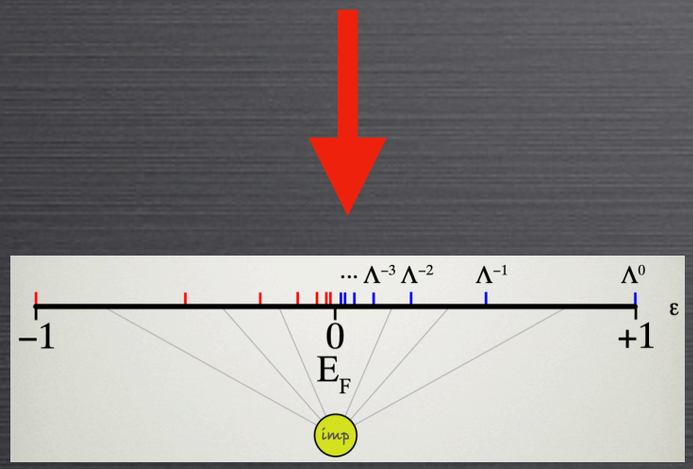
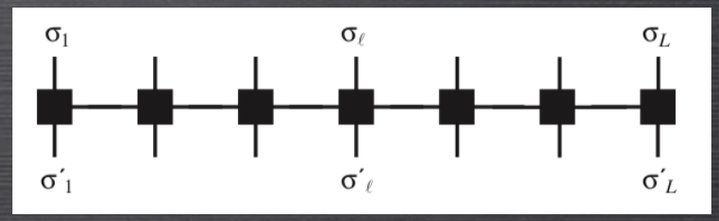
Solvers for quantum impurity problems (with superconducting baths)

Tutorial 3: NRG advanced





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University of Copenhagen, Oct 2021

Anatomy of impurity Green's function

$$G(z) = \frac{1}{z - \epsilon - \Delta(z) - \Sigma(z)}$$

hybridisation function

self-energy function

Hybridisation function

$$\Delta(z) = \sum_k |V_k|^2 \frac{1}{z - \epsilon_k}$$

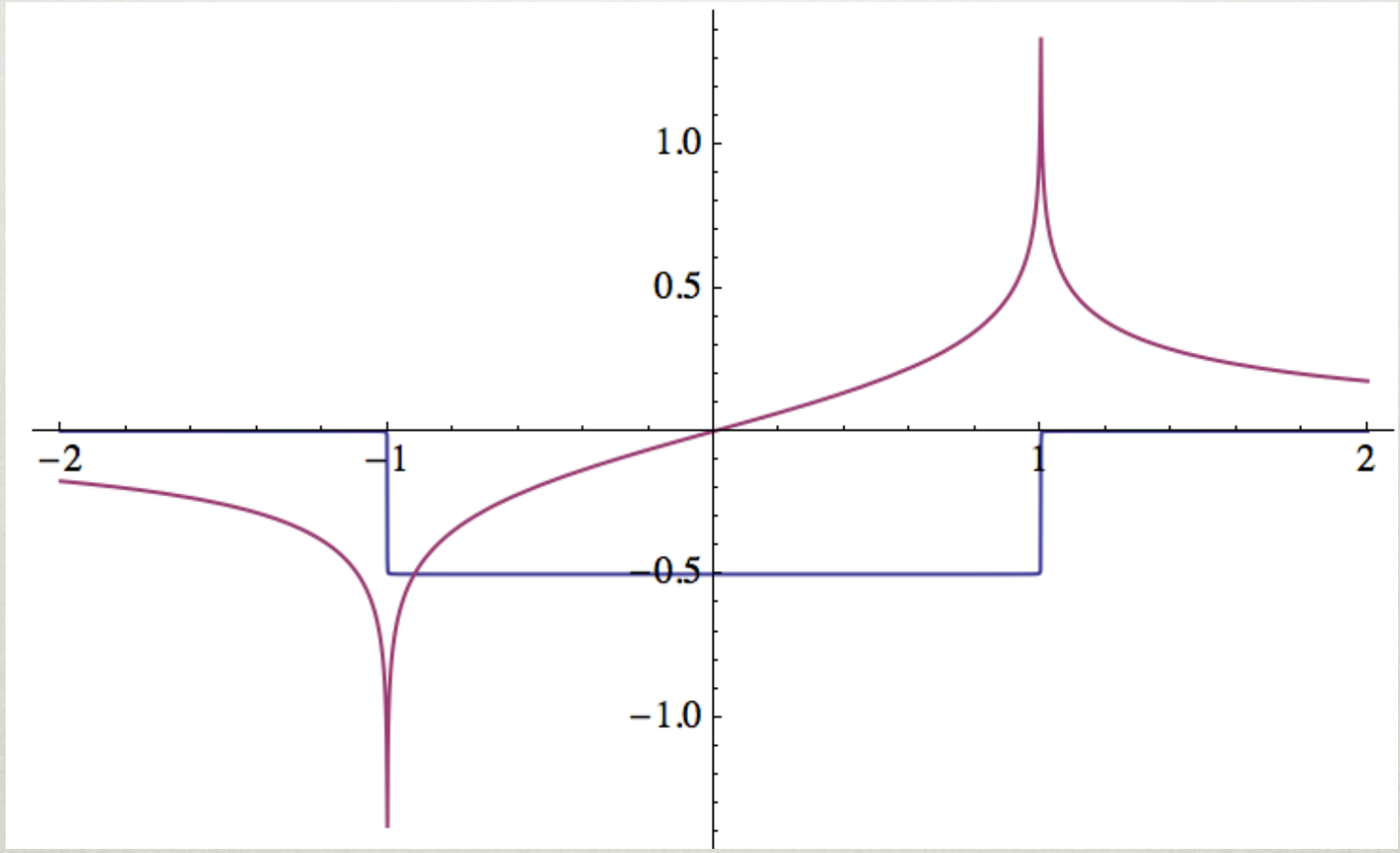
$$\Gamma(\omega) = -\mathrm{Im}\,\Delta(z + i0^+)$$

$$\Gamma(\omega) = \pi \sum_k |V_k|^2 \delta(\omega - \epsilon_k) \approx \pi \rho_0 |V_{k_F}|^2$$

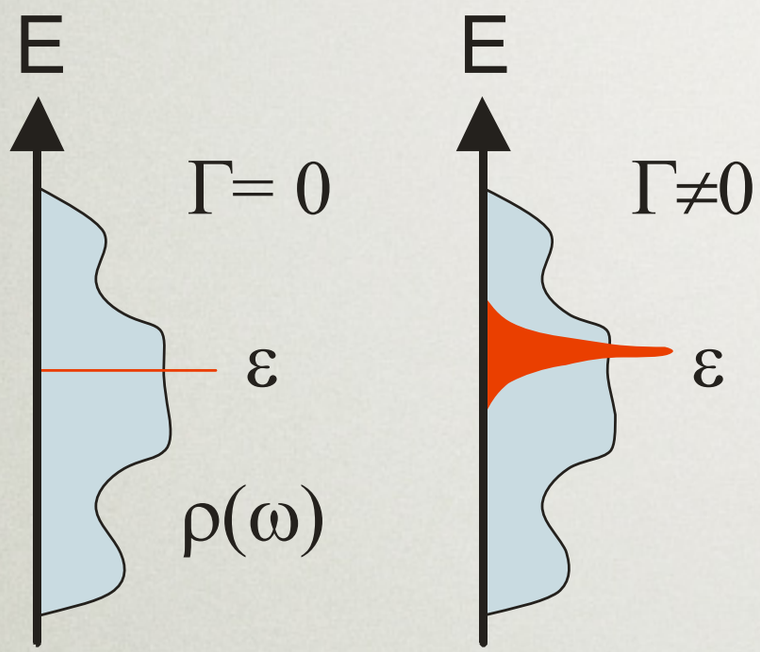
Hybridization function fully describes the effect of the conduction band on the impurity.
This is possible because the band is non-interacting.

HYBRIDISATION FUNCTION FOR FLAT BAND

$$\Delta(z) = \frac{\Gamma}{2\pi} \ln \frac{z+1}{z-1}$$



Resonant-level model



$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}\left(\frac{1}{\omega - \epsilon + \Delta(\omega)}\right)$$

$$\Delta(\omega) = \Gamma\left[i + \frac{1}{\pi}\ln\left(\frac{1-\omega/D}{1+\omega/D}\right)\right]$$

T=0 vs. T≠0

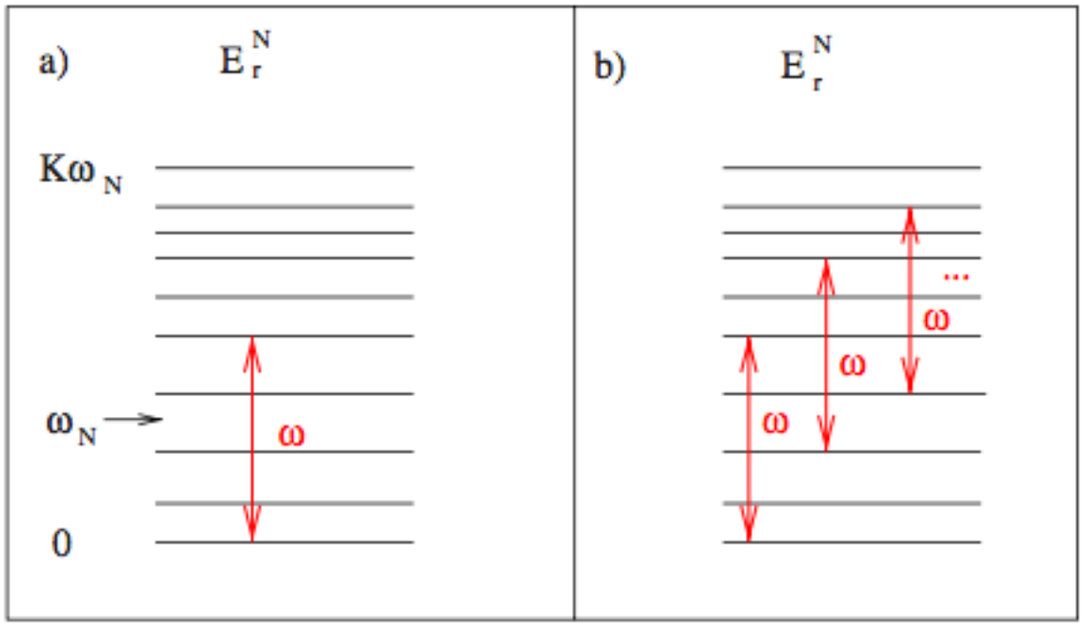
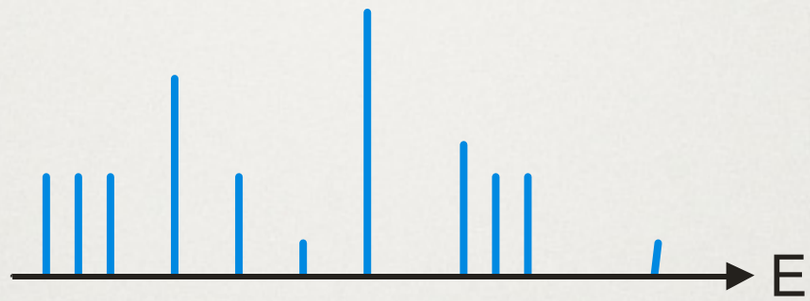


FIG. 9. (Color online) Excitations of H_N contributing to the spectral function at frequency ω for (a) $T=0$ and (b) $T>0$.

