Tutorial 4: Kondo peak splitting in magnetic field, transport integrals, conductance and thermopower

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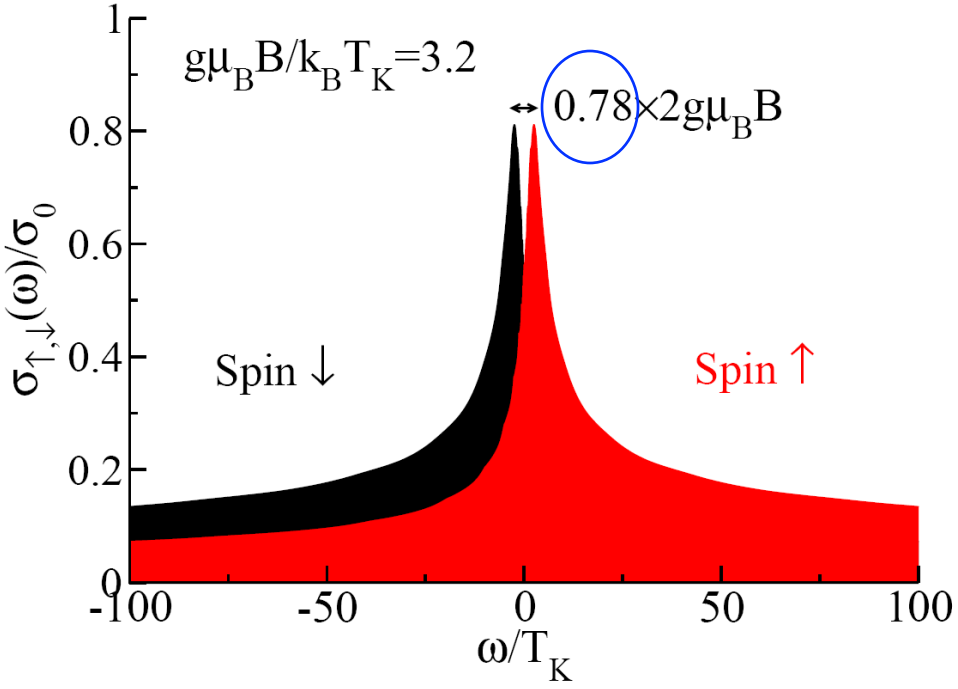
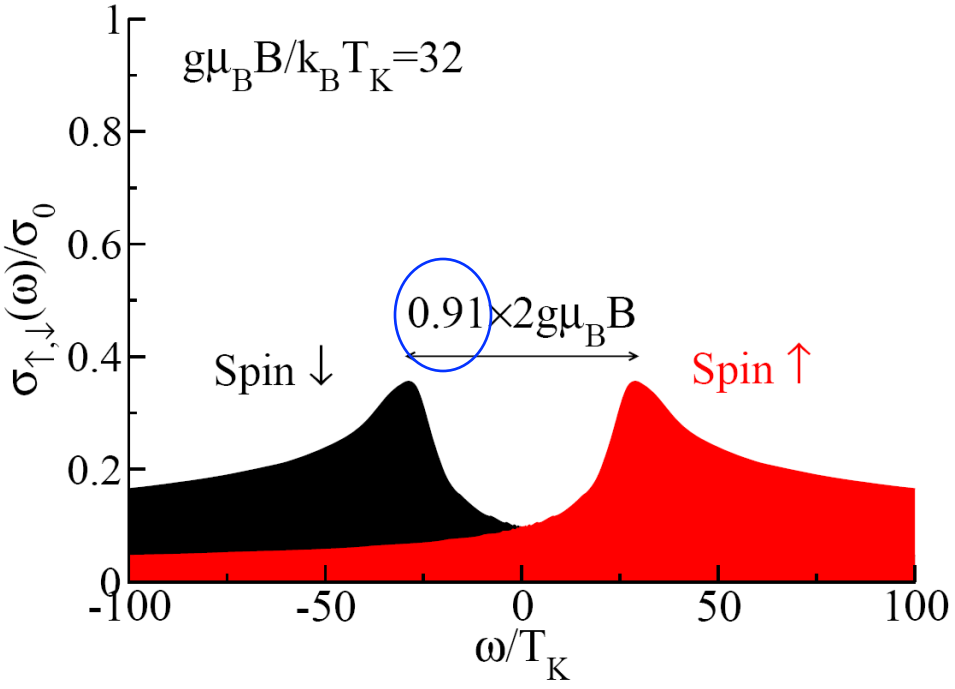
Kondo resonance splitting

