Tutorial 3: spectral functions for SIAM, arbitrary DOS, finite-tempratures, T-matrix for Kondo model

Rok Žitko

Institute Jožef Stefan

Ljubljana, Slovenia

Spectral funcion

05_spec

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

model=SIAM
U=0.01
Gamma=0.001
delta=0
```

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

creation/annihilation operator

spectral function <<d;d†>>

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

grid for the broadened (smooth) spectral function

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

full-density-matrix method

temperature for the spectral-function calculation

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

broadening parameters

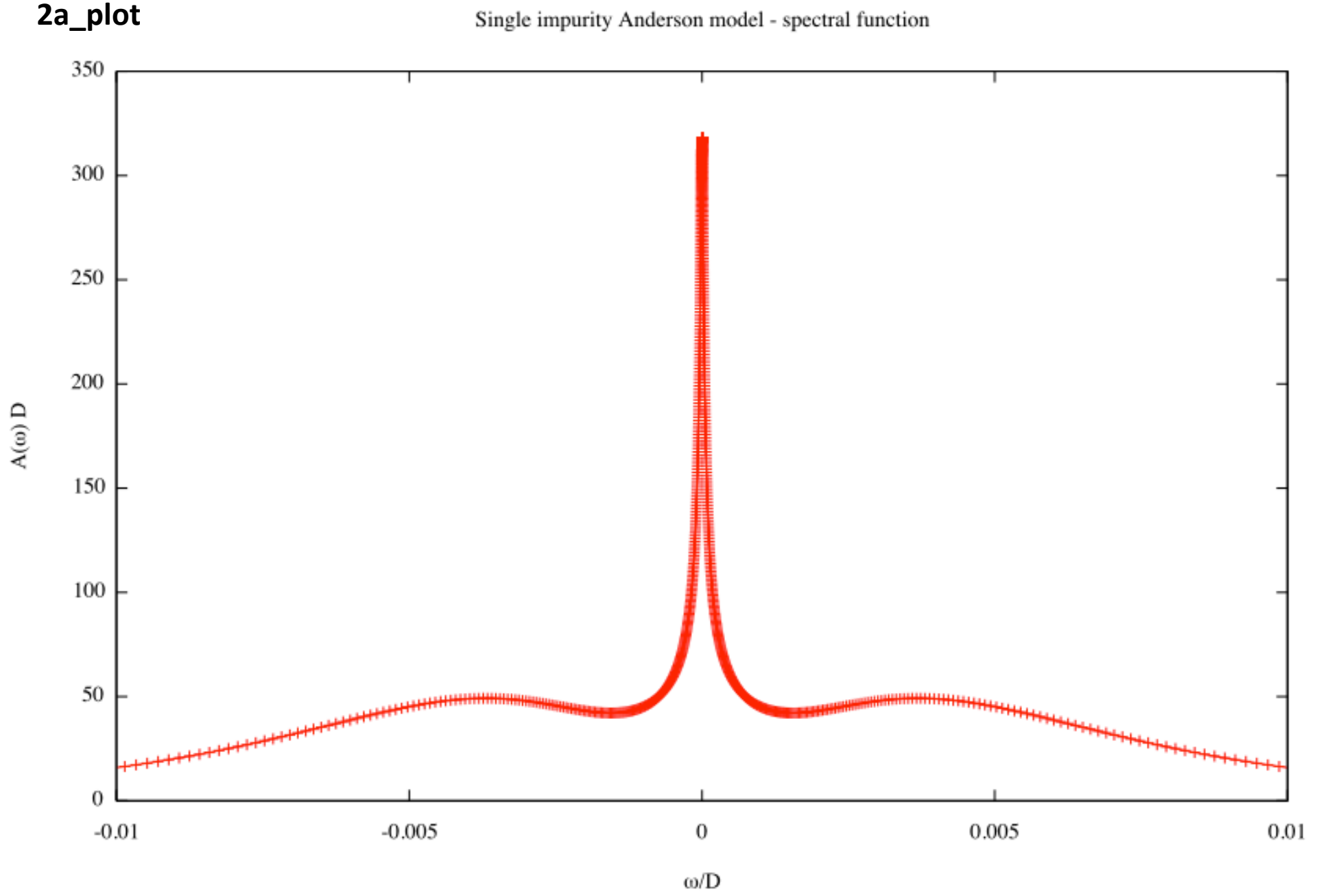
$$\omega_n = \text{broaden\_max} \times \text{broaden\_ratio}^{-n}$$

Output: spectral function = imaginary part of the Green's function

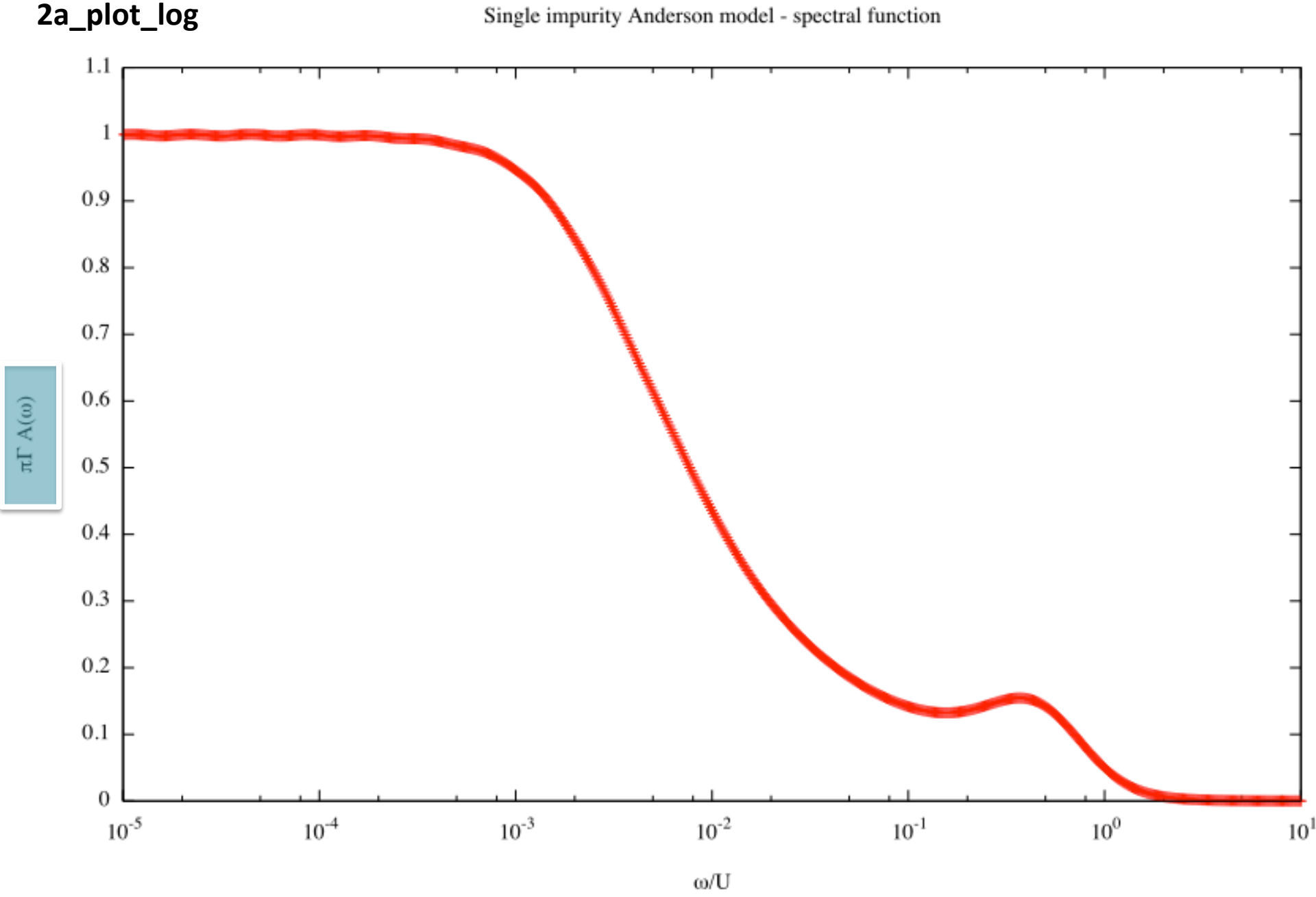
$$\rho_{AB}(\omega) = -\frac{1}{\pi}\mathrm{Im}\left[\langle\langle A; B^{\dagger}\rangle\rangle_{\omega+i\delta}\right]$$

The corresponding real part can be computed using the Kramers-Kronig transformation tool "`kk`", which comes bundled as part of the NRG Ljubljana package.

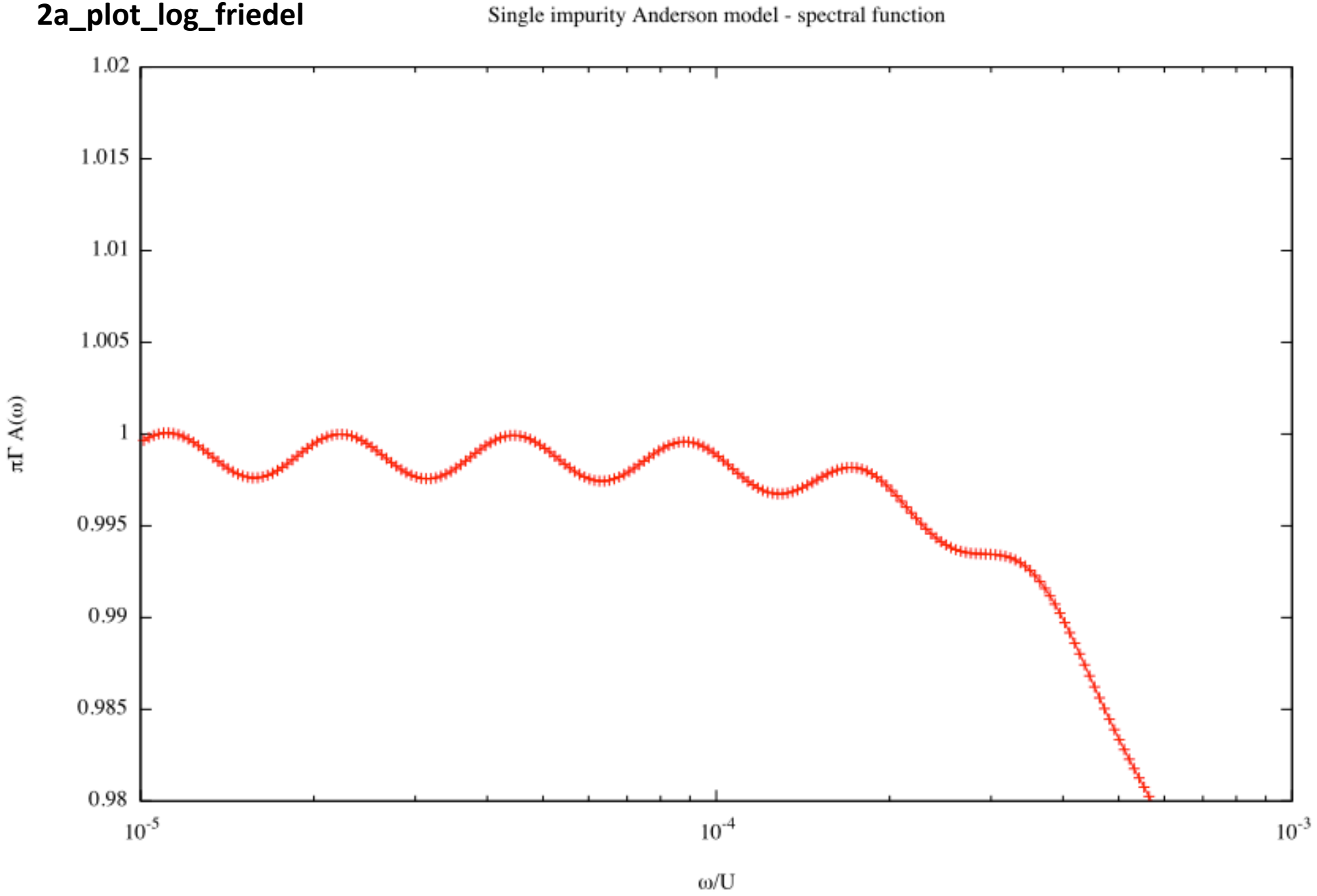
2a_plot


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

2a_plot_log


Single impurity Anderson model - spectral function
πΓ A(ω)
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
10^-5
10^-4
10^-3
10^-2
10^-1
10^0
10^1
ω/U

2a_plot_log_friedel



Removing oscillations using the z-averaging