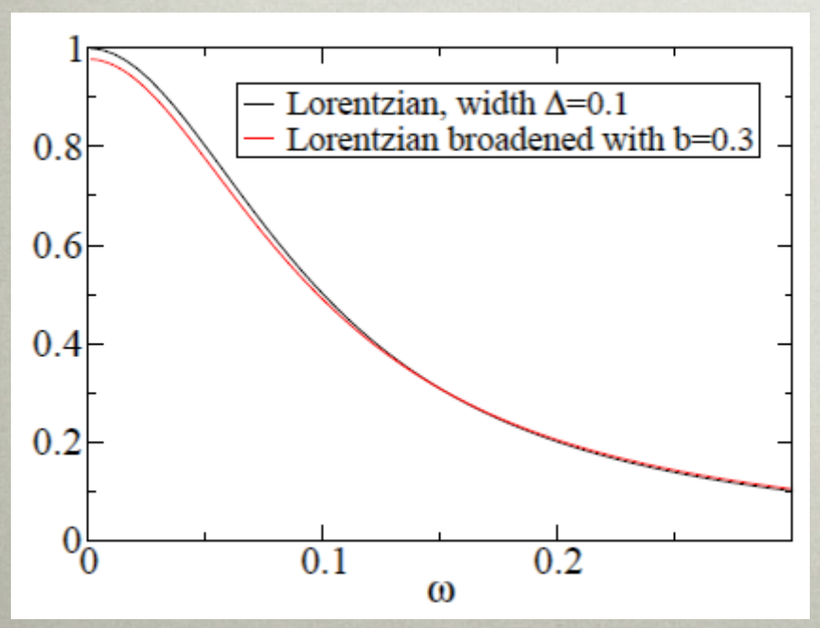
Broadening





Traditional log-Gaussian

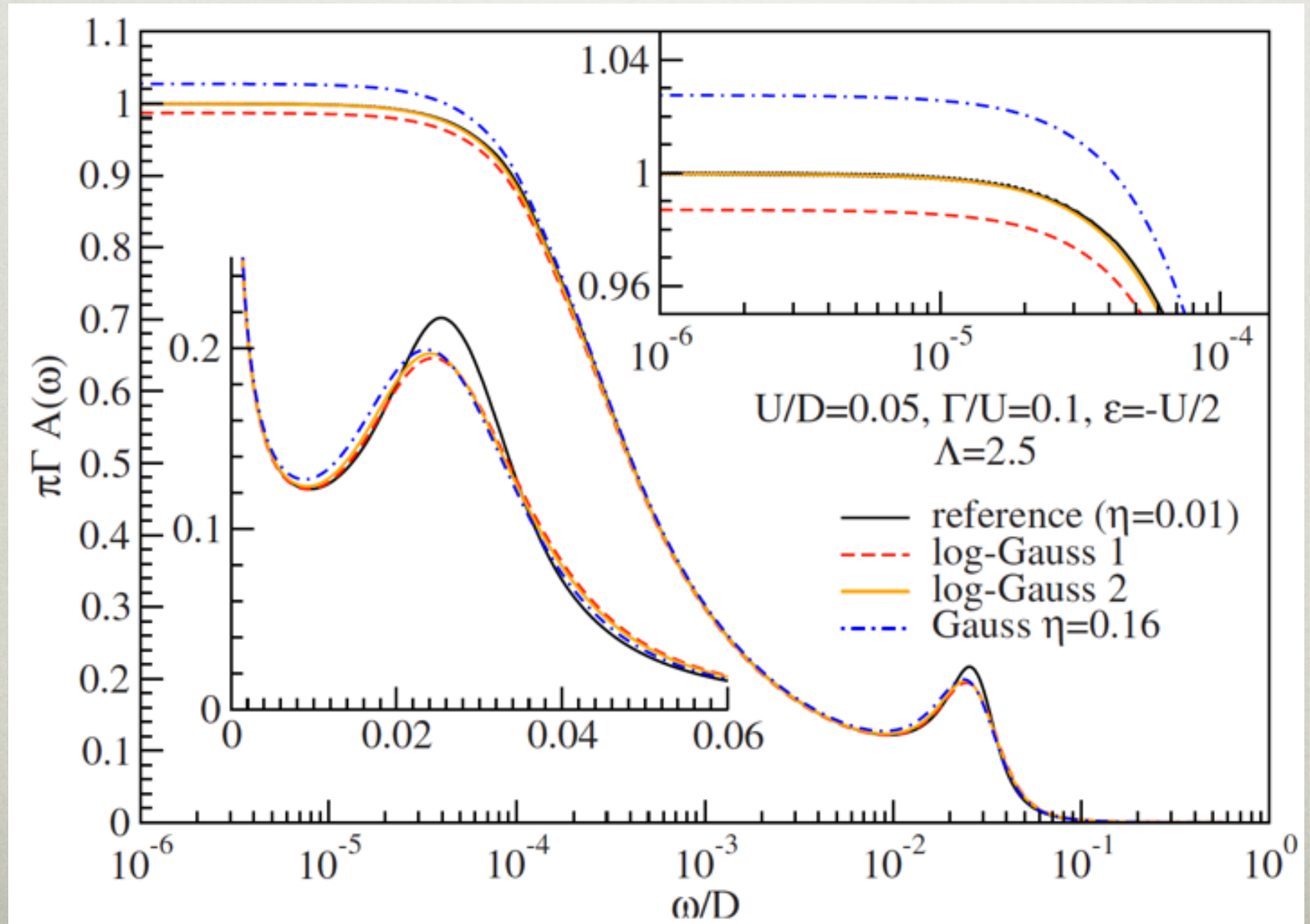
$$lG(\omega, E) = \frac{e^{-b^2/4}}{bE\sqrt{\pi}} \exp\left[-\left(\frac{(\log\omega - \log E}{b}\right)^2\right]$$



$$\delta\omega_+ = \omega\left(e^{b\sqrt{\ln 2}} - 1\right)$$
$$\delta\omega_- = \omega\left(1 - e^{-b\sqrt{\ln 2}}\right)$$

MODIFIED LOG-GAUSSIAN

$$mLG(\omega, E) = \frac{1}{\alpha|\omega|\sqrt{\pi}} \exp\left[-\left(\frac{\log(\omega/E)}{\alpha} - \frac{\alpha}{4}\right)^2\right]$$



Broadening at finite temperatures

Second stage of broadening:

$$G(\omega, E) = \frac{1}{\omega_0 \sqrt{\pi}} \exp\left[- \left(\frac{\omega - E}{\omega_0} \right)^2 \right]$$

$$\omega_0 \propto T$$

```
[extra]
U=0.01
Gamma=0.001
delta=0

[param]
symtype=QS
discretization=Z
Lambda=2
Tmin=1e-10
keepenergy=10
keep=5000

model=SIAM
```

```
ops=A_d
specd=A_d-A_d
```

choice of operators / spectra

A_d $\langle m|d_\sigma^\dagger|n\rangle$

A_d-A_d $\langle\langle d_\sigma; d_\sigma^\dagger\rangle\rangle_\omega$

```
broaden_max=0.1
broaden_min=1e-7
broaden_ratio=1.02
```

frequency mesh for output

$$\omega_n = \text{broaden_max} \times \text{broaden_ratio}^{-n}$$

```
fdm=true
T=1e-10
```

algorithm

```
smooth=new
alpha=0.6
omega0=1e-99
```

spectral smoothing

CFS & FDM-NRG

CFS = complete Fock space
FDM = full density matrix

Anders, Schiller, PRL 2005, PRB 2006

Peters, Pruschke, Anders, PRB 2006

Weichselbam, von Dellt, PRL 2007

COMPLETE BASIS SET FOR WILSON CHAIN

$$|\alpha_{\rm imp}, \alpha_0, \ldots, \alpha_N\rangle$$

m: shell label

$$|r, e; m\rangle \qquad e = \{\alpha_{m+1}, \ldots, \alpha_N\}$$

$$|k, e; m\rangle_{\rm kp} \qquad |l, e; m\rangle_{\rm dis}$$

$$\mathcal{F}_N = {\rm span}\{|l, e; m\rangle_{\rm dis}\}$$

Anders, Schiller, PRL 2005, PRB 2006

$$\rho = \sum_m \sum_{le} |le; m\rangle \frac{e^{-\beta E_l^m}}{Z} \langle le; m|$$

Weichselbam, von Dellt, PRL 2007

CFS vs FDM vs DMNRG

- CFS and FDM equivalent at T=0
- FDM recommended at T>0
- CFS and FDM are slower than DMNRG
  (all states need to be determined, more complex expressions for spectral functions)
- No patching, thus no arbitrary parameter as in DMNRG

param

```
finite=true
dmnrg=true
fdm=true
cfs=true
```

$$\rho_{AB}(\omega) = -\frac{1}{\pi}\mathrm{Im}\left[\langle\langle A^\dagger; B\rangle\rangle_\omega\right]$$

`spec_FDM_dens_A_d-A_d.dat`

This is the spectral function = imaginary part of the Green's function.
Real part can be obtained using the Kramers-Kronig transformation.

Validation: are spectral functions correct?