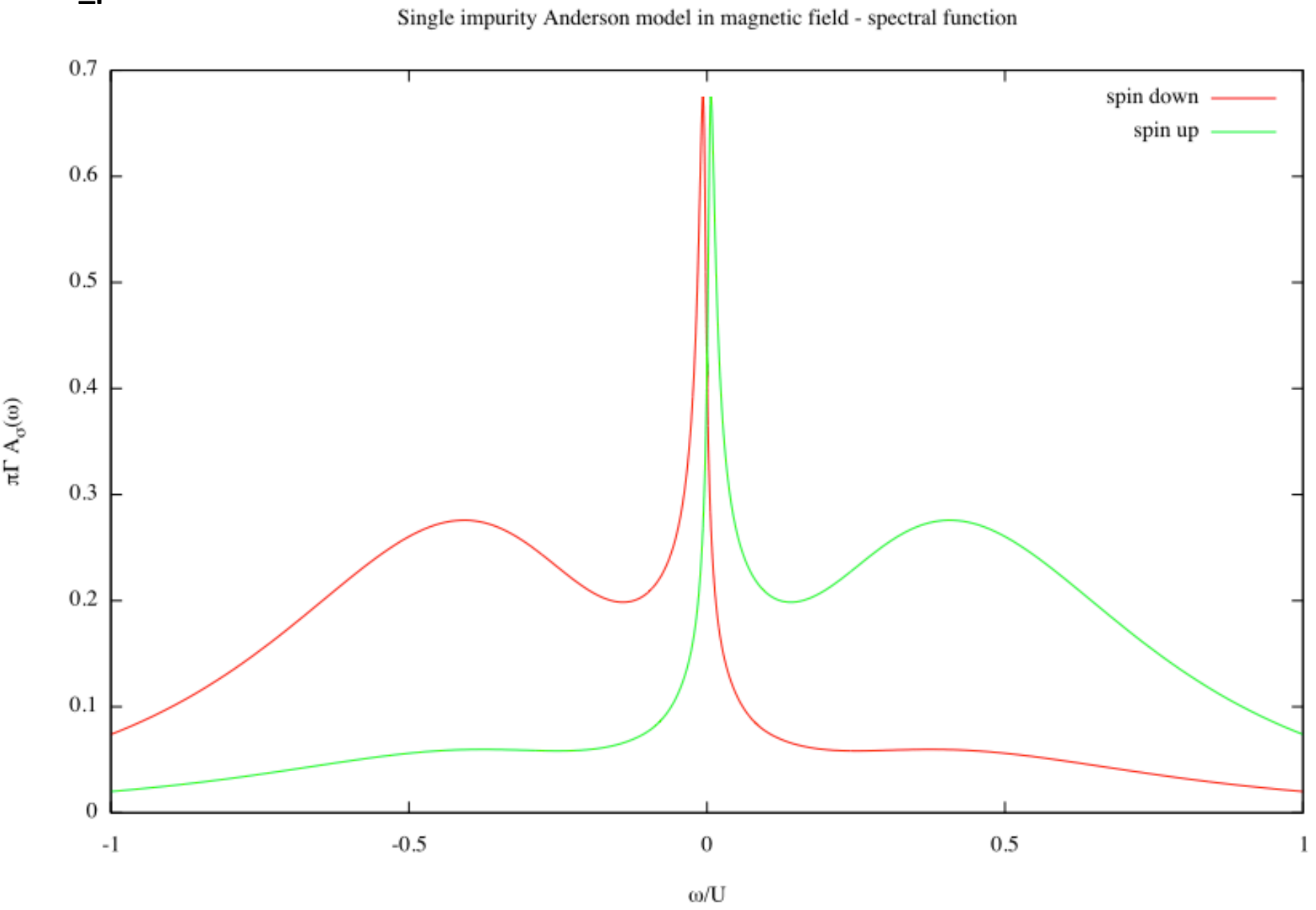




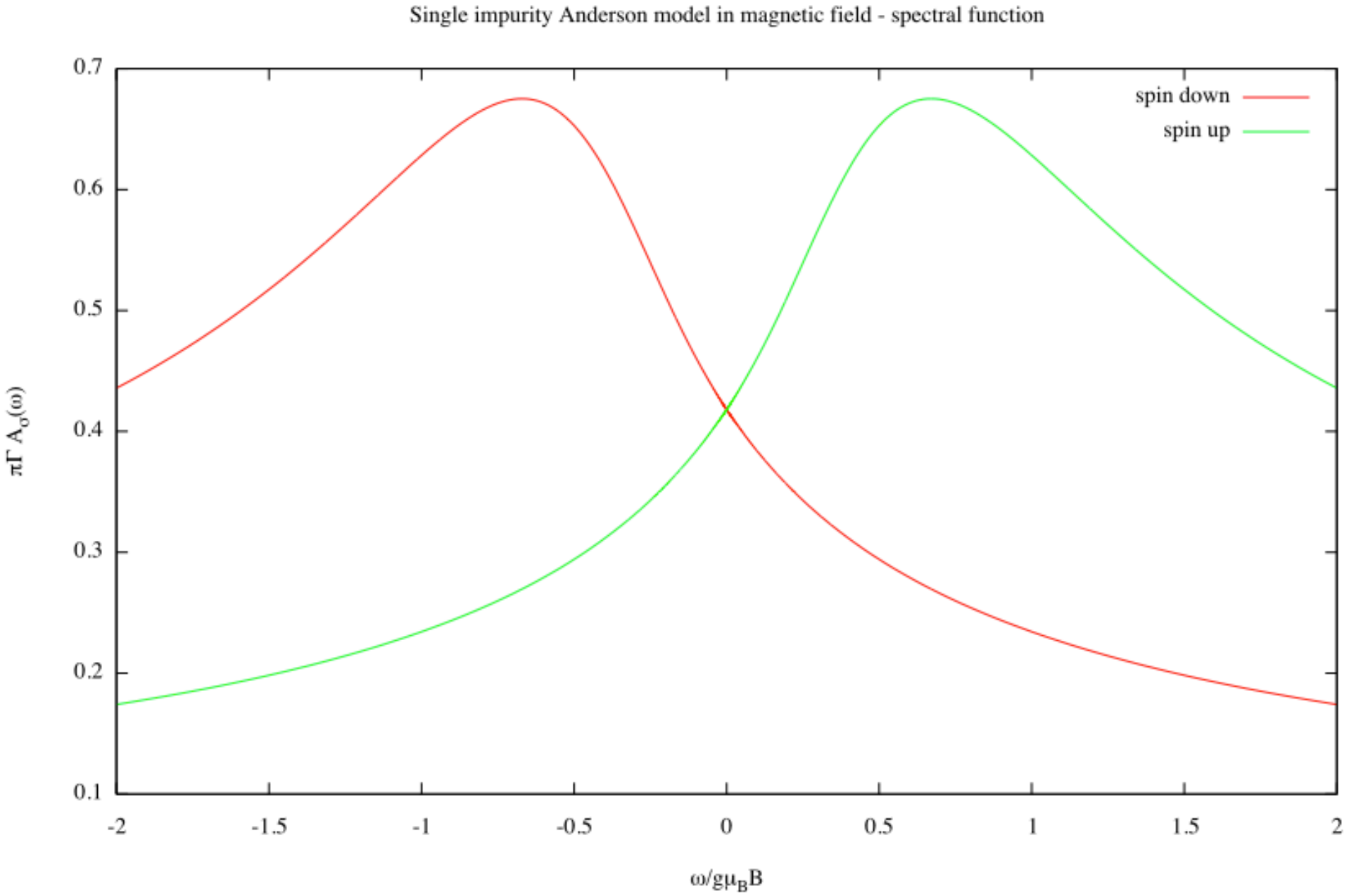
```
#!/usr/bin/env looper
#AUTOLOOP: nrginit ; nrgrun
#OVERWRITE

[extra]
B=1e-4

[param]
symtype=QSZ
discretization=Z
@$z = 1/4; $z <= 1; $z += 1/4
z=$z
Lambda=3
Tmin=1e-10
keepenergy=10
keep=10000

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

ops=A_d SZd
specd=A_d-A_d-u A_d-A_d-d

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

fdm=true
T=1e-10

smooth=new
alpha=0.5
omega0=1e-99
```

06_splitting/1_zloop

2a_plot


Single impurity Anderson model in magnetic field - spectral function
spin down
spin up
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
πΓ A_σ(ω)
-1
-0.5
0
0.5
1
ω/U