```
#!/usr/bin/env looper
#AUTOLOOP: nrginit ; nrgrun
#OVERWRITE

[param]
symtype=QS
discretization=Z
@$z = 1/4; $z <= 1; $z += 1/4
z=$z
Lambda=2
Tmin=1e-10
keepenergy=10
keep=10000

model=SIAM
U=0.01
Gamma=0.001
delta=0

ops=A_d
specd=A_d-A_d

broaden_max=0.1
broaden_min=1e-8
broaden_ratio=1.02

fdm=true
T=1e-10

smooth=new
alpha=0.3
omega0=1e-99
```

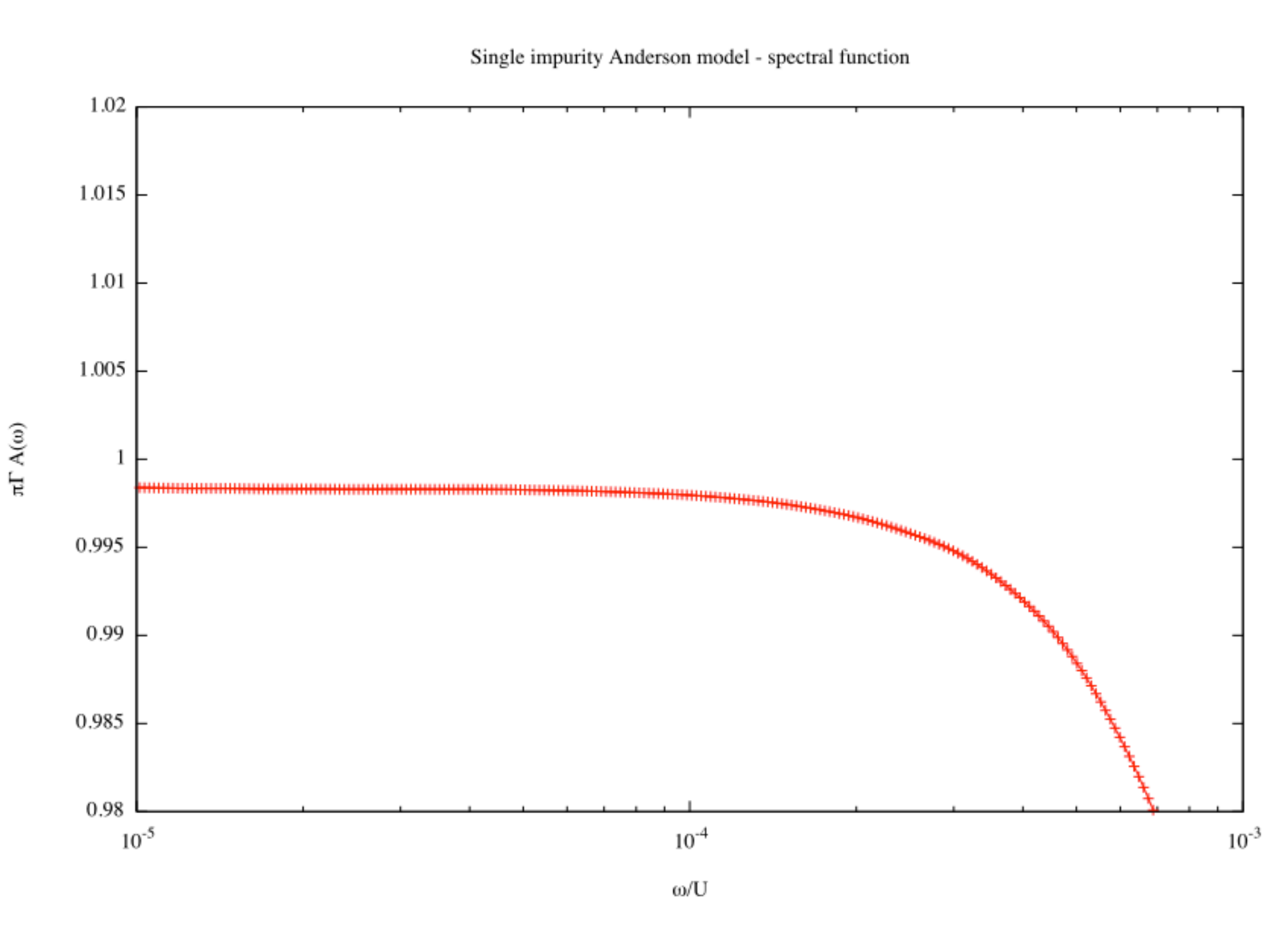
May be reduced!

05_spec_z/1_zloop

05_spec_z/2_proc

```
#!/bin/sh
FN=spec_FDM_dens_A_d-A_d.dat
Nz=4
intavg ${FN} ${Nz}
Gamma=`getparam Gamma 1_zloop`
U=`getparam U 1_zloop`
scaley=`echo 3.14159*${Gamma} | bc`
scalex=`echo 1/${U} | bc`
scalexy ${scalex} ${scaley} ${FN} >A-rescaled.dat
```

`intavg` is a tool for z-averaging the spectral functions


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

Exercises

1. Try increasing Λ. How do the results deteriorate? **2a1**

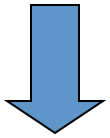
2. Try changing the broadening α and the number of z points. When do the oscillations appear?

3. How does the Kondo resonance evolve as U is decreased toward 0?

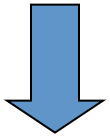
Self-energy (Σ) trick

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

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



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



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

12_self_energy_trick/1_zloop

```
#!/usr/bin/env looper
#PRELUDE: $Nz=8;
#AUTOLOOP: nrginit ; nrgrun
#OVERWRITE

[sweep]
Nz=8

[param]
symtype=QS
Lambda=2.0
Tmin=1e-8
keepmin=200
keepenergy=10.0
keep=10000

discretization=Z
@$z = 1/$Nz; $z <= 1.00001; $z
+= 1/$Nz
z=$z
```

```
model=../model.m
U=0.5
Gamma=0.03
delta=0.1

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

dmnrg=true
goodE=2.3
NN2avg=true

# Broadening is performed by
an external tool
broaden_max=2
broaden_ratio=1.01
broaden_min=1e-6
bins=1000
broaden=false
savebins=true

T=1e-10
```

12_self_energy_trick/model.m

```
def1ch[1];

H = H0 + Hc + H1;