- normalization to 1 (follows directly from the canonical anticommutation relations)
- fluctuation-dissipation theorem
- spectral moments (high-frequency expansion)

Fluctuation-dissipation theorem

$$\langle A(t)B\rangle = -\int_{-\infty}^{\infty} \frac{d\omega}{\pi} e^{-i\omega t} \frac{G''_{AB}(\omega)}{1+\epsilon e^{-\beta\omega}}$$

ε=+1 for fermions

$$\langle AB\rangle = -\int_{0}^{\infty} d\omega \left[-\frac{1}{\pi} G''_{AB}(\omega)\right]$$

at T=0

Caveat: G"(ω) may have a delta peak at ω=0, which NRG will not capture.

Not an issue when calculating with fluctuation parts, A-⟨A⟩.

$$C^{>}_{AB}(t) = \langle A(t)B \rangle$$

$$C^{<}_{AB}(t) = \langle BA(t) \rangle$$

$$C^{>,<}_{AB}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} C^{>,<}_{AB}(t)$$

$$C^{<}_{AB}(\omega) = e^{-\beta\omega} C^{>}_{AB}(\omega)$$

$$C^{>}_{AB}(\omega) = \sum_{nm} p_n A_{nm} B_{mn} 2\pi\delta(\omega + E_n - E_m)$$

$$C^{<}_{AB}(\omega) = \sum_{nm} p_m B_{mn} A_{nm} 2\pi\delta(\omega + E_n - E_m)$$

$$G''_{AB}(\omega) = -\pi \sum_{nm} p_n A_{nm} B_{mn} \delta(\omega + E_n - E_m)(1 + \epsilon e^{-\beta\omega})$$

$$\langle A(t)B \rangle = -\int_{-\infty}^{\infty} \frac{d\omega}{\pi} e^{-i\omega t} \frac{G''_{AB}(\omega)}{1 + \epsilon e^{-\beta\omega}}$$

Well satisfied in NRG at T=0, at T>0 some issues.

Spectral sum-rules

$$\mu_m = \int_{-\infty}^{\infty} \omega^m A_\sigma(\omega) \mathrm{d}\omega$$

$$\mu_0 = 1 \qquad \mu_m = \left\langle \left\{ [d_\sigma, H]_m , d_\sigma^\dagger \right\} \right\rangle$$

$$[A, B]_1 = [A, B] = AB - BA$$
$$[A, B]_{n+1} = [[A, B]_n, B]$$

"well-known", but first published by S. White, PRB 1991

ALTERNATIVE VERSION

$$\bar{\mu}_m = \int_{-\infty}^{\infty} \omega^m A_\sigma(\omega)/(1+\exp(\beta\omega))\mathrm{d}\omega$$

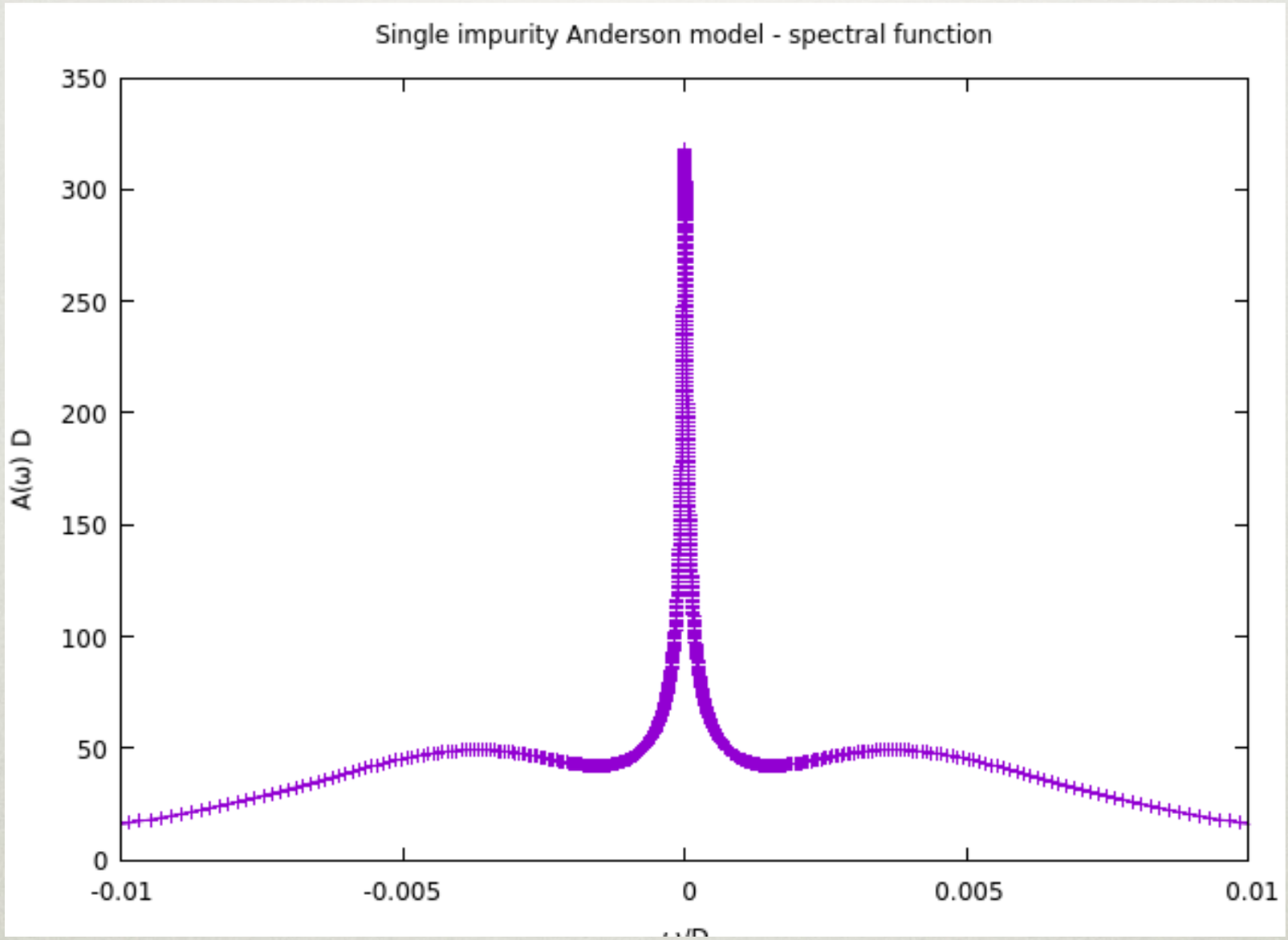
$$\bar{\mu}_m = \langle d_\sigma^\dagger, [d_\sigma, H] \rangle$$

$$\mu_1 = \epsilon + U \langle n_{-\sigma} \rangle$$

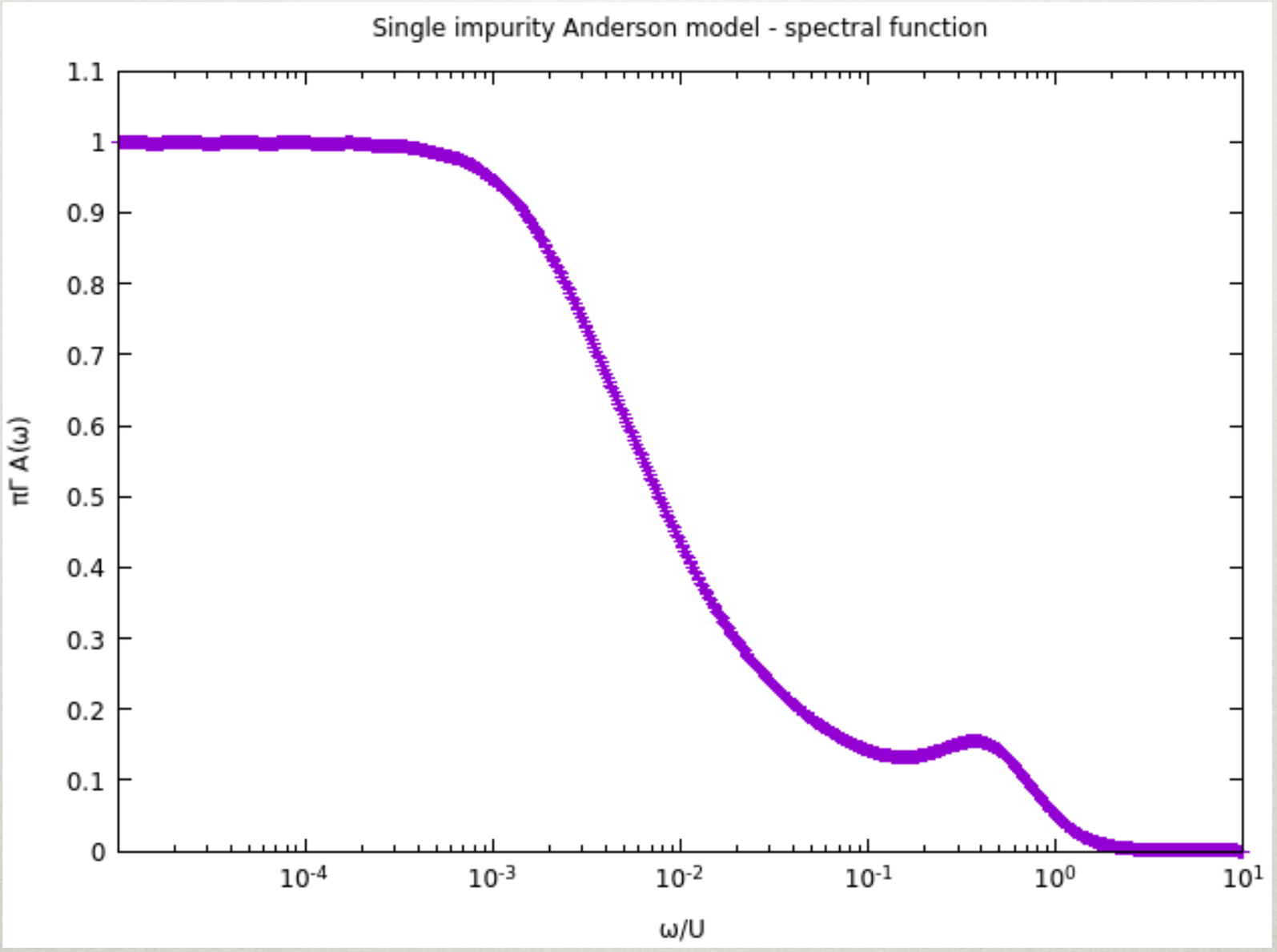
$$\mu_2 = V^2 + \epsilon^2 + (U + 2\epsilon)U \langle n_{-\sigma} \rangle$$

