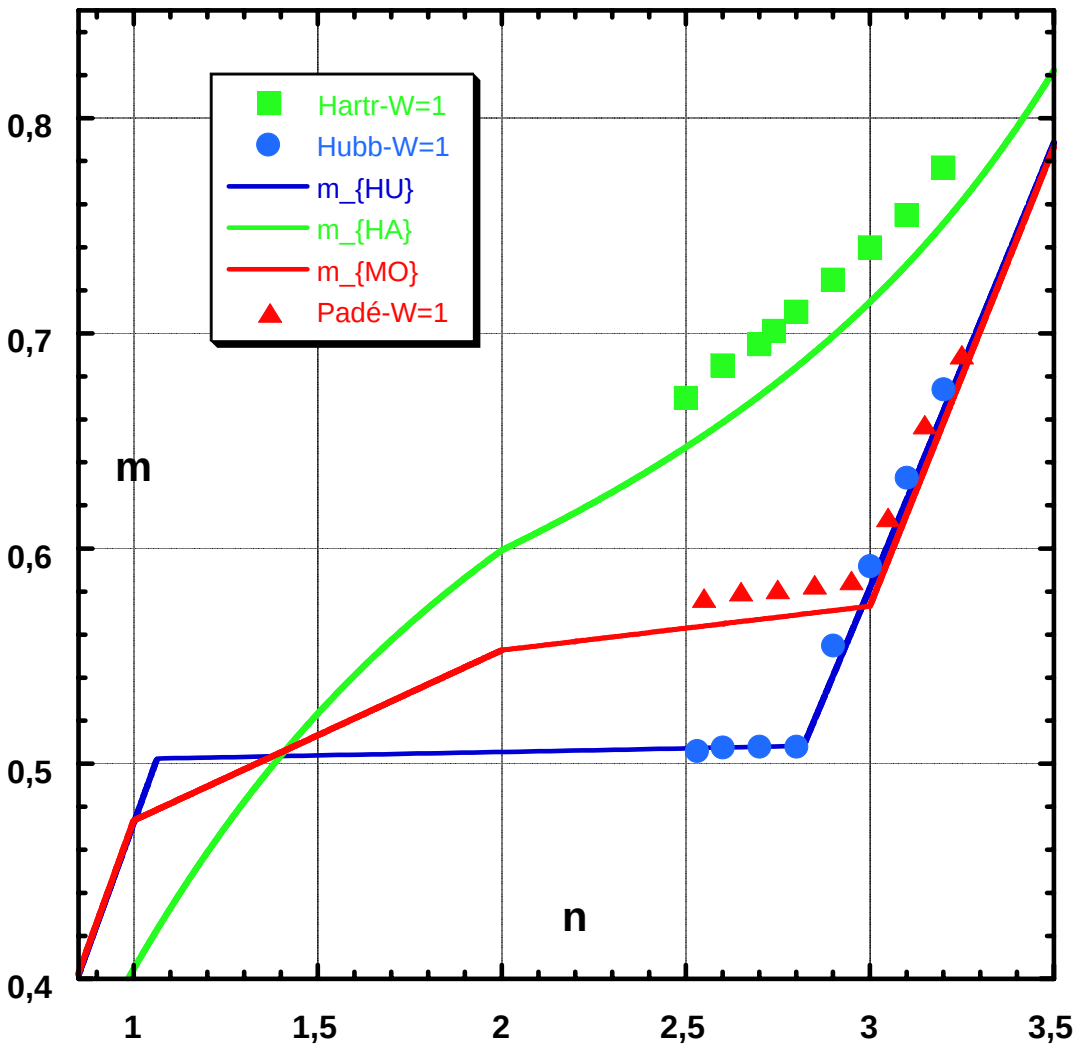
Selfconsistent d-filling m: Outcome for m depends crucially on Padé order, not crucially on bandwidth 0≤W≤1

Hartree: No correlations. Bad everywhere, except in low hole density limit n --> 4. Warning for density functional method!

Hubbard-1: Correlation effect overestimated.
O.k. for particle doping, bad for hole doping. CT-crossover not at integer n=3 !

Sumrules up to Padé <3/4> taken over from molecule (MO): Yields selfconsistent analytical solution for PAM at finite bandwidth.
Correct CT- crossover at n=3.
Proposal: Check closeness to exact solution by NRG

Partial filling m: A revealing problem
Approximate solution with {4/5}



The continuous curves are the selfconsistent W=0 limits