(* 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]];
```

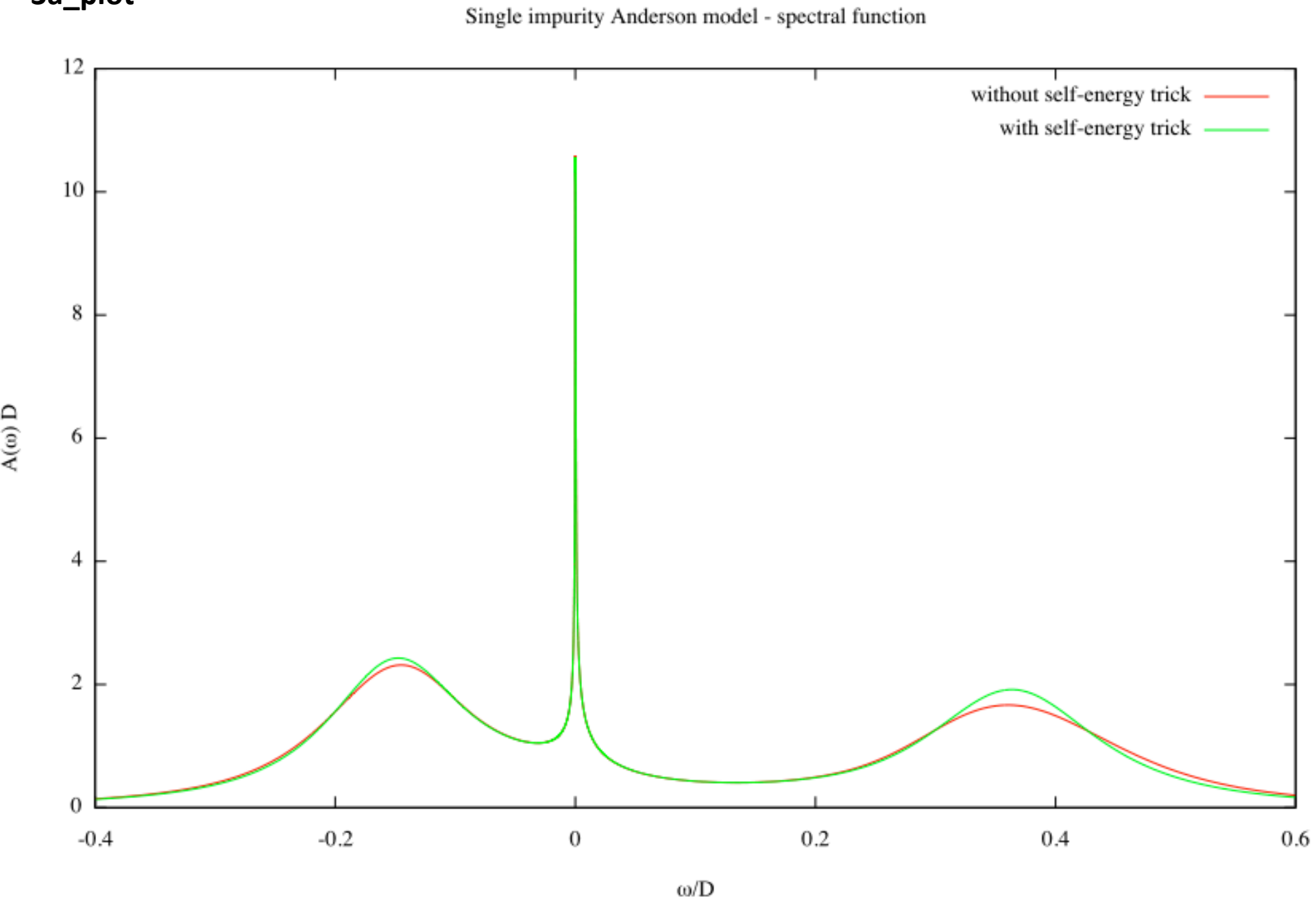
H0 = Hamiltonian for the first site (index 0) of the Wilson chain
Hc = hybridization part of the Hamiltonian, hopping between the impurity and the first site of the Wilson chain
H1 = the impurity Hamiltonian

$$H1 = \sum_\sigma \epsilon_d d_\sigma^\dagger d_\sigma + U n_\uparrow n_\downarrow = \delta(n-1) + \frac{U}{2}(n-1)^2 + \text{const.}$$

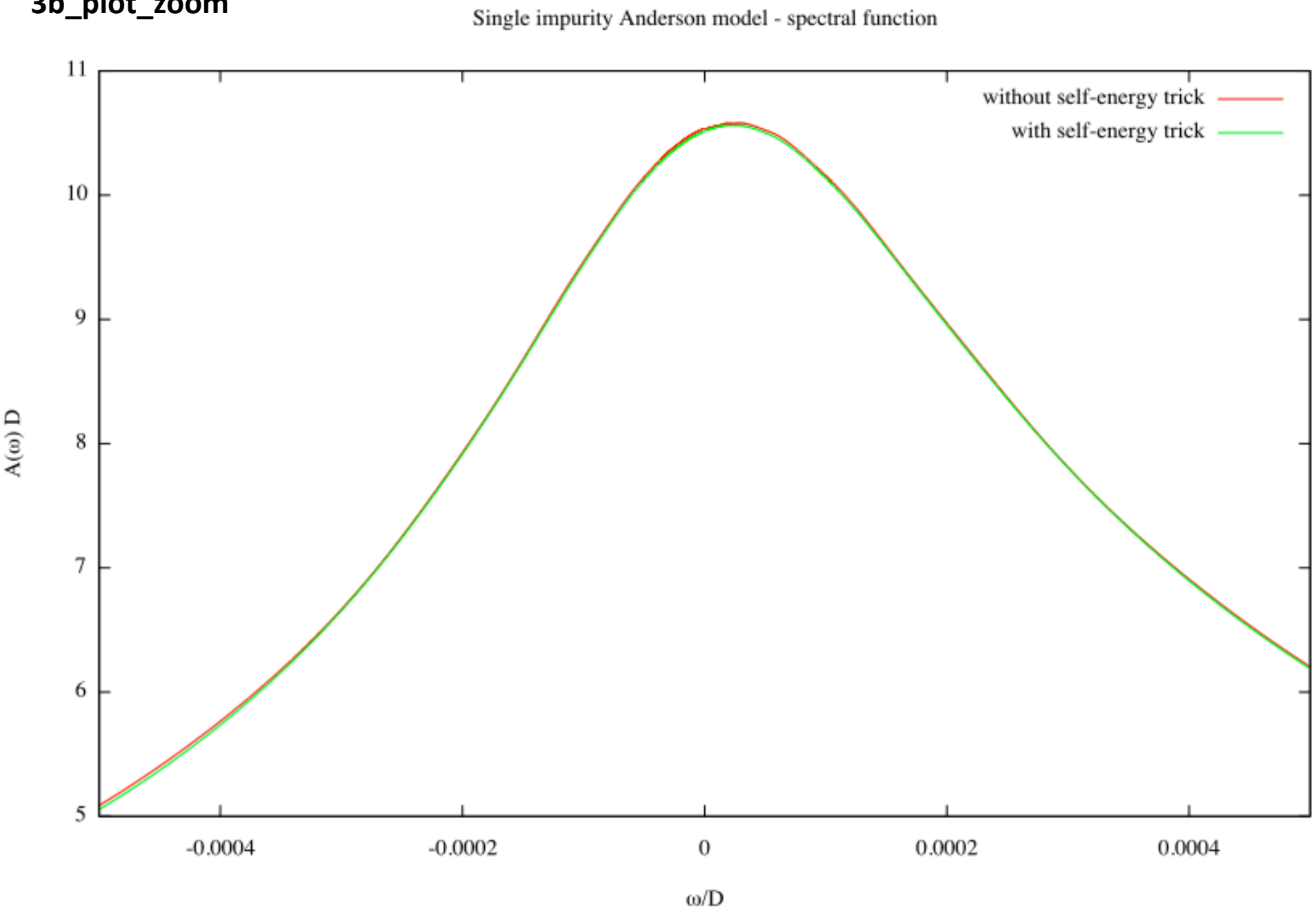
Postprocessing

- z-averaging of both spectral functions, A_G (`A_d-A_d`) and A_F (`self_d-A_d`) — **average**
- compute the corresponding real parts to obtain the full Green's functions: G=Re G-iπ A_G, similarly for F — **realparts**
- compute the self-energy — **sigmatrick**
- calculate the improved spectral function

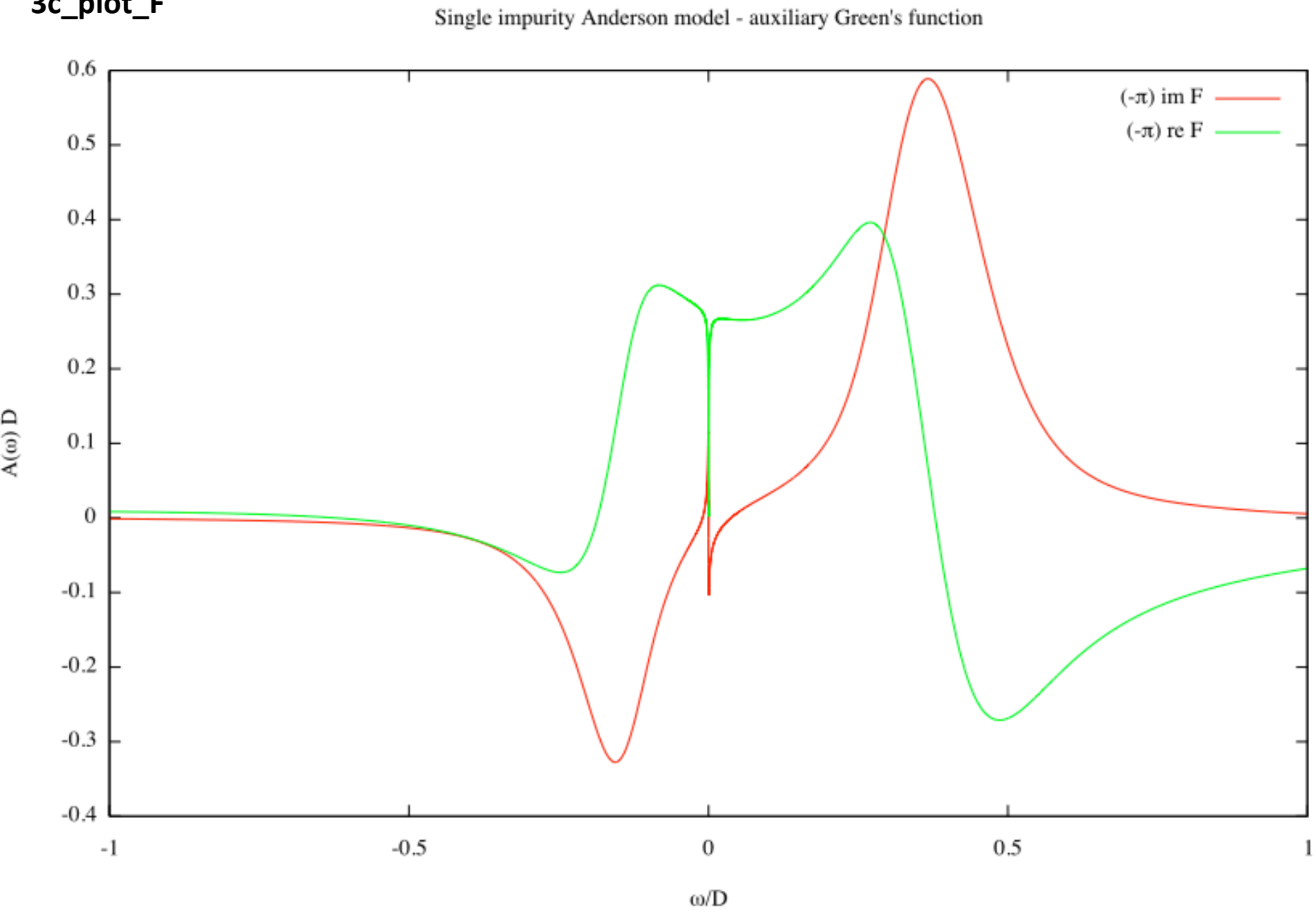