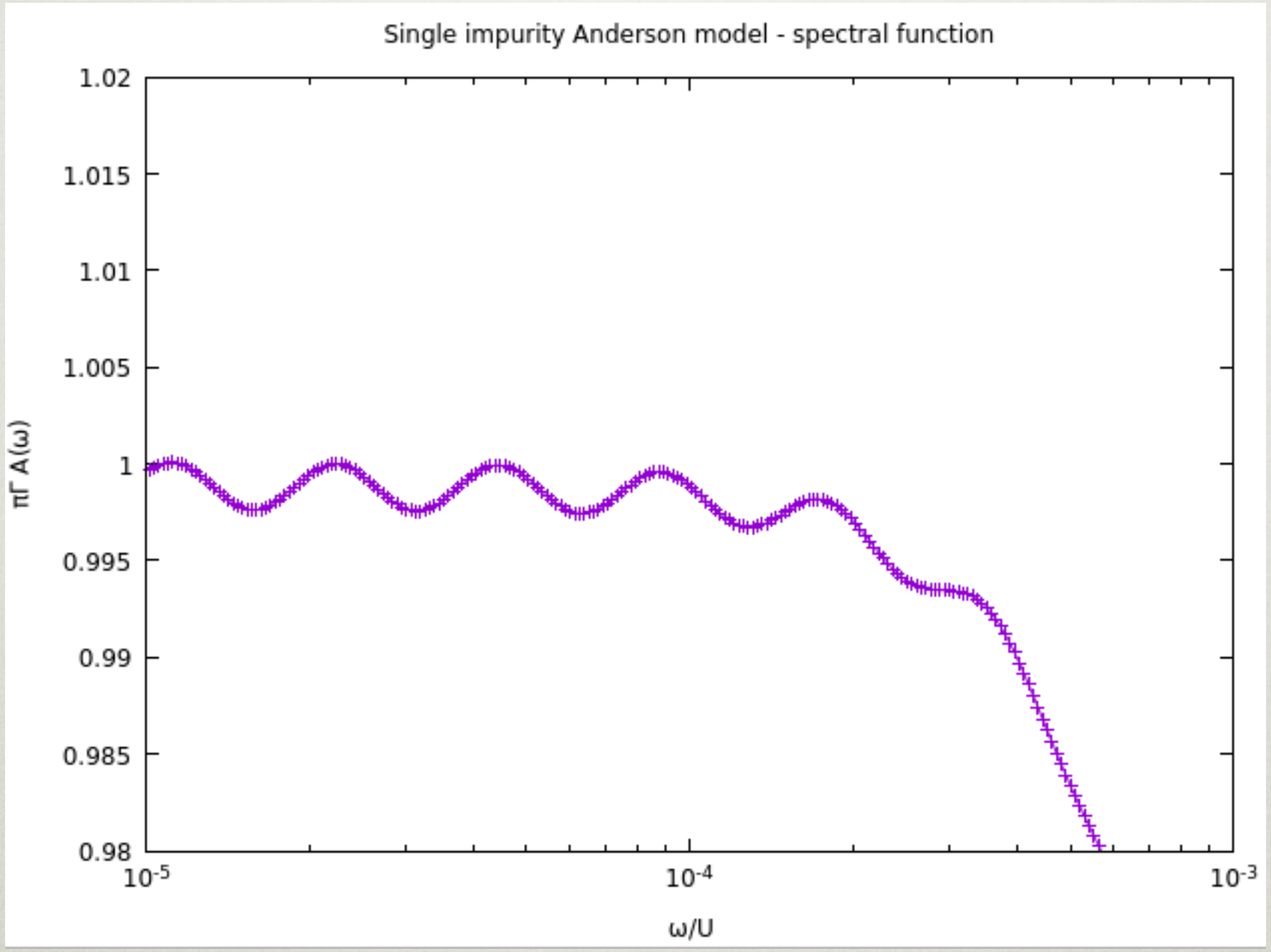
$$\begin{aligned}\mu_3 =& \epsilon^3 + 2\epsilon V^2 + U(3\epsilon^2 + 3\epsilon U + U^2 + 4V^2) \langle n_{-\sigma} \rangle \\ & - \frac{UV}{2}\left(4V \langle n_{f,-\sigma} \rangle + (U + 2\epsilon) \left\langle h^{(0)}_{-\sigma} \right\rangle\right) \\ & + t_0 UV \left\langle h^{(1)}_{-\sigma} \right\rangle .\end{aligned}$$

$$\begin{aligned}\mu_4 =& \epsilon^4 + 3\epsilon^2 V^2 + V^4 + U\left(4\epsilon^3 + 6\epsilon^2 U + 4\epsilon U^2 + U^3 + 2(7\epsilon + 4U)V^2\right) \langle n_{-\sigma} \rangle \\ & + \quad UV\left[(U + 2\epsilon)^2 \left\langle h^{(0)}_{-\sigma} \right\rangle + V\left((8\epsilon + 3U) \langle n_{f,-\sigma} \rangle + U \langle g_{-\sigma} \rangle\right)\right] + t_0^2 V^2 + 2t_0 U(U + 2\epsilon) \left\langle h^{(1)}_{-\sigma} \right\rangle\end{aligned}$$


Single impurity Anderson model - spectral function
A(ω) D
350
300
250
200
150
100
50
0
-0.01
-0.005
0
0.005
0.01

Friedel sum rule




Single impurity Anderson model - spectral function
πΓ A(ω)
1.02
1.015
1.01
1.005
1
0.995
0.99
0.985
0.98
10-5
10-4
10-3
ω/U

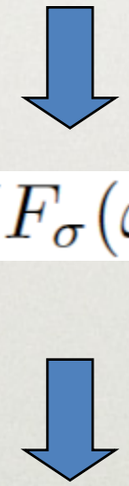
Self-energy trick

$$G_\sigma(\omega) = \langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle_\omega$$

A=-1/π Im[G]

$$F_\sigma(\omega) = \langle\langle n_{-\sigma} d_\sigma; d_\sigma^\dagger \rangle\rangle_\omega$$

B=-1/π Im[F]



$$\Sigma_\sigma(\omega) = U F_\sigma(\omega)/G_\sigma(\omega)$$

$$G_\sigma^{\text{improved}}(\omega) = \frac{1}{\omega - \epsilon - \Sigma(\omega) + \Delta(\omega)}$$

Bulla, Hewson, Pruschke 1998

param

```
ops=A_d self_d
specd=A_d-A_d self_d-A_d
```

model.m

```
(* All operators which contain d[], except hybridization (Hc). *)
Hselfd = H1;

selfopd = ( Chop @ Expand @ komutator[Hselfd /. params, d[#1, #2]] )&;

(* Evaluate *)
Print["selfopd[CR,UP]=", selfopd[CR, UP]];
Print["selfopd[CR,DO]=", selfopd[CR, DO]];
Print["selfopd[AN,UP]=", selfopd[AN, UP]];
Print["selfopd[AN,DO]=", selfopd[AN, DO]];
```

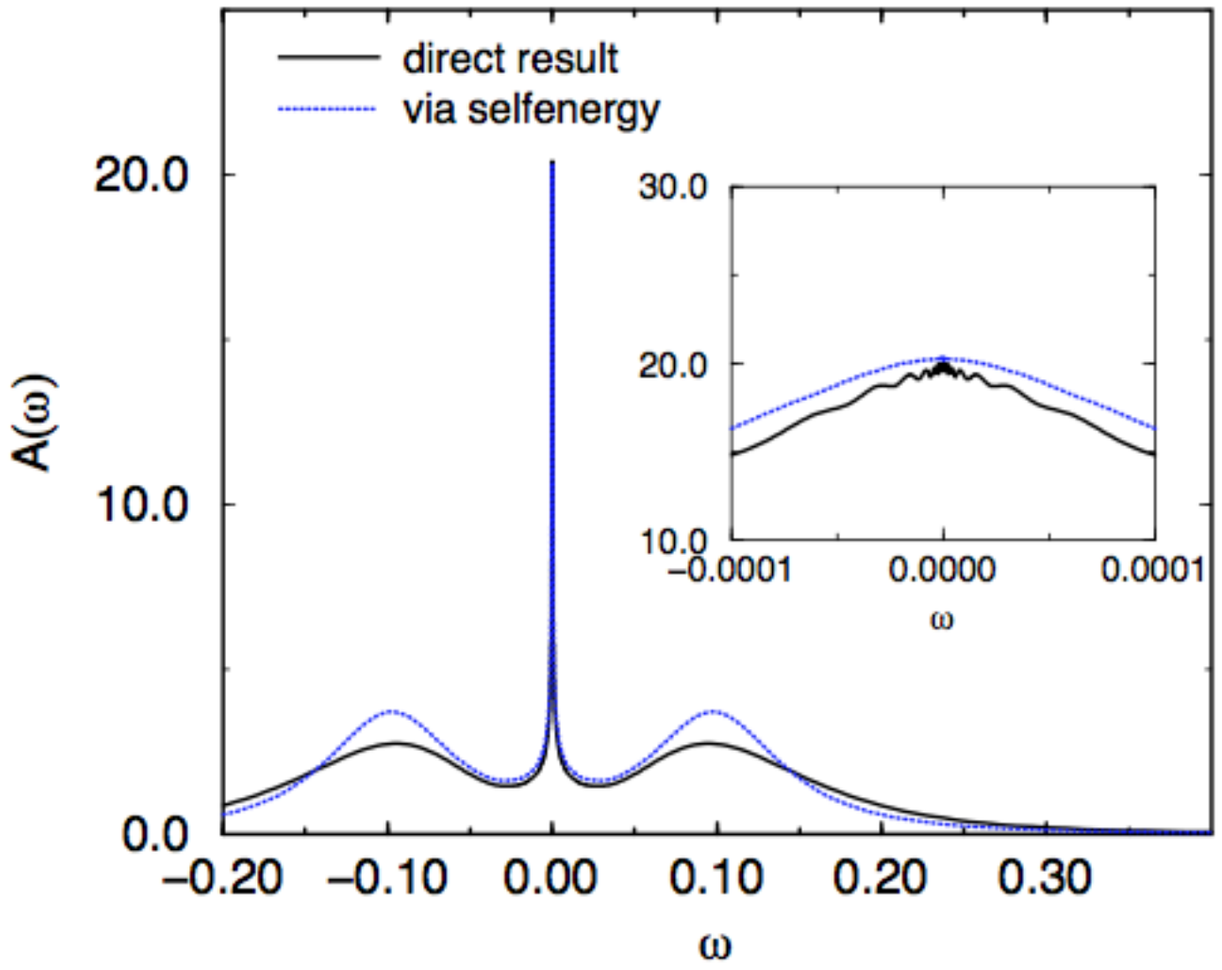


Figure 1. The impurity spectral function for $\varepsilon_f = -0.1, U = 0.2, T = 0$ and $-\mathrm{Im}\,\Delta(\omega+\mathrm{i}0^+) = 0.015$ in units of the conduction electron bandwidth. $\bar{A}(\omega)$ (solid line) is the result obtained directly from the NRG method and $A(\omega)$ (dashed line) is calculated via the self-energy equation (8). The inset shows the region around the Fermi level.