2a_plot_zoom_B



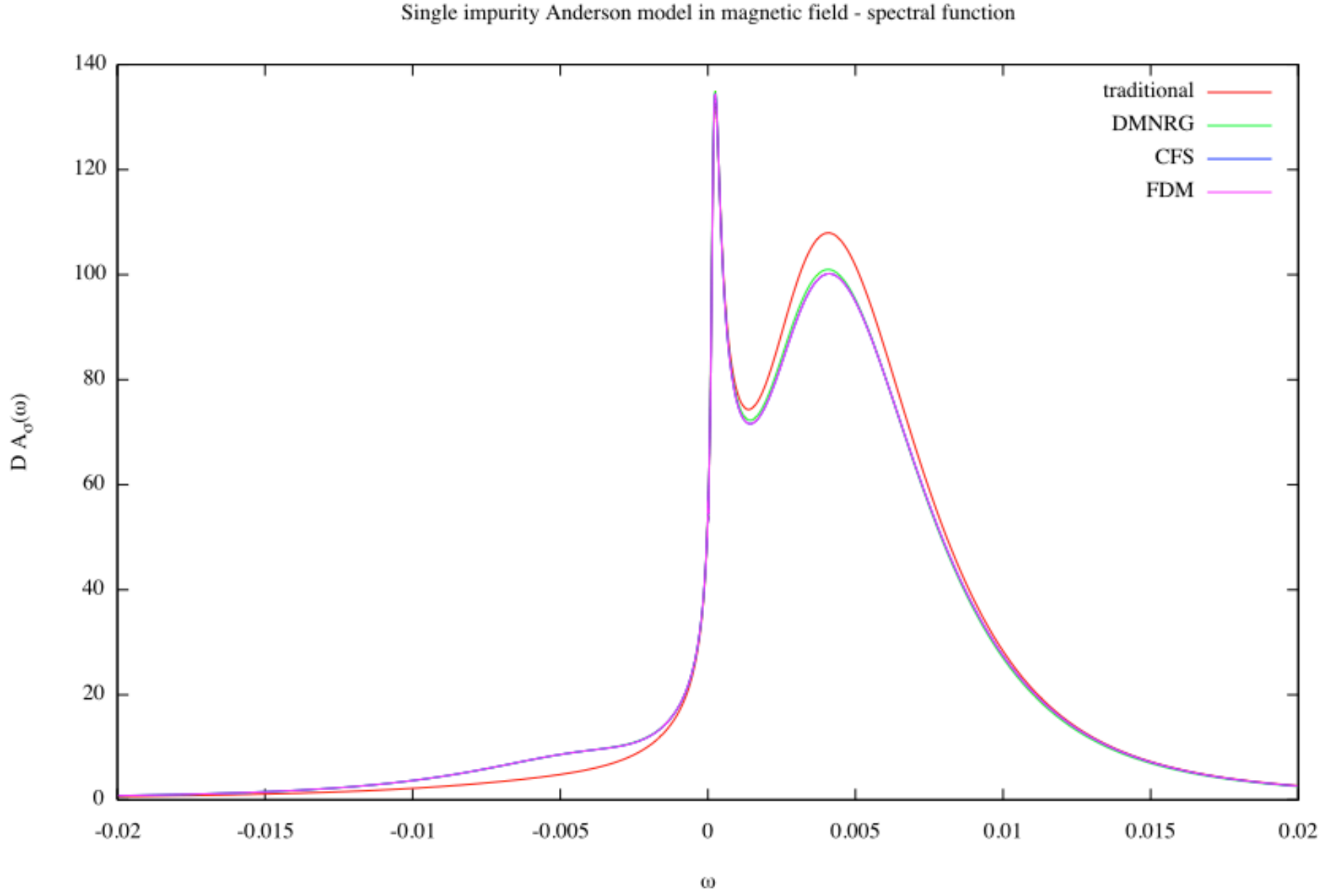
FT vs. DMNRG vs. CFS vs. FDM

FT = traditional approach, no density matrix
DMNRG = density matrix evaluated at the last NRG iteration, necessary for cases where the low-energy fixed point affects the high-energy part of the spectral function; recommended in the presence of magnetic field or other marginal and relevant perturbations.
CFS = complete Fock space, similar to DMNRG, but fulfills the normalization sum rule by construction, no overcounting; recommended at higher values of Λ.
FDM = full density matrix, ρ is constructed on all energy shells; recommended for finite-temperature calculations.

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

[extra]
B=3e-4

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

model=SIAM
variant=MAGFIELD
U=0.01
Gamma=0.001
delta=0
ops=A_d SZd
specd=A_d-A_d-u A_d-A_d-d

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

finite=true
dmnrg=true
cfs=true
fdm=true
T=1e-10

goodE=2.1

smooth=new
alpha=0.5
omega0=1e-99
```

06_splitting_methods

3_plot


Single impurity Anderson model in magnetic field - spectral function
traditional
DMNRG
CFS
FDM
D A_σ(ω)
ω
140
120
100
80
60
40
20
0
-0.02
-0.015
-0.01
-0.005
0
0.005
0.01
0.015
0.02

```
bash-3.2$ ./4_sum_rule
Sz (custom) = -0.3646425
Sz (FT) = -0.402076352947836  diff=10.265905084524%
Sz (DMNRG) = -0.364642938937181  diff=0.00012037466312647 9%
Sz (CFS) = -0.364479526193025  diff=-0.044694133836565 3%
```

Transport integrals for SIAM