3a_plot


Single impurity Anderson model - spectral function
without self-energy trick
with self-energy trick
A(ω) D
ω/D
12
10
8
6
4
2
0
-0.4
-0.2
0
0.2
0.4
0.6

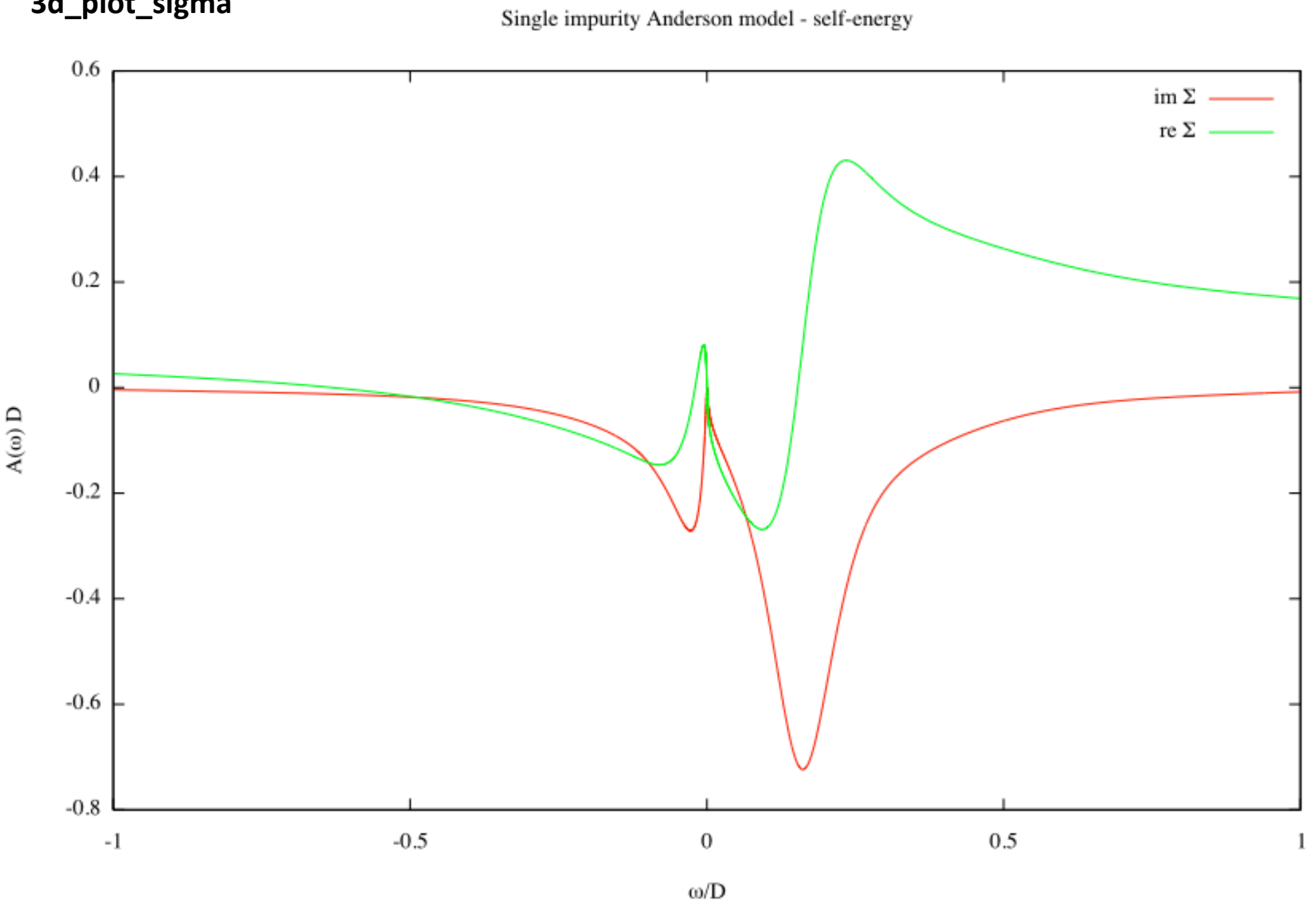
3b_plot_zoom


Single impurity Anderson model - spectral function
without self-energy trick
with self-energy trick
A(ω) D
ω/D
11
10
9
8
7
6
5
-0.0004
-0.0002
0
0.0002
0.0004

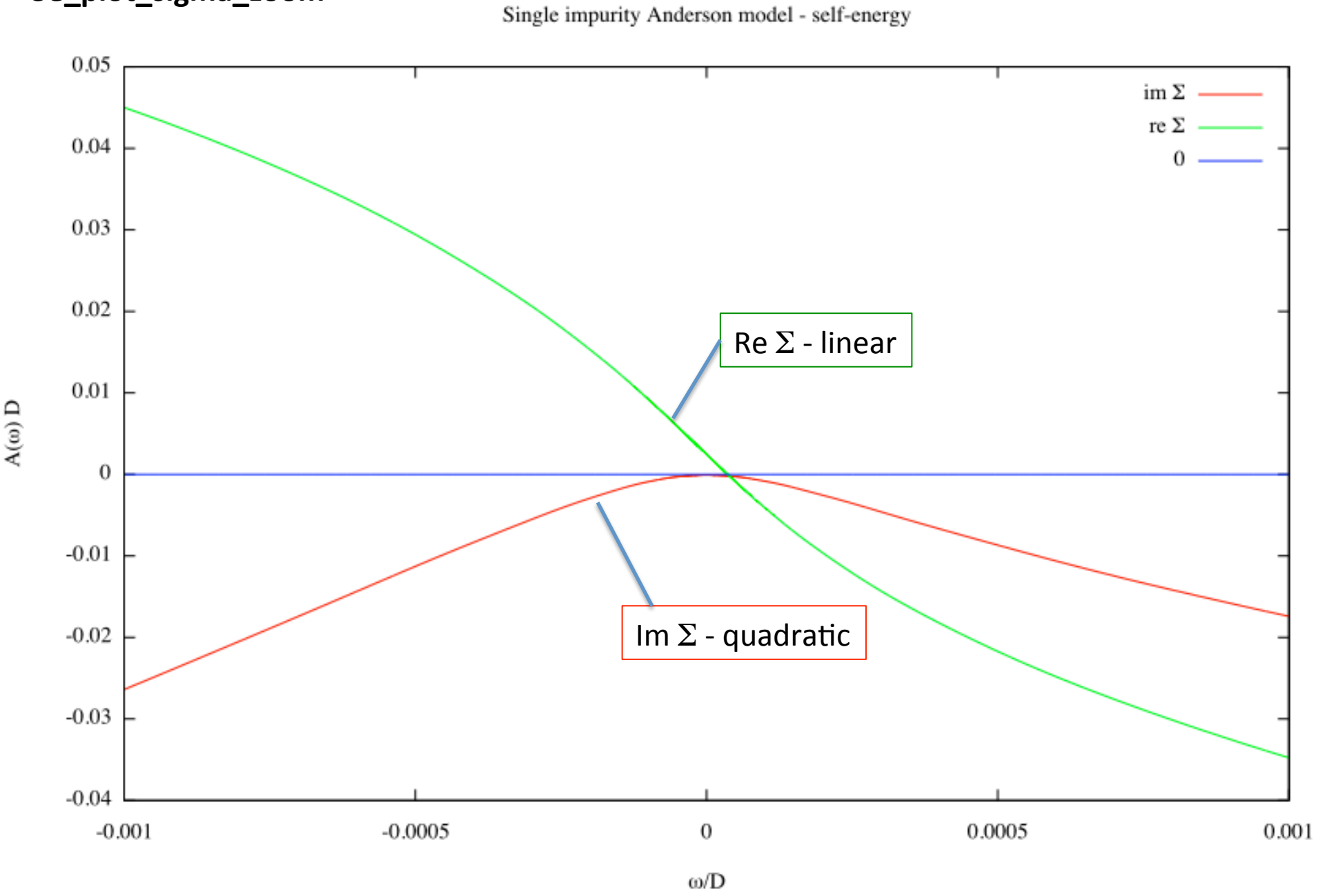
3c_plot_F


Single impurity Anderson model - auxiliary Green's function
(-π) im F
(-π) re F
A(ω) D
ω/D
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-1
-0.5
0
0.5
1

3d_plot_sigma



3e_plot_sigma_zoom



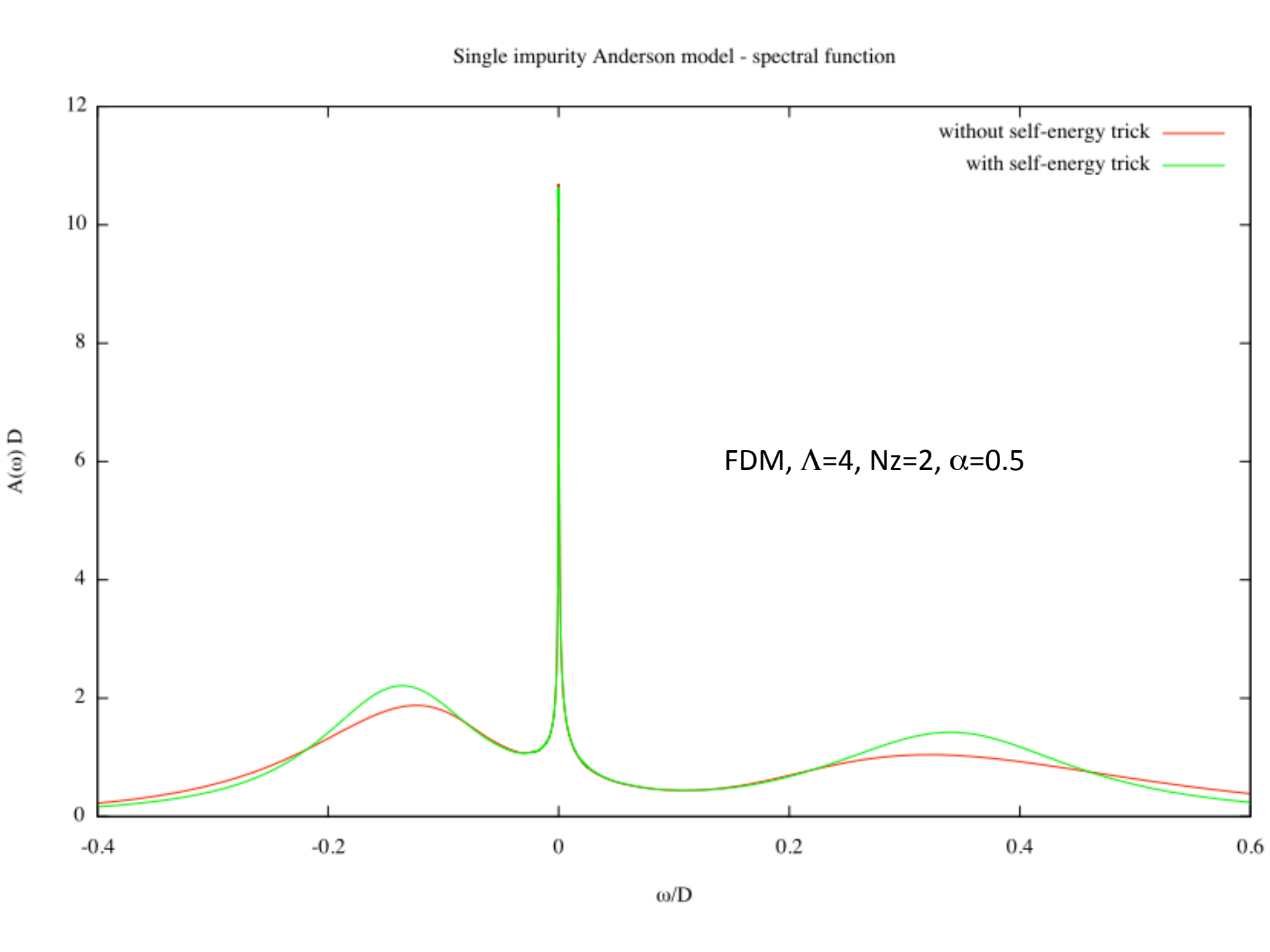
Exercises

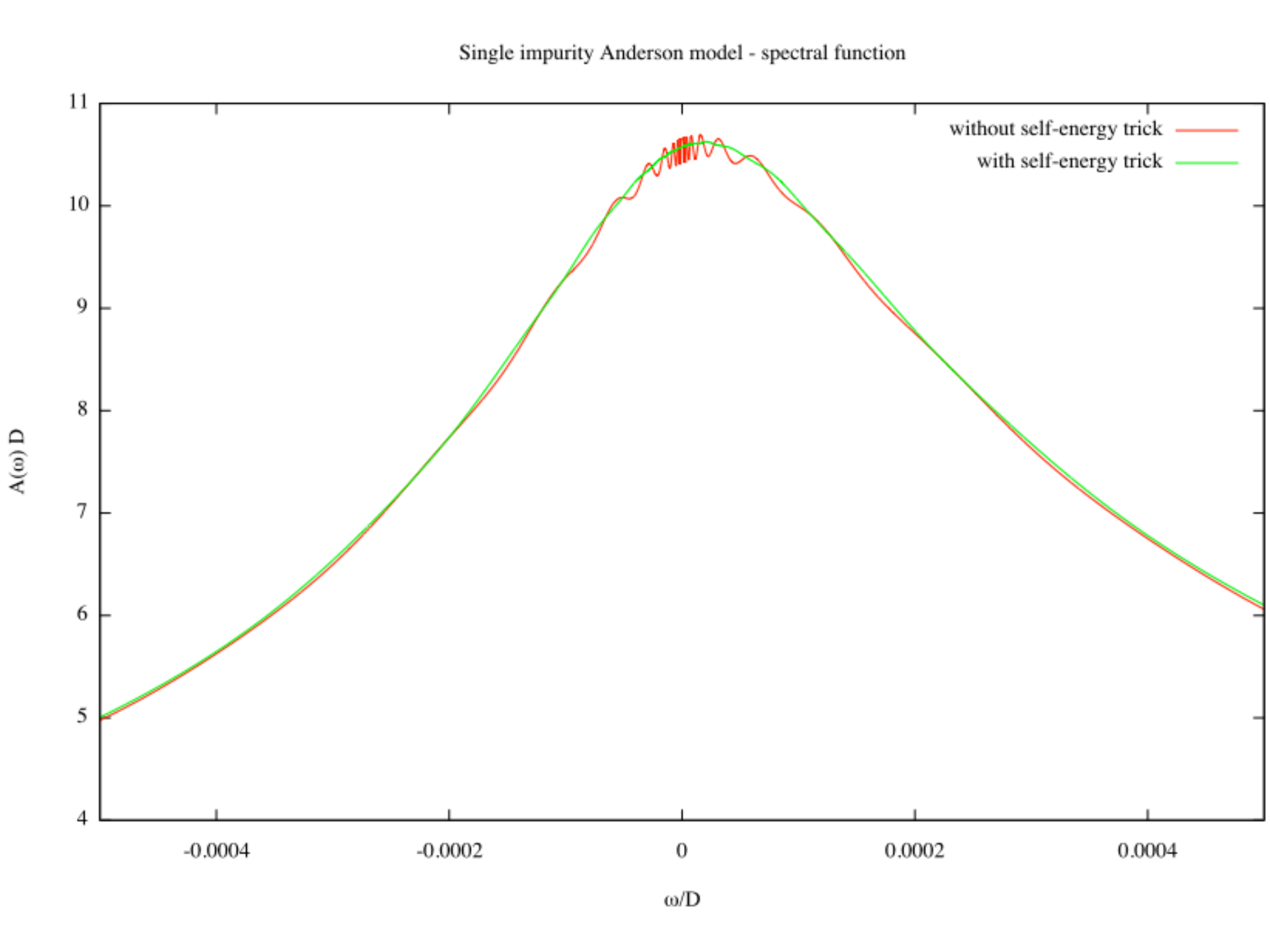
1. Extract the quasiparticle renormalization factor Z, defined as

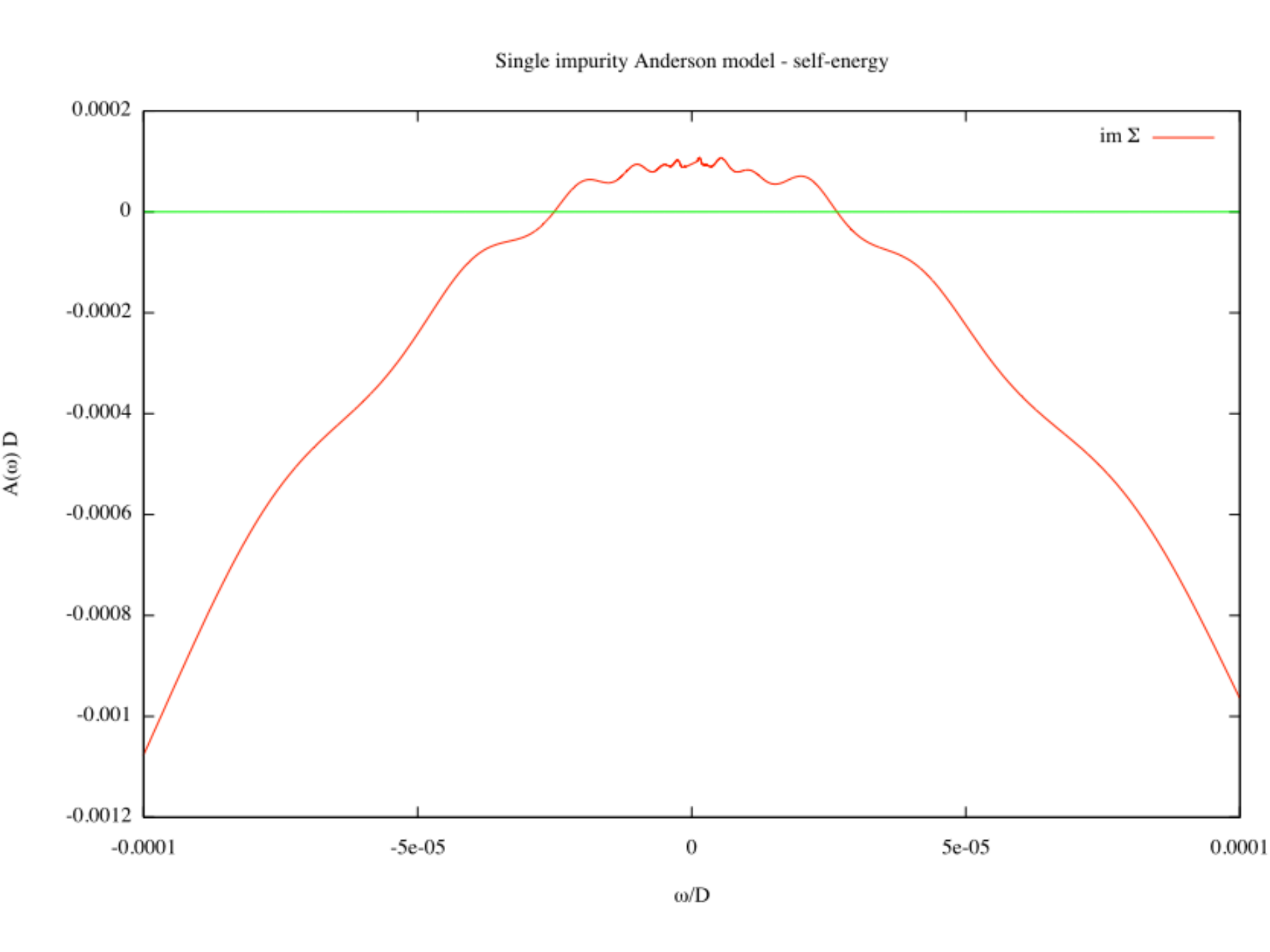