(i) We find for the total spectral weight

$$\int \mathrm{d}\omega\ \bar{A}(\omega) = \bar{w} = 0.93 \qquad \text{and} \qquad \int \mathrm{d}\omega\ A(\omega) = w = 0.9993.$$

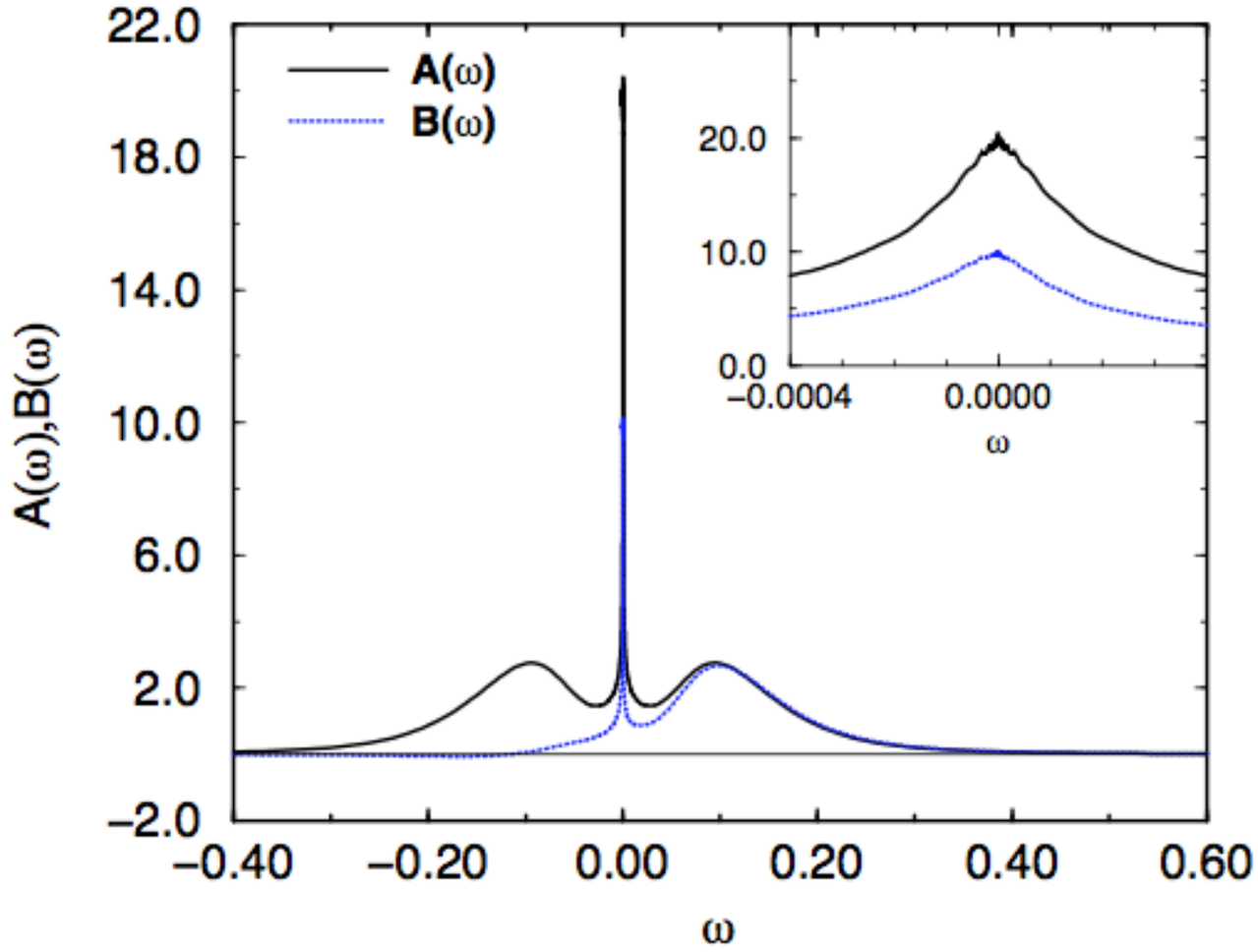


Figure 2. The spectral functions $A(\omega)$ (solid line) and $B(\omega)$ (dotted line) for the same parameters as in figure 1 (directly from the NRG method, not via the self-energy). The inset shows the region around the Fermi level.

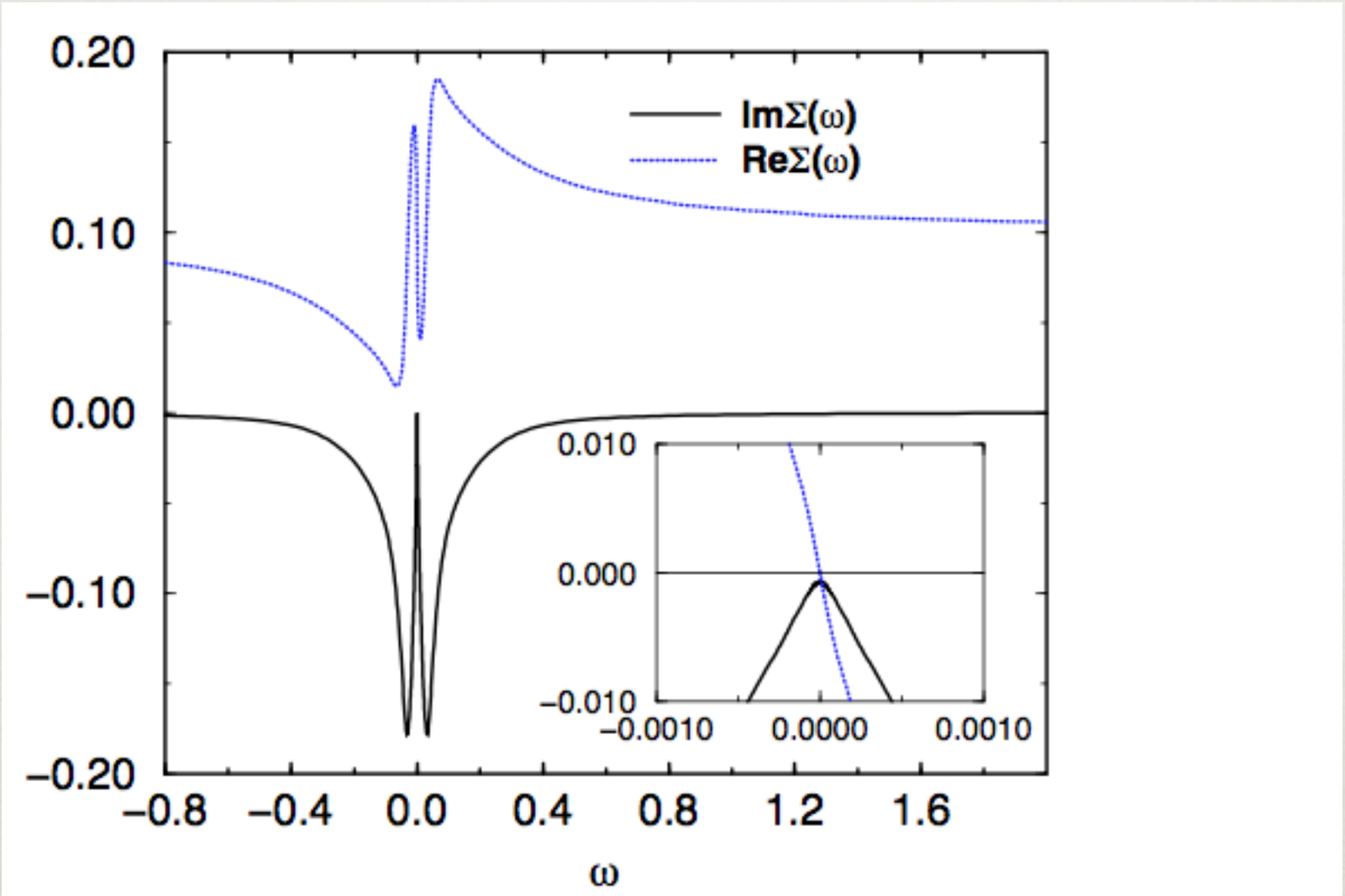


Figure 3. Real and imaginary parts of the self-energy for $\varepsilon_f = -0.1$, $U = 0.2$ and a constant $\Delta_0 = 0.015$. The inset shows the region around the Fermi level where the Hartree term was subtracted from the real part.

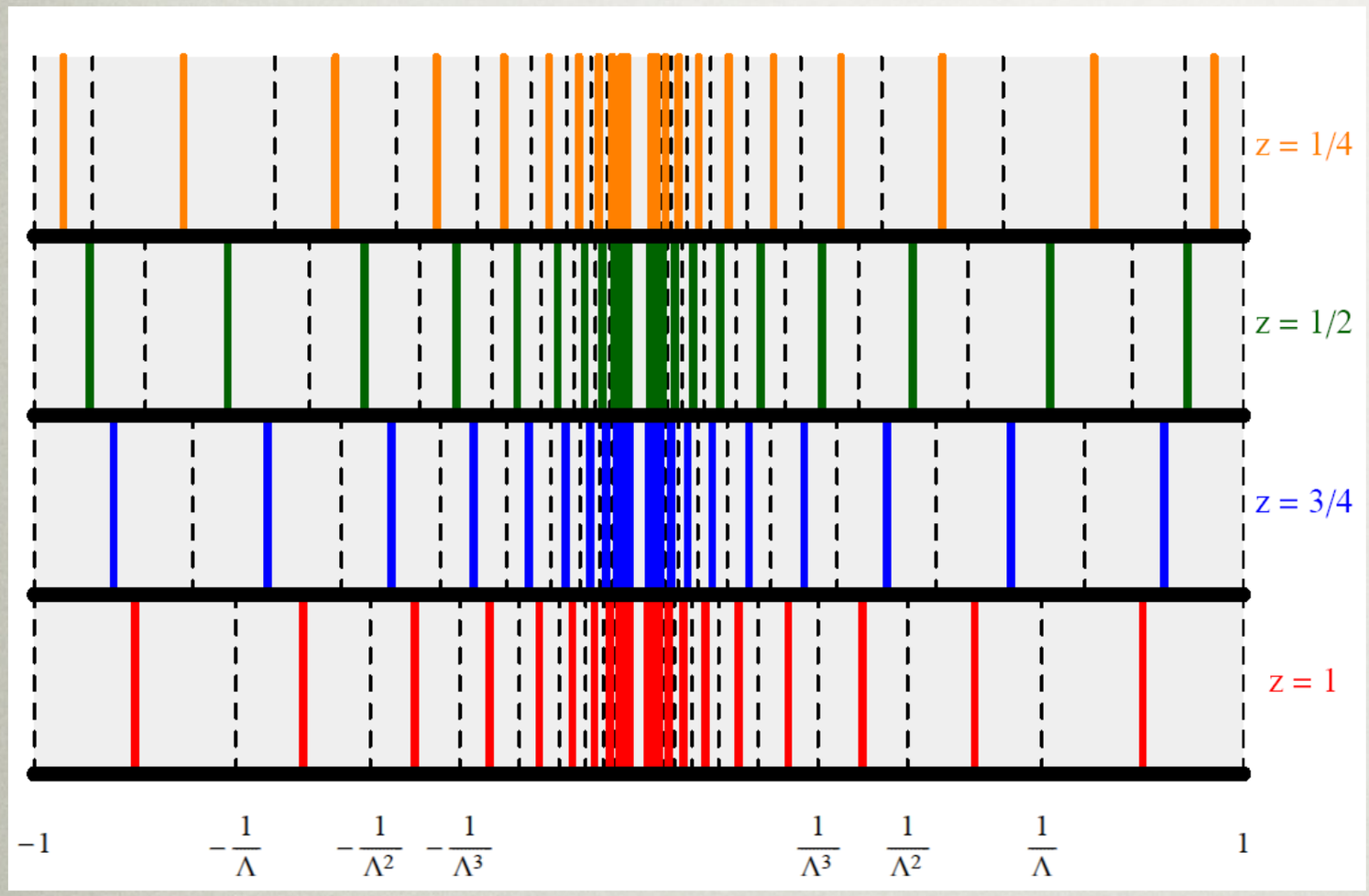
In the case of the standard single-impurity Anderson model, we furthermore know that the Friedel sum rule $\mathrm{Im}\,\Sigma^U(\mathrm{i}0^+) = 0$ has to be fulfilled, which implies that

$$\mathrm{Re}\,F(\mathrm{i}0^+) = -\int_{-\infty}^{\infty} \mathrm{d}\omega\; B(\omega)\,\mathcal{P}\frac{1}{\omega} = 0 \tag{15}$$

where $\mathcal{P}(\cdots)$ denotes the principal value. Relation (15) is obviously not trivial as regards the unusual shape of $B(\omega)$. Indeed, it turns out that $\mathrm{Re}\,F(\mathrm{i}0^+)$ is numerically zero as long as the *full* spectrum of the Hamiltonian can be used. However, as soon as a truncation of states sets in, the calculated value for $\mathrm{Re}\,F(\mathrm{i}0^+)$ suddenly jumps to a finite value, eventually leading to a violation of the Friedel sum rule as observed e.g. in figure 1.

This observation suggests that high-energy states are also important to guarantee that $\mathrm{Re}\,F(\mathrm{i}0^+) = 0$ and also that a slight violation of the Friedel sum rule is almost unavoidable in this method.

Z-AVERAGING



$$\epsilon_1^z = D$$

$$\epsilon_j^z = D\Lambda^{2-j-z}$$

$$z \in (0:1]$$

works best for $N_z=2^N$

similar to *twist averaging* over different boundary conditions in finite clusters to reduce the finite-size effects (better k-space sampling)