$$Z = \left(1 - \frac{\partial \mathrm{Re}\Sigma(\omega)}{\partial \omega}\Big|_{\omega=0}\right)^{-1}$$

How does it vary with U? Is it related to T_K?

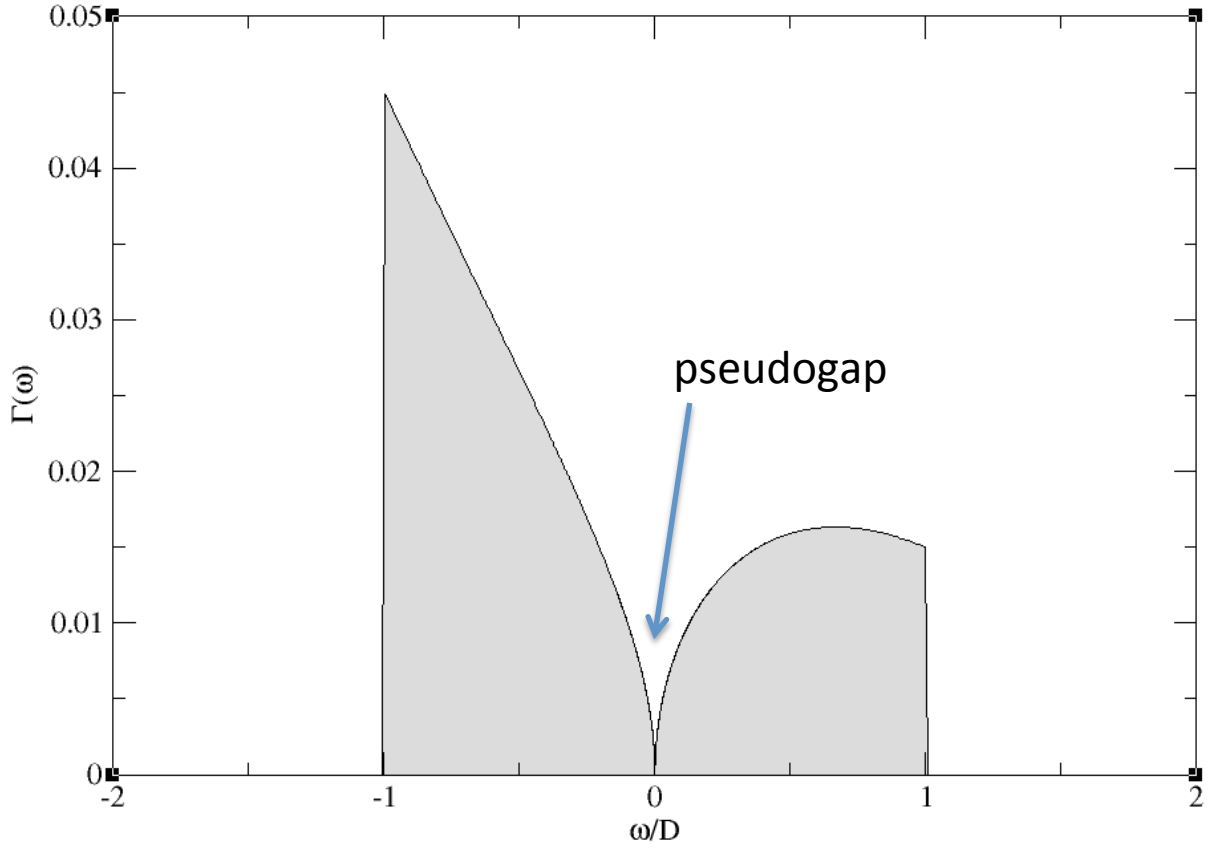
2. Is Im Σ really quadratic? Is its curvature related to Z?


Single impurity Anderson model - spectral function
without self-energy trick
with self-energy trick
FDM, Λ=4, Nz=2, α=0.5
A(ω) D
ω/D
12
10
8
6
4
2
0
-0.4
-0.2
0
0.2
0.4
0.6


Single impurity Anderson model - spectral function
without self-energy trick
with self-energy trick
A(ω) D
ω/D
11
10
9
8
7
6
5
4
-0.0004
-0.0002
0
0.0002
0.0004


Single impurity Anderson model - self-energy
im Σ
0.0002
0
-0.0002
-0.0004
-0.0006
-0.0008
-0.001
-0.0012
A(ω) D
-0.0001
-5e-05
0
5e-05
0.0001
ω/D

Arbitrary density of states



$$\Gamma = \Gamma_0 \theta(D - |\omega|) \left(\sqrt{|\omega|/D}(1 - \omega/2D) \right)$$

13_arbitrary_DOS

02_zloop