Frota, Oliveira, PRB 33, 7871 (1986)
Oliveira, Oliveira, PRB 49, 11986 (1994)

```
#!/usr/bin/env looper
#PRELUDE: $Nz=4;
#AUTOLOOP: ${NRGPREFIX} nrginit ; ${NRGPREFIX} nrgrun
#OVERWRITE

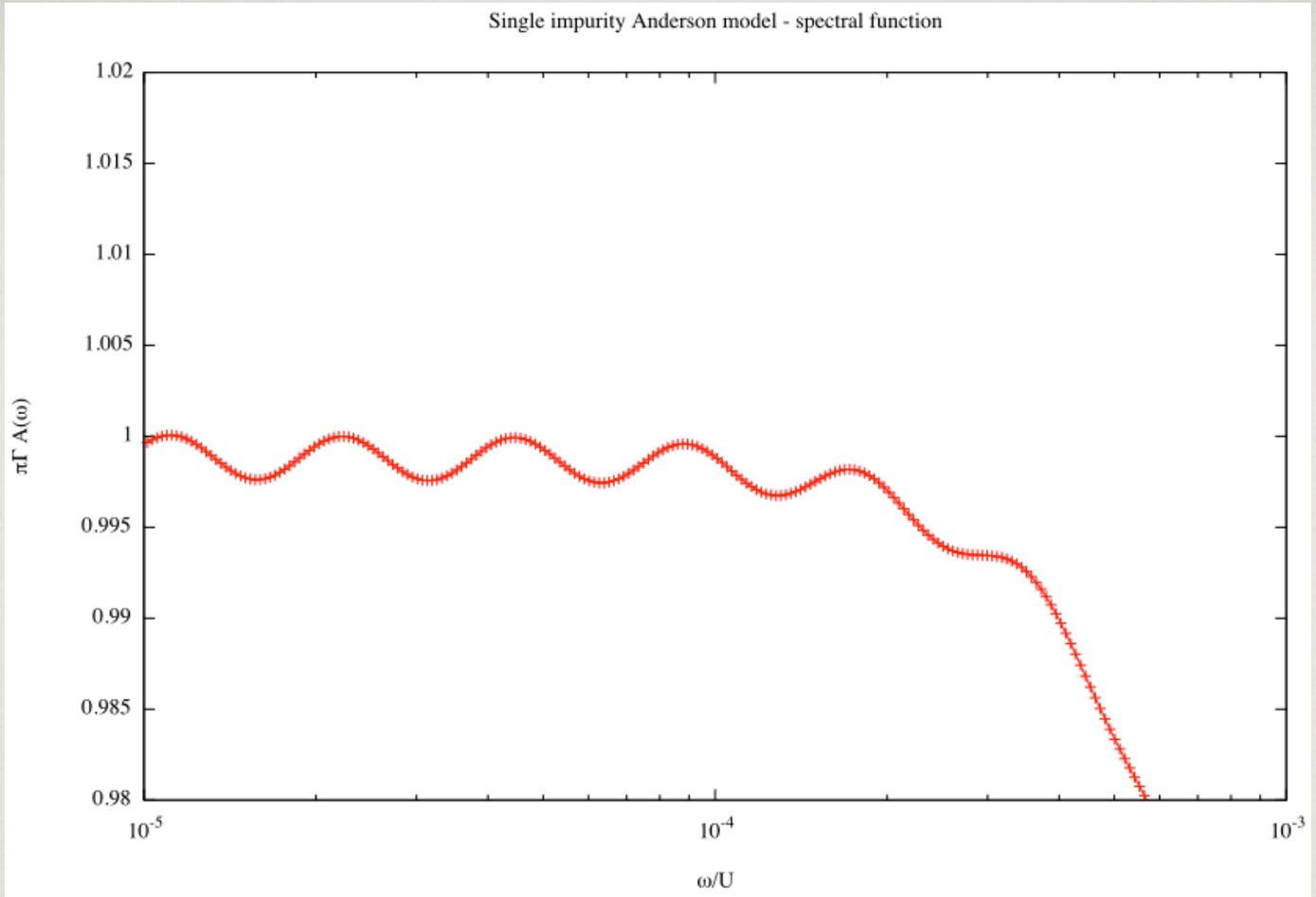
[extra]
U=0.01
Gamma=0.001
delta=0

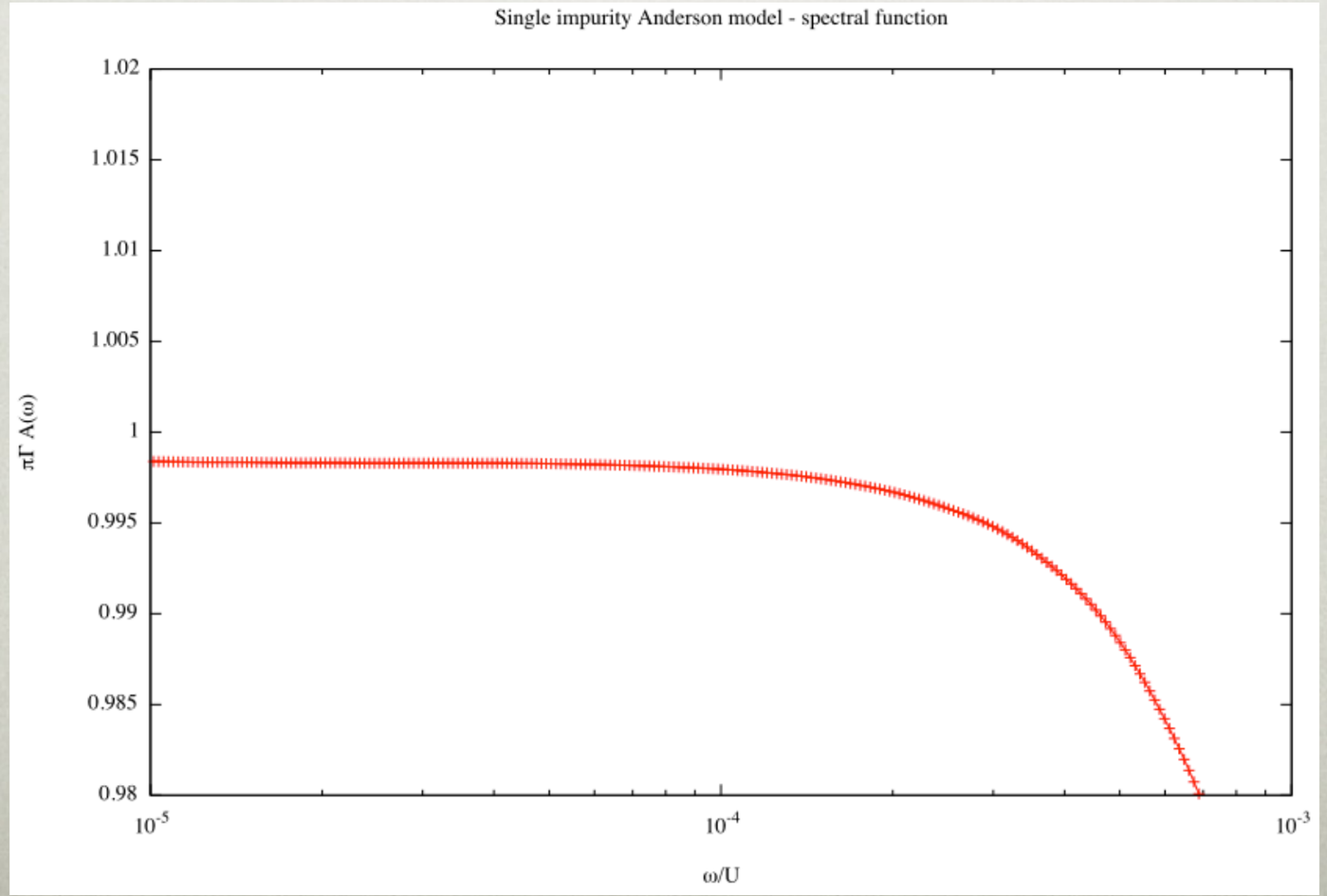
[param]
symtype=QS
discretization=Z
@$z = 1/$Nz; $z <= 1; $z += 1/$Nz
z=$z

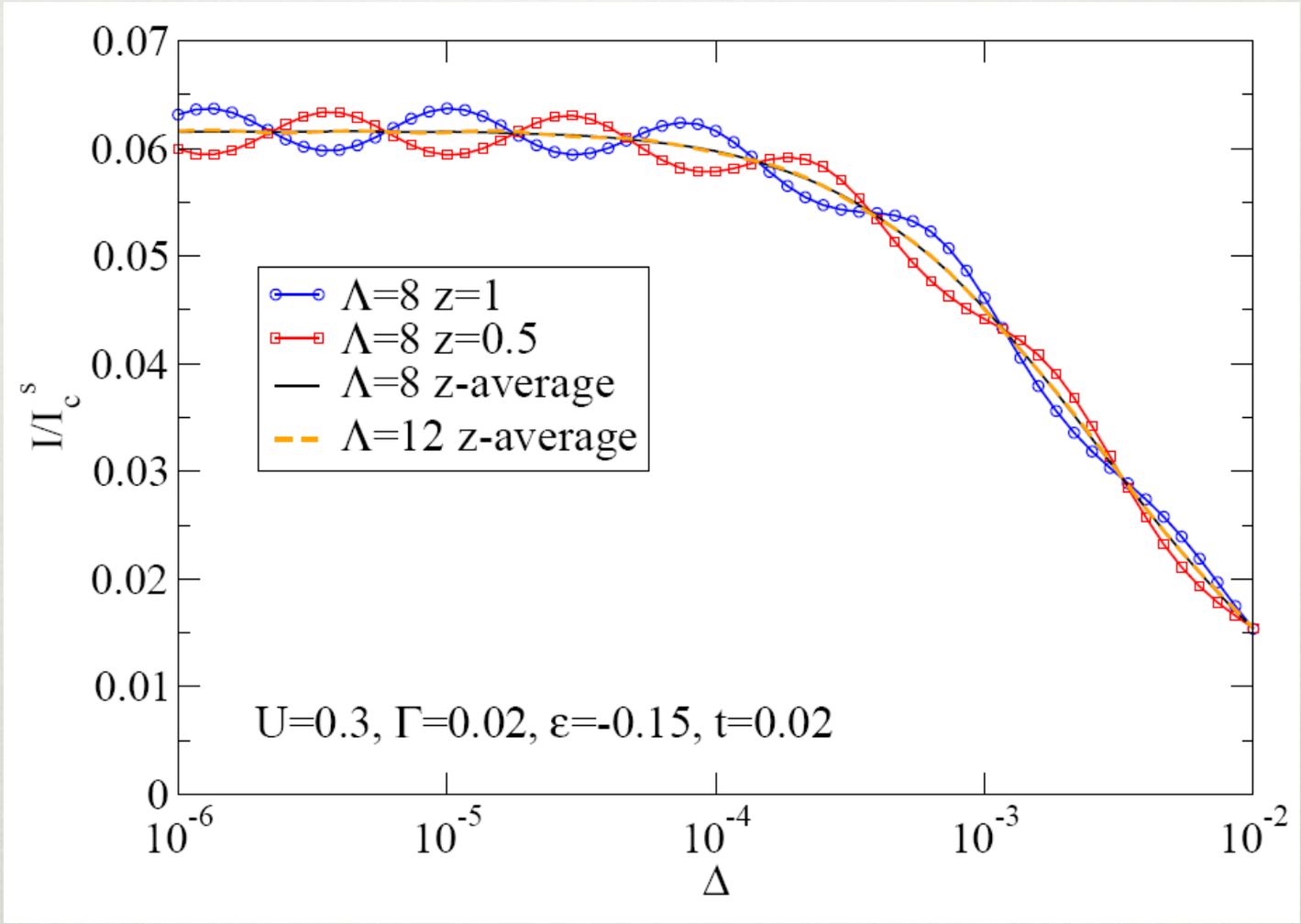
Lambda=2
Tmin=1e-10
keepenergy=10
keep=5000

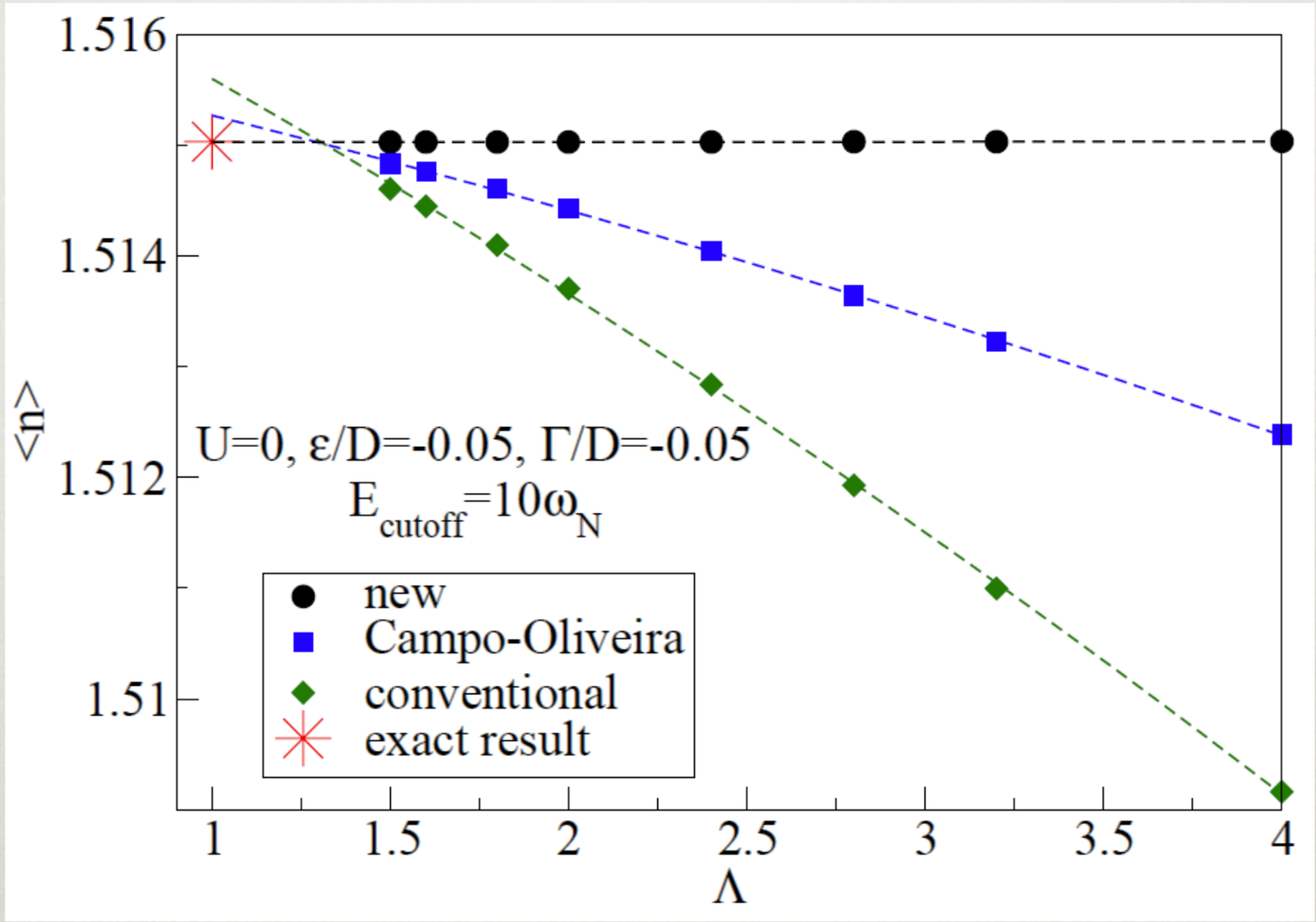
model=SIAM
```