```
[param]
symtype=QS
Lambda=2.0
Tmin=1e-8
keepmin=200
keepenergy=10.0
keep=10000

band=asymode
dos=../Delta.dat

discretization=Z
@$z = 1/$Nz; $z <= 1.00001; $z += 1/$Nz
z=$z
```

param

```
[param]
xmax=20
dos=Delta.dat
```

for "adapt" tool which solves the discretization ODE

Diagonalization tool "adapt"

Input: **Delta.dat**

$$x = j + z \qquad \mathcal{E}(x) = Df(x)\Lambda^{2-x}$$

$$\frac{df(x)}{dx} = \ln\Lambda\, f(x) - \frac{\int_{\epsilon(x+1)}^{\epsilon(x)} \rho(\omega)d\omega}{\Lambda^{2-x}\rho[\mathcal{E}(x)]}$$

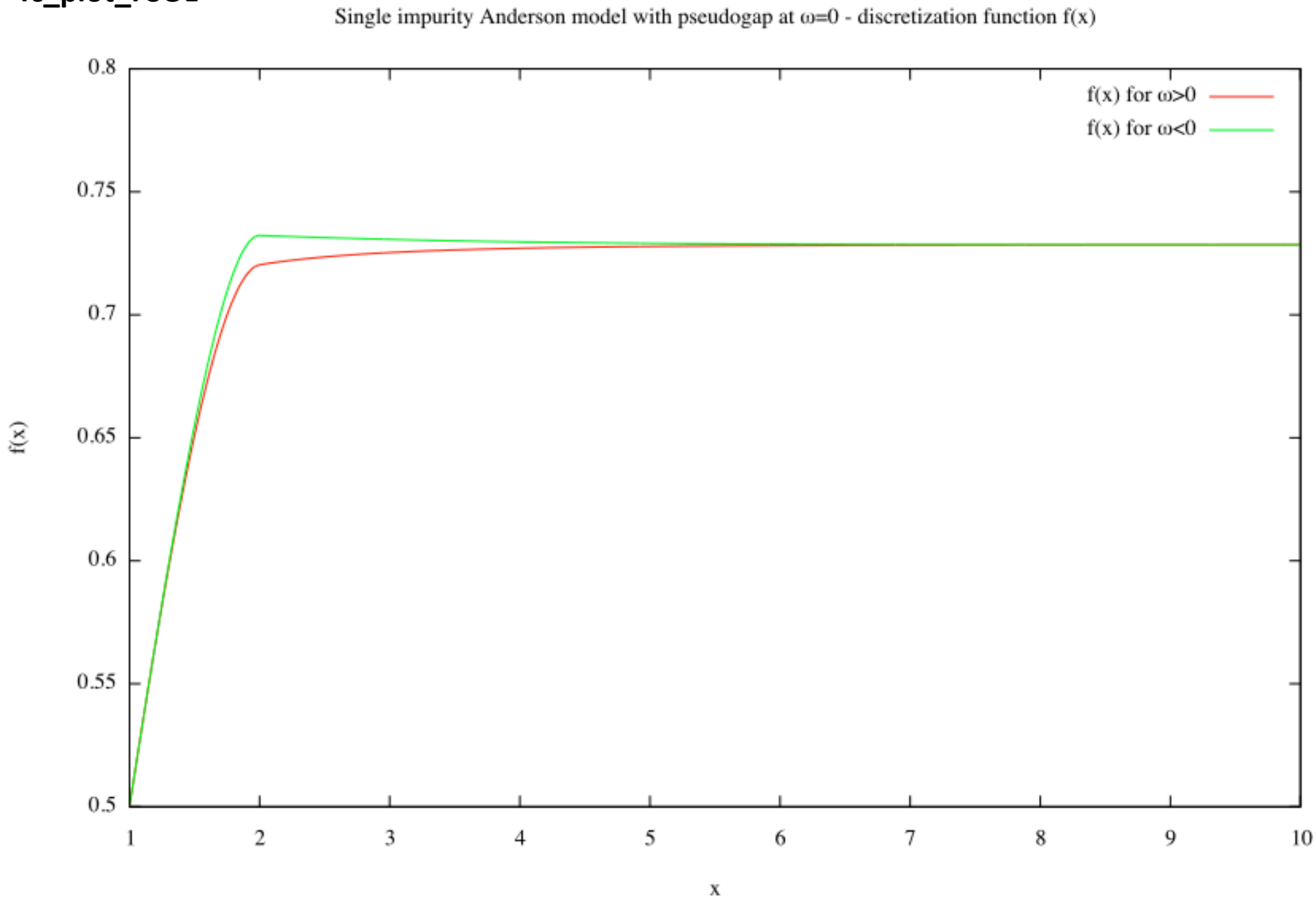
Output: **FSOL.dat**, **FSOLNEG.dat**

f(x) for positive and negative frequencies

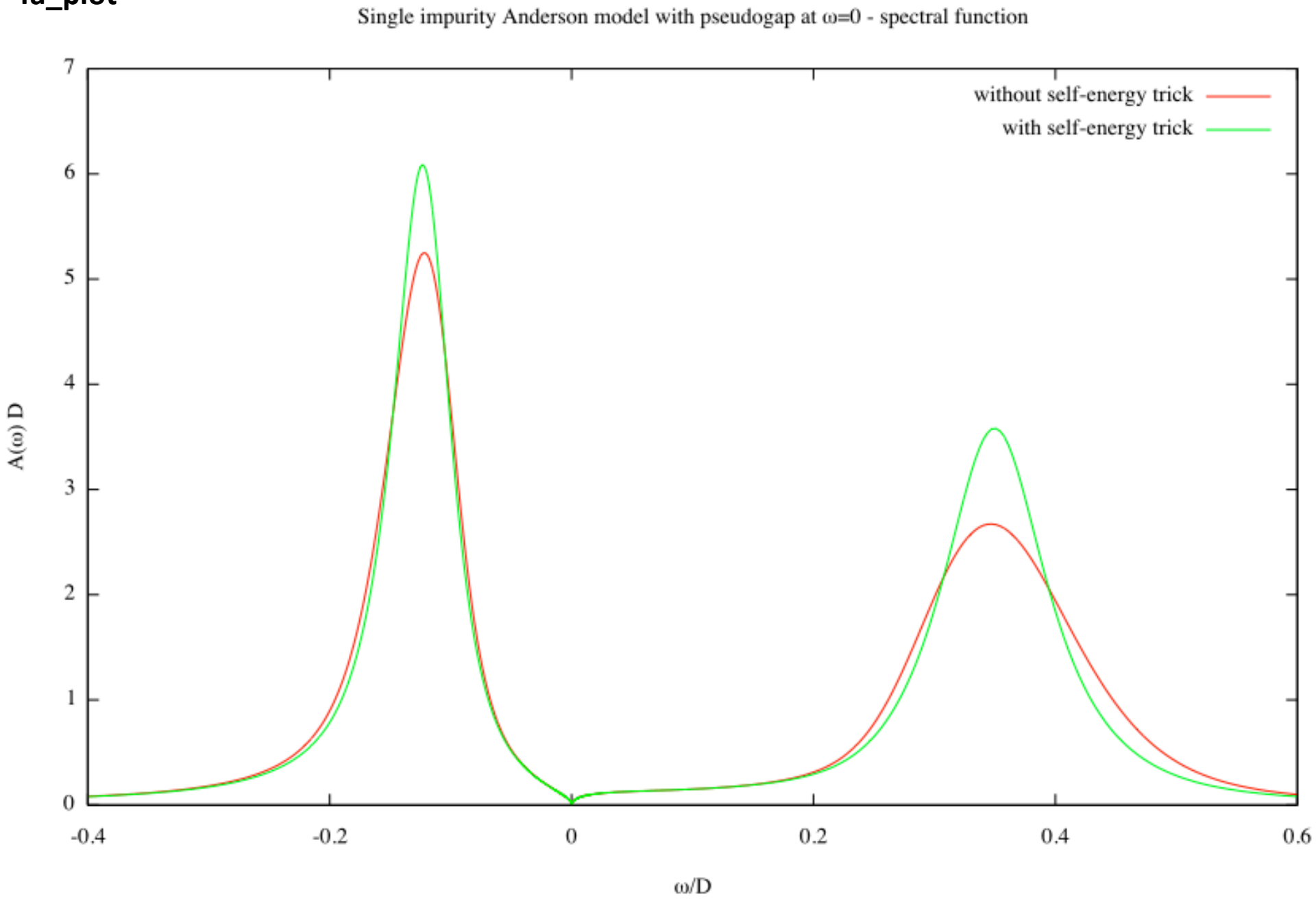
Invocation:

```
adapt P
adapt N
```

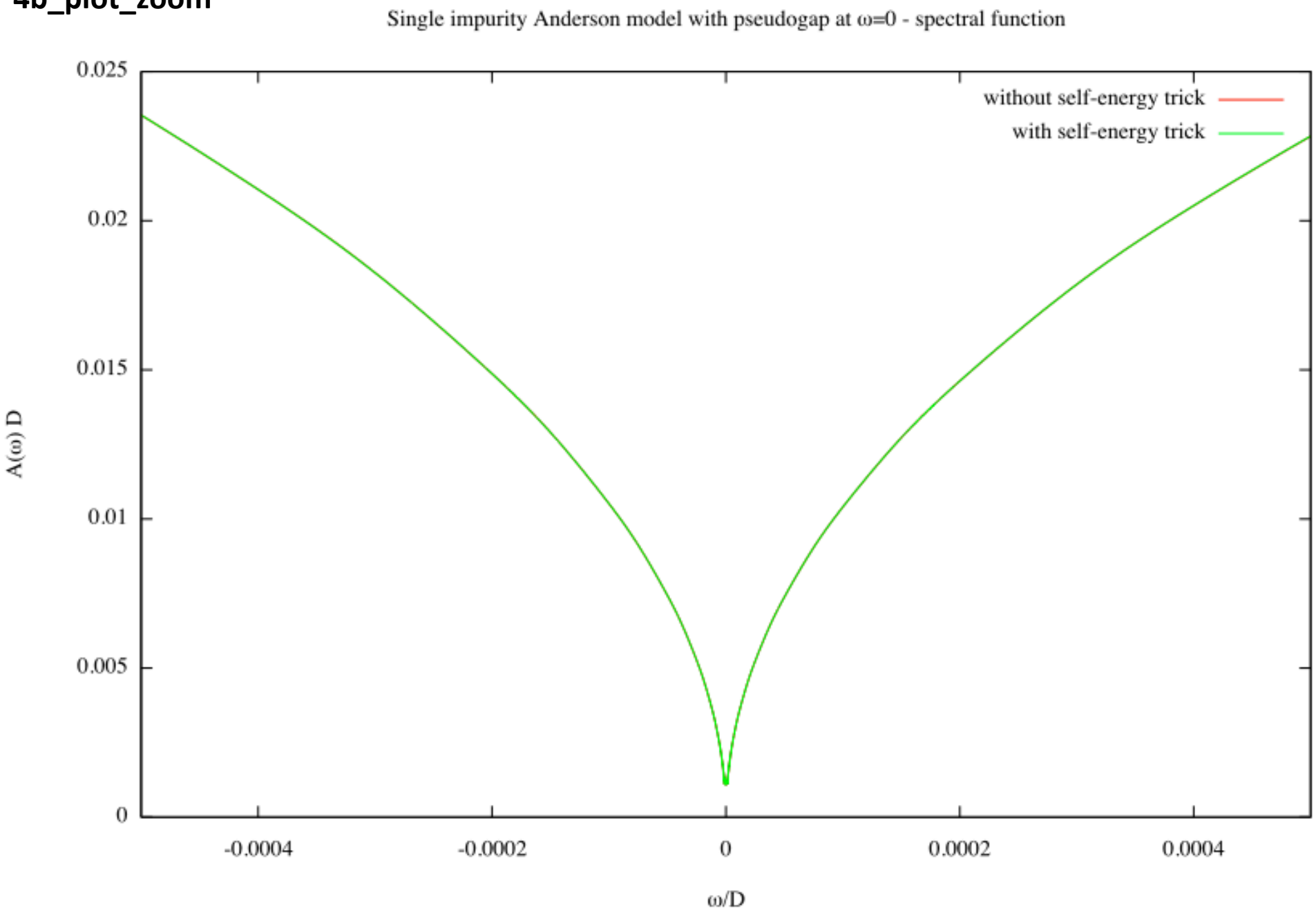
4c_plot_FSOL


Single impurity Anderson model with pseudogap at ω=0 - discretization function f(x)
f(x) for ω>0
f(x) for ω<0
f(x)
x
0.8
0.75
0.7
0.65
0.6
0.55
0.5
1
2
3
4
5
6
7
8
9
10

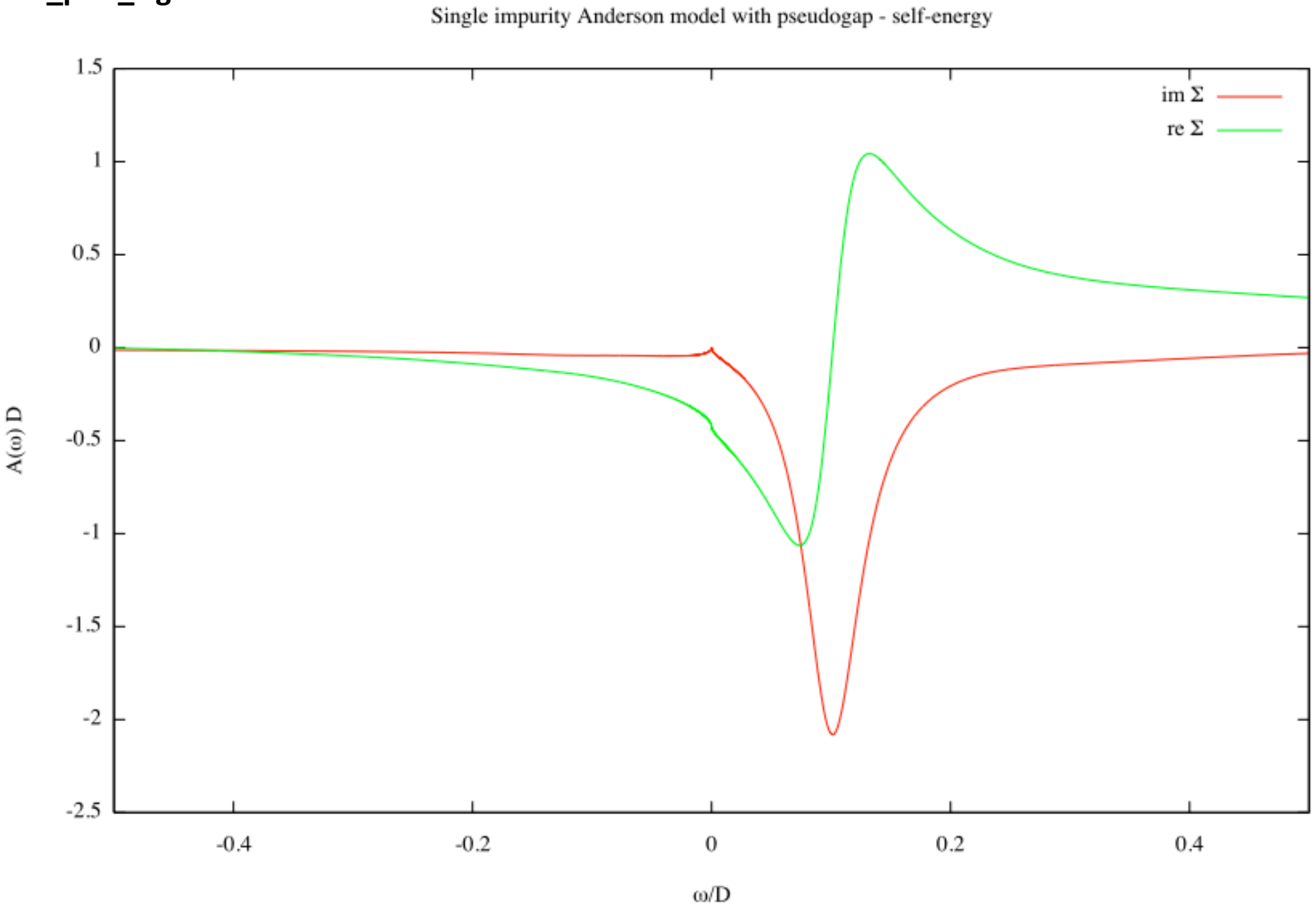
4a_plot


Single impurity Anderson model with pseudogap at ω=0 - spectral function
without self-energy trick
with self-energy trick
A(ω) D
ω/D
7
6
5
4
3
2
1
0
-0.4
-0.2
0
0.2
0.4
0.6

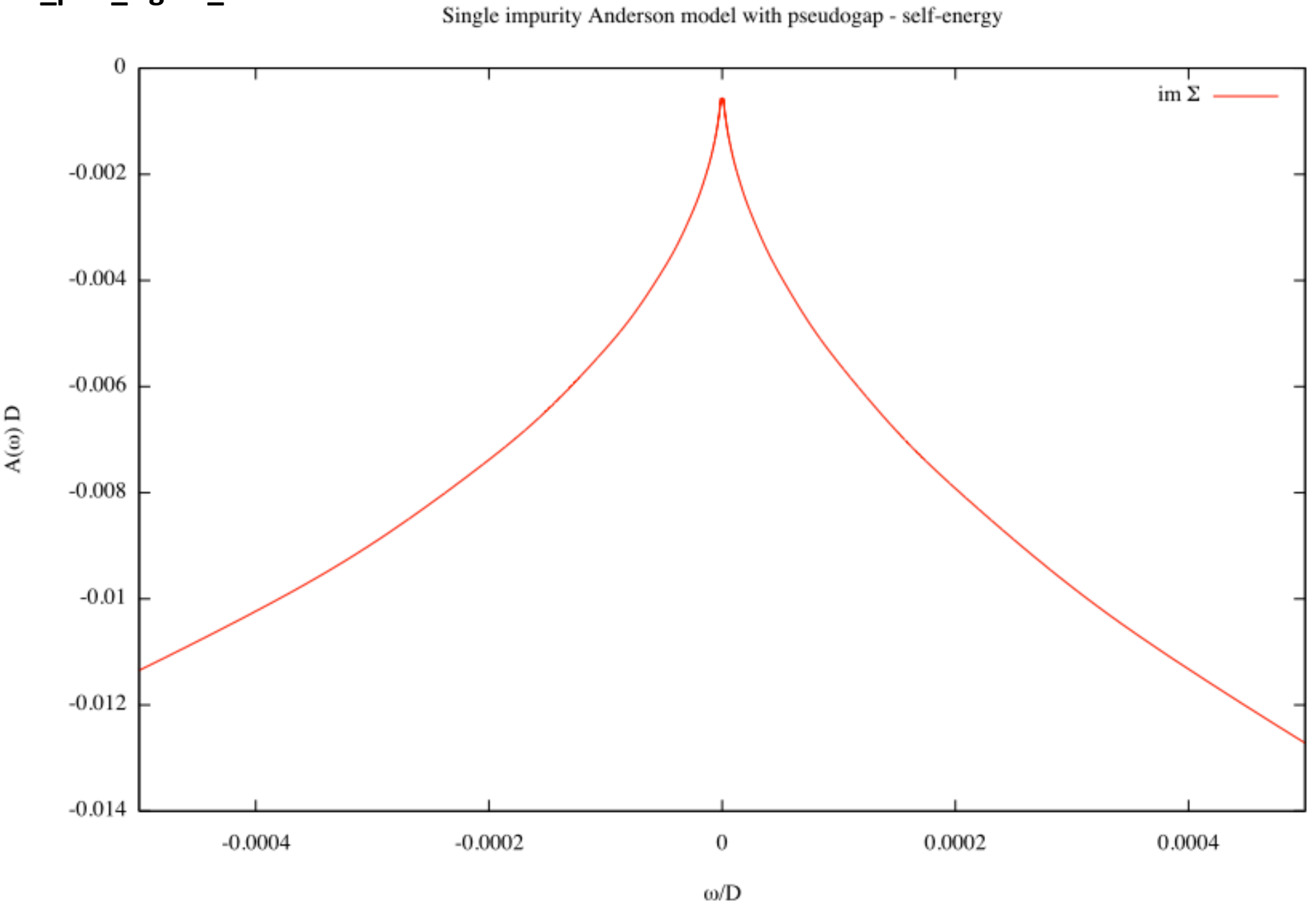
4b_plot_zoom


Single impurity Anderson model with pseudogap at ω=0 - spectral function
without self-energy trick
with self-energy trick
A(ω) D
ω/D
0.025
0.02
0.015
0.01
0.005
0
-0.0004
-0.0002
0
0.0002
0.0004

4e_plot_sigma



4f_plot_sigma_zoom



Exercises

- Try some other densities of states in the band. How robust is the Kondo resonance?
- When δ=0, show that the model is not particle-hole symmetric if the band isn't.
- Can the code handle discontinuities in DOS? What about divergencies in DOS?

Finite-temperature spectral functions

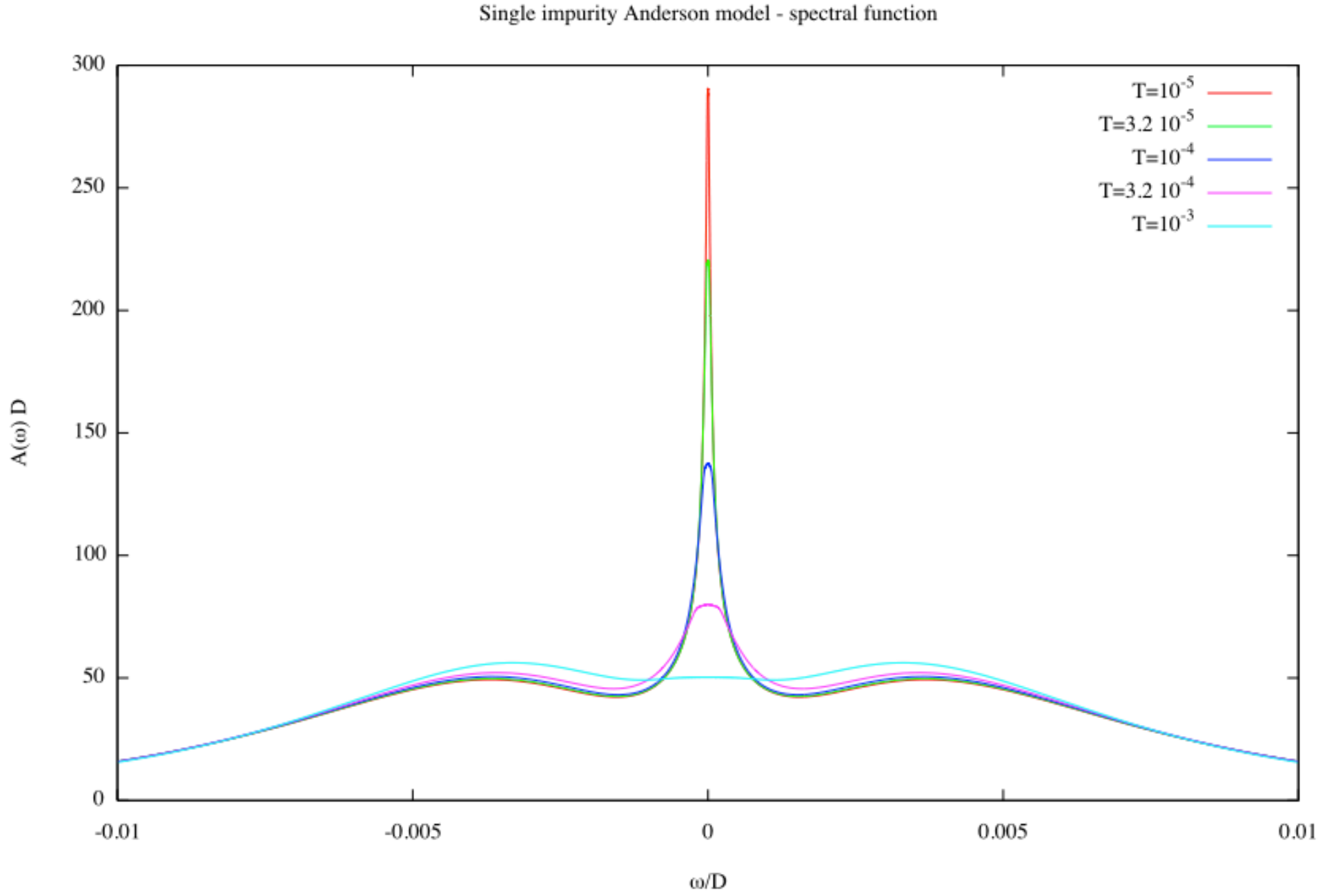
05_spec_ft/1e-3

```
ops=A_d
specd=A_d-A_d

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

fdm=true
T=1e-3

smooth=new
alpha=0.6
```

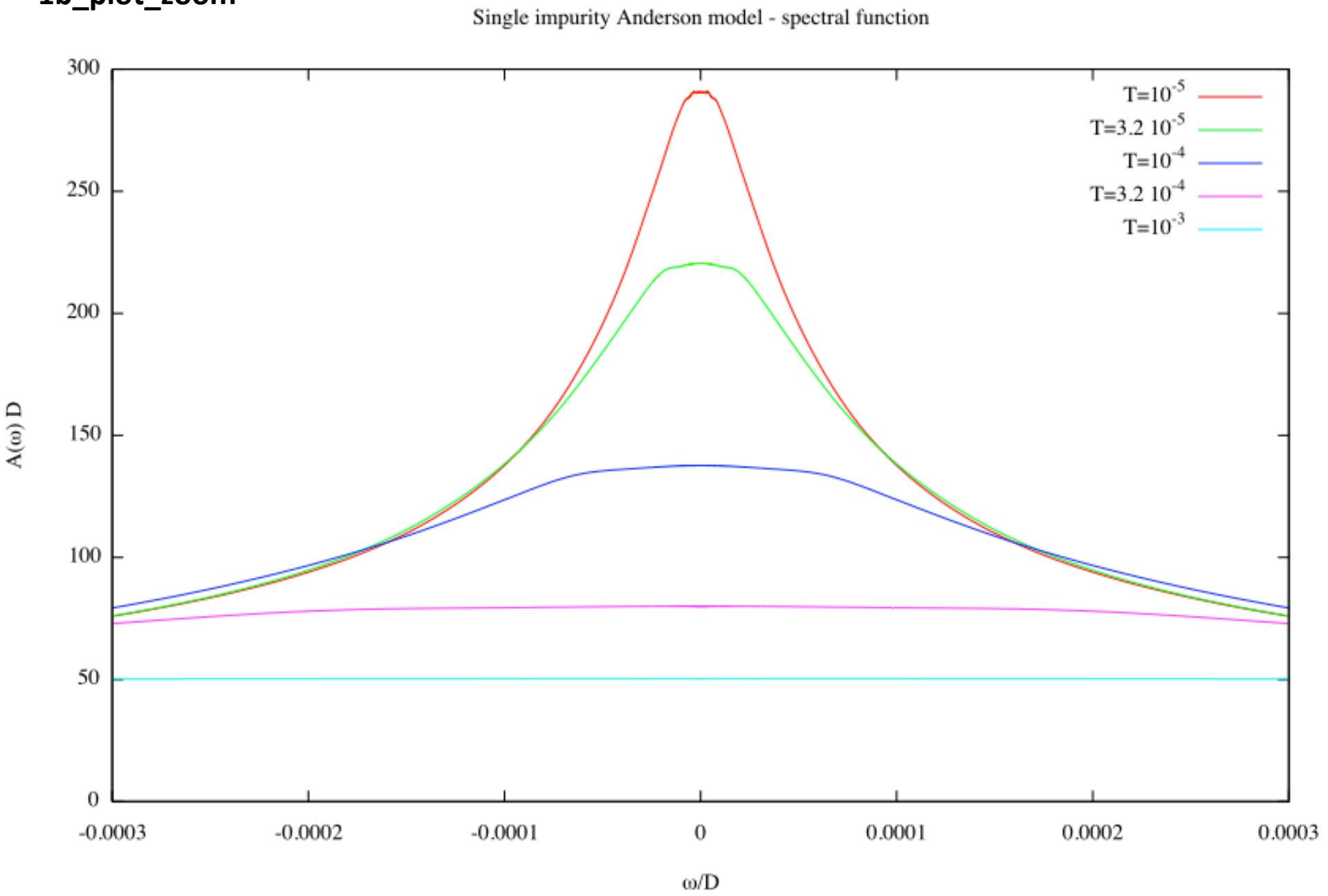
Full density matrix method (recommended for finite T)

Broadening kernel for finite T

1a_plot


Single impurity Anderson model - spectral function
A(ω) D
ω/D
300
250
200
150
100
50
0
-0.01
-0.005
0
0.005
0.01
T=10^-5
T=3.2 10^-5
T=10^-4
T=3.2 10^-4
T=10^-3

1b_plot_zoom


Single impurity Anderson model - spectral function
A(ω) D
ω/D
300
250
200
150
100
50
0
-0.0003
-0.0002
-0.0001
0
0.0001
0.0002
0.0003
T=10-5
T=3.2 10-5
T=10-4
T=3.2 10-4
T=10-3

Exercises

- Combine the code for the self-energy trick with that for finite-T calculations (using FDM NRG). How does Im Σ evolve with increasing temperature?

Kondo model

$$G = G_0 + G_0 T G_0$$

$$T_\sigma = \langle\langle O_\sigma ; O_\sigma^\dagger \rangle\rangle$$

$$O_\sigma = [H_{\mathrm{coupling}}, f_{0,\sigma}]$$

$$H_{\mathrm{K}} = \left(\frac{1}{2} f_{0,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} f_{0,\beta} \right) \cdot \mathbf{S}$$

$$O_\sigma = \left(\frac{1}{2} \boldsymbol{\sigma}_{\alpha\beta} f_{0,\beta} \right) \cdot \mathbf{S}$$