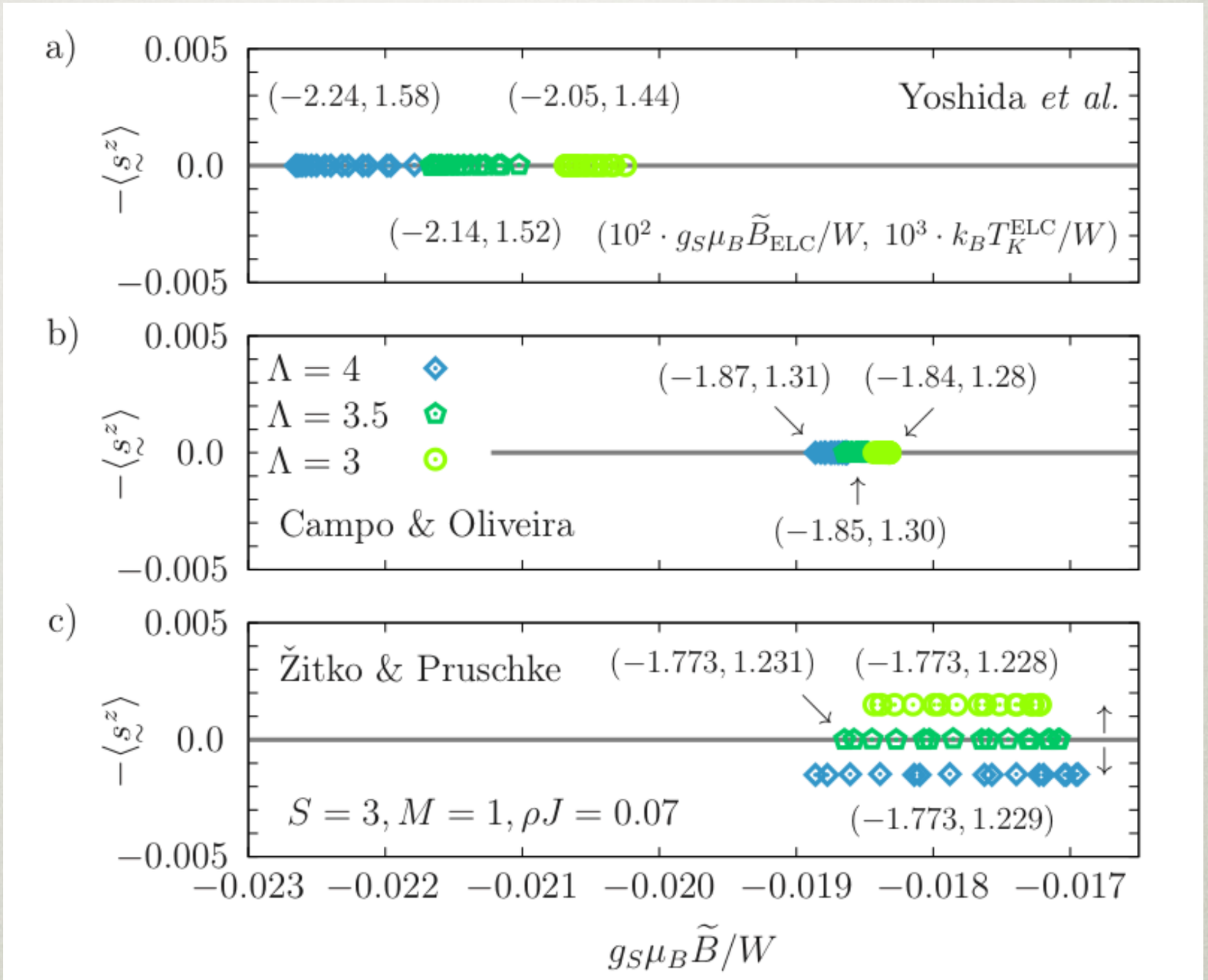
```
#!/bin/bash
FN=spec_FDM_dens_A_d-A_d.dat
Nz=`getNz`
${NRGPREFIX} intavg ${FN} ${Nz}
```


Single impurity Anderson model - spectral function
πΓ A(ω)
1.02
1.015
1.01
1.005
1
0.995
0.99
0.985
0.98
10^-5
10^-4
10^-3
ω/U


Single impurity Anderson model - spectral function
πΓ A(ω)
1.02
1.015
1.01
1.005
1
0.995
0.99
0.985
0.98
10^-5
10^-4
10^-3
ω/U


0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
I/I_c^s
Λ=8 z=1
Λ=8 z=0.5
Λ=8 z-average
Λ=12 z-average
U=0.3, Γ=0.02, ε=-0.15, t=0.02
10^-6
10^-5
10^-4
10^-3
10^-2
Δ


1.516
1.514
1.512
1.51
⟨n⟩
U=0, ε/D=-0.05, Γ/D=-0.05
E_cutoff=10ω_N
new
Campo-Oliveira
conventional
exact result
1
1.5
2
2.5
3
3.5
4
Λ



Höck, Schnack, PRB 2013

There are several schemes for logarithmically discretizing the continuum of the bath degrees of freedom:

- `Y` - the scheme proposed in the paper by Yoshida, Whitaker, Oliveira, Phys. Rev. B 41, 9403 (1990).
- `C` - the scheme proposed in the paper by Campo, Oliveira, Phys. Rev. B 72, 104432 (2005). It corrects the systematic underestimation of the bath density of states of scheme `Y`.
- `Z` - the scheme proposed in the paper by Zitko, Pruschke, Phys. Rev. B 79, 085106 (2009). It corrects the systematic error in the first energy interval of scheme `C`.

Recommendation: **`discretization=Z`**

When things go wrong

- Code doesn't start at all. Library problems? Wrong CPU optimization?
- No Mathematica licence available (in network licence environments).
- Typos in input file. Case is important. Spaces are important.
- Errors in model definition file (code is not valid Mathematica language code).
- Convergence? Increase truncation cutoffs, if memory/time allows.
- Suitable Λ? Too small, too large?
- Wrong `symtype`
- Truncation within clusters (`safeguard`)
- Floating-point errors (`fixeps`)
- Inappropriate `Tmin` (should be some orders of magnitude smaller than the lowest energy scale in the problem)

...CONTINUED

- Model parameters must be in [extra] block, NRG parameters in [param] block
- Model definition is not what you think it is.
- Path problems (files are not where you think they are)
- Operators used in `specd` missing in `ops`
- Inappropriate broadening parameter (N_z vs α)
- Confusion between `T` (physical parameter) and `Tmin` (chain length)
- Too slow? Are parameters sensible? Use parallelization.
- Running out of disk space during calculation? Set `workdir`.

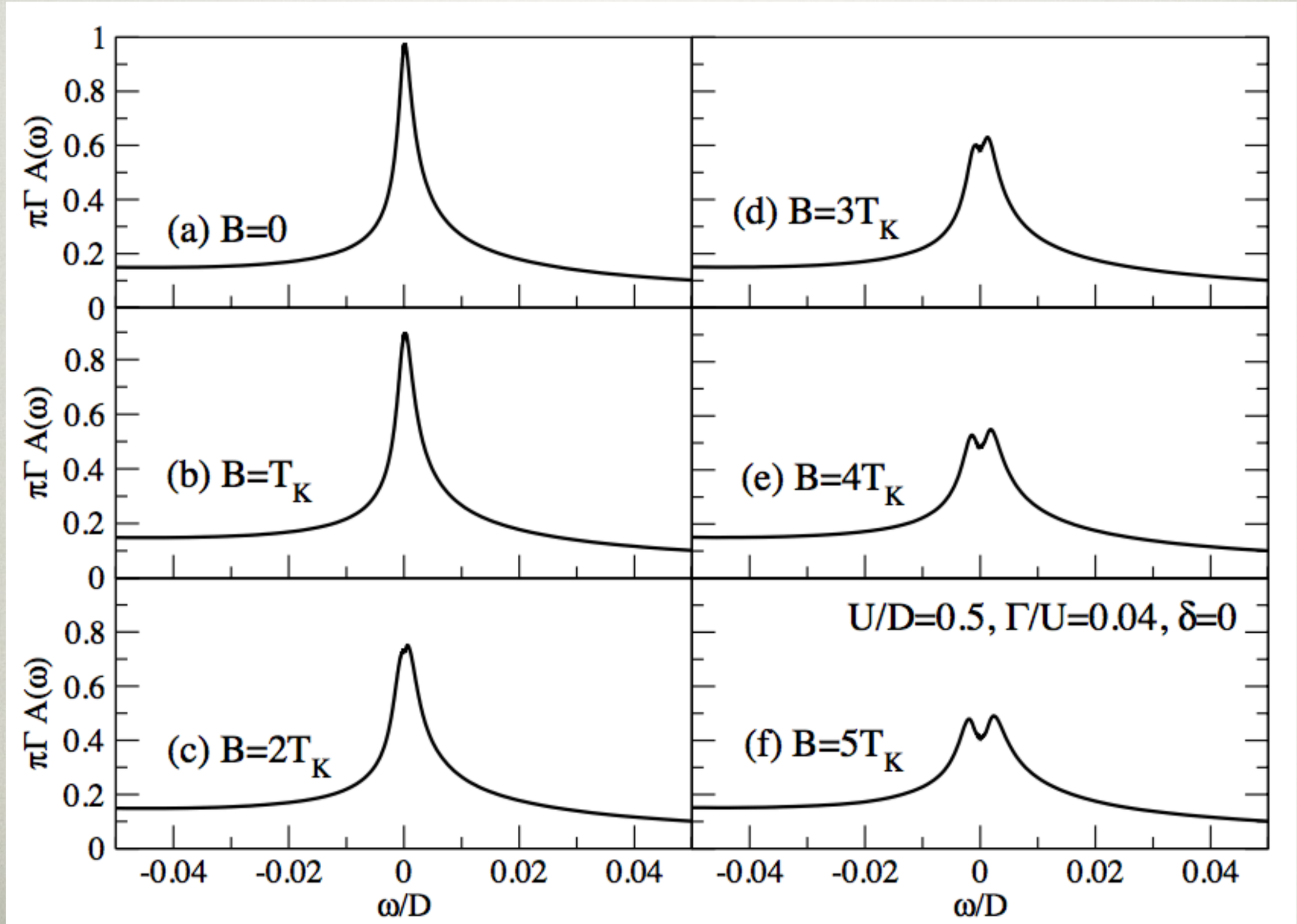
Troubleshooting

- Run code manually, without scripts. Call `nrginit` and `nrgrun` separately.
- Inspect log files (`mmalog`, `log`).
- Increase the verbosity of output (`log=` setting, see `param.cc` for documentation).
- Do results make physical sense?
- Check the details (sum rules, compare with different methods, etc.)
- If the results are “interesting”, check twice! Then check again!

Good to know

- Interleaved iteration (`substeps=true`)
- Different unit? Use `bandrescale`
-

Kondo resonance splitting



Problems

1. Spectral function of SIAM at large Λ=10. How does it compare to that at Λ=2?
2. Study the magnetic field dependence of the spectral function in SIAM, both in the B~T_K range, and in the B~U range.
3. Compute the spectral function for U>2D. What is the width of the atomic peaks?
4. How does the Kondo peak disappear with increasing temperature?
5. What is the T-dependence of conductance at finite magnetic field?
6. Write a model definition file for a "side-coupled double quantum dot".
7. How does the "binding energy" in the Kondo model depend on J?