```
#!/usr/bin/env looper
#AUTOLOOP: nrginit ; nrgrun
#OVERWRITE

[extra]
spin=1/2
Jkondo=0.2

[param]
symtype=QS
discretization=Z
@$z = 1/4; $z <= 1; $z += 1/4
z=$z
Lambda=2
Tmin=1e-10
keepenergy=10
keep=10000
```

```
model=../kondo.m

ops=hyb_f SfSk
specd=hyb_f-hyb_f

broaden_max=0.1
broaden_min=1e-8
broaden_ratio=1.02

fdm=true
T=1e-11

smooth=new
alpha=0.3
omega0=1e-99
```

05_spec_kondo/1_zloop

05_spec_kondo/model.m

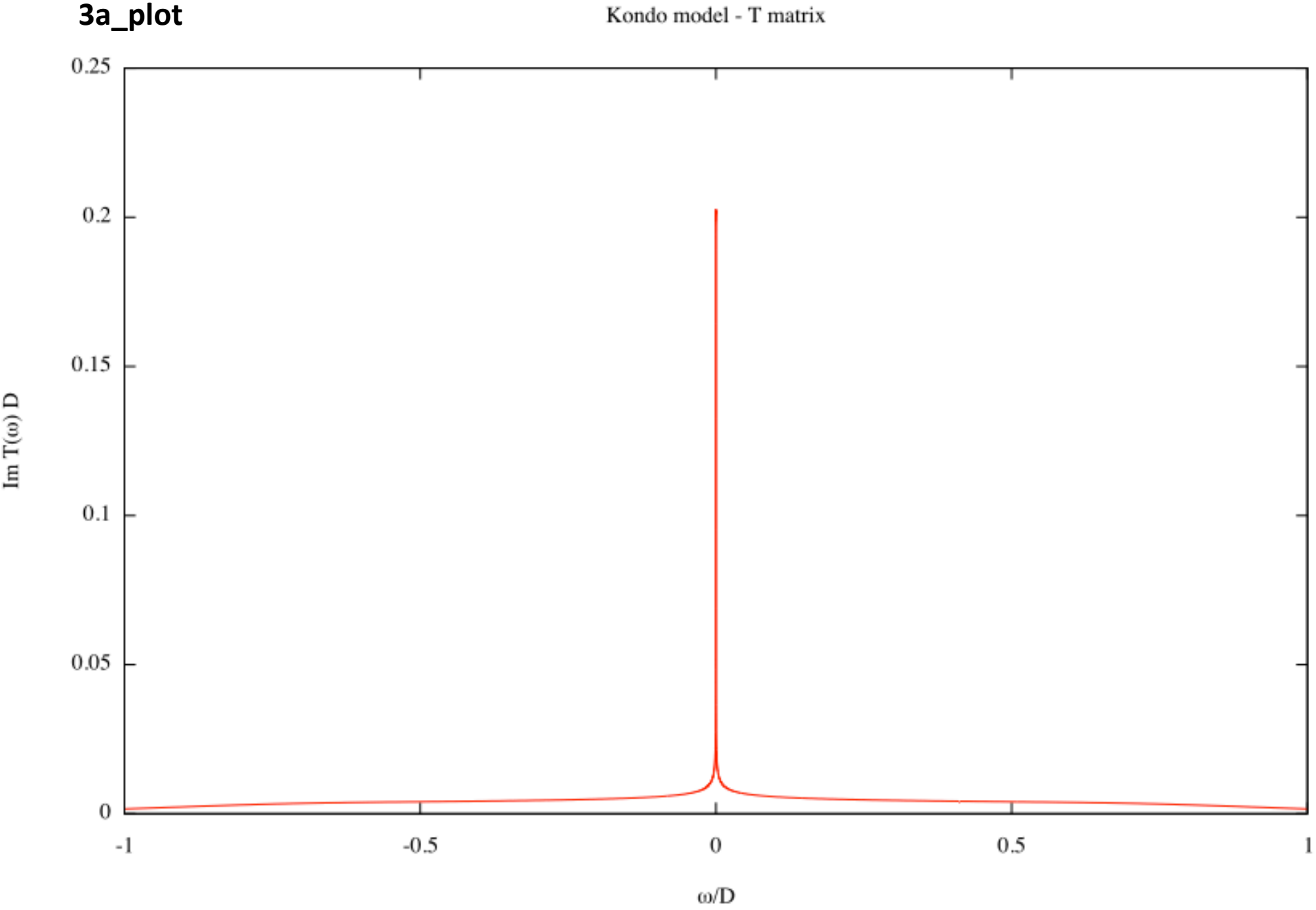
```
def1ch[0];

SPIN = ToExpression @ param["spin", "extra"];

Module[{sx, sy, sz, ox, oy, oz, ss},
 sx = spinketbraX[SPIN];
 sy = spinketbraY[SPIN];
 sz = spinketbraZ[SPIN];

 ox = nc[ sx, spinx[ f[0] ] ];
 oy = nc[ sy, spiny[ f[0] ] ];
 oz = nc[ sz, spinz[ f[0] ] ];

 ss = Expand[ox + oy + oz];
 Hk = Jkondo ss;
];

H = H0 + Hk;
Hhyb = Hk;

MAKESPINKET = SPIN;

hybopf = ( Chop @ Expand @ komutator[Hhyb /. params, f[#1, 0, #2]] )&;
```

NOTE: this is different from what we did in SIAM for the self-energy trick, where we computed the commutator with the interaction part of the Hamiltonian.

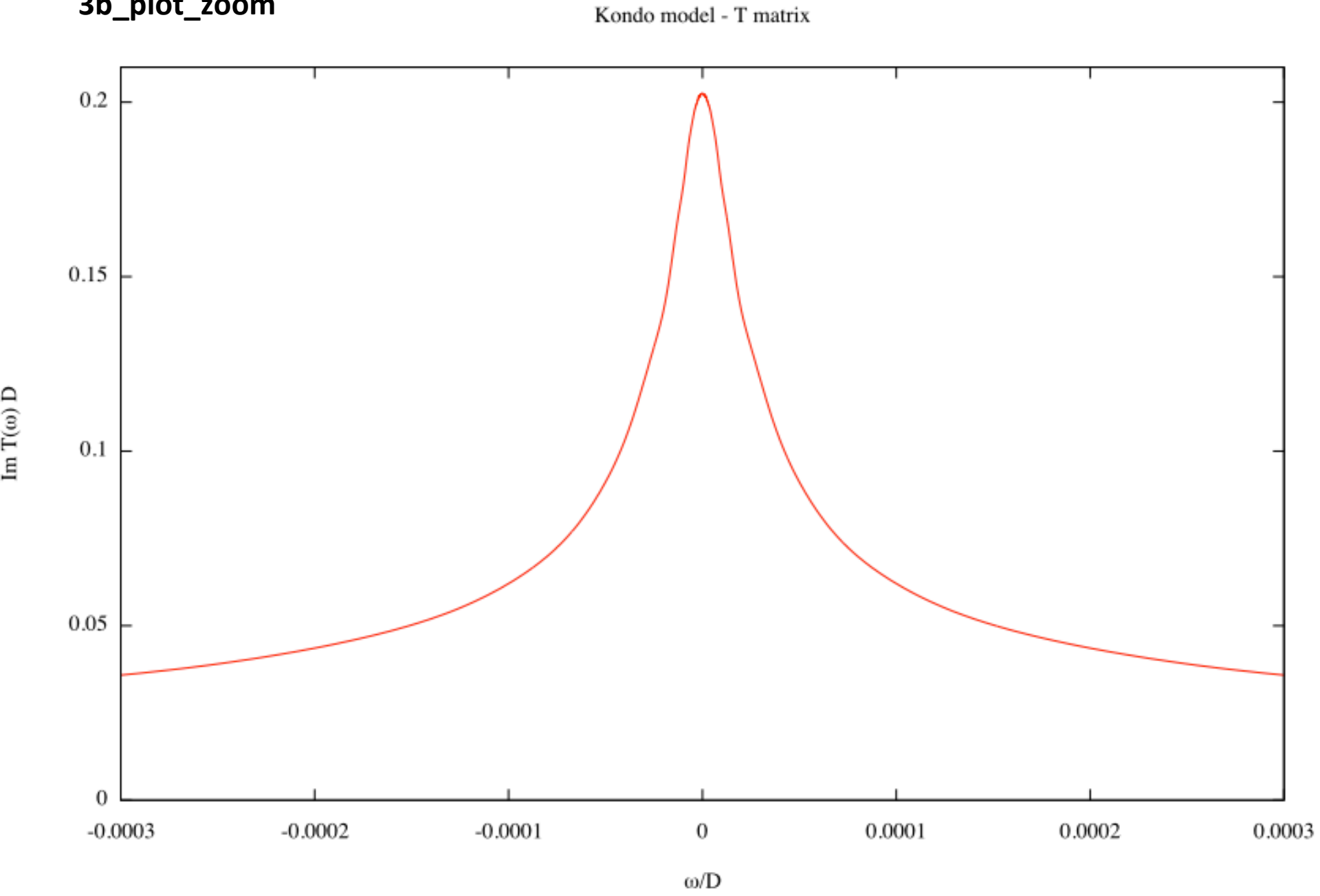
```
Module[{t={}},

 If[calcopq["hyb_f"],
   AppendTo[t, {"dhyb_f"}];
   MPVCFAST = False;
   t = Join[t, ireducTable[ hybopf ]];
   MPVCFAST = True;
 ];

 texportable = t;
];

texportable
```

05_spec_kondo/modeloperators.m

3a_plot



3b_plot_zoom


Kondo model - T matrix
Im T(ω) D
0.2
0.15
0.1
0.05
0
-0.0003
-0.0002
-0.0001
0
0.0001
0.0002
0.0003
ω/D

Exercises

- How is the width (HWHM) of the Kondo resonance related to the Kondo temperature T_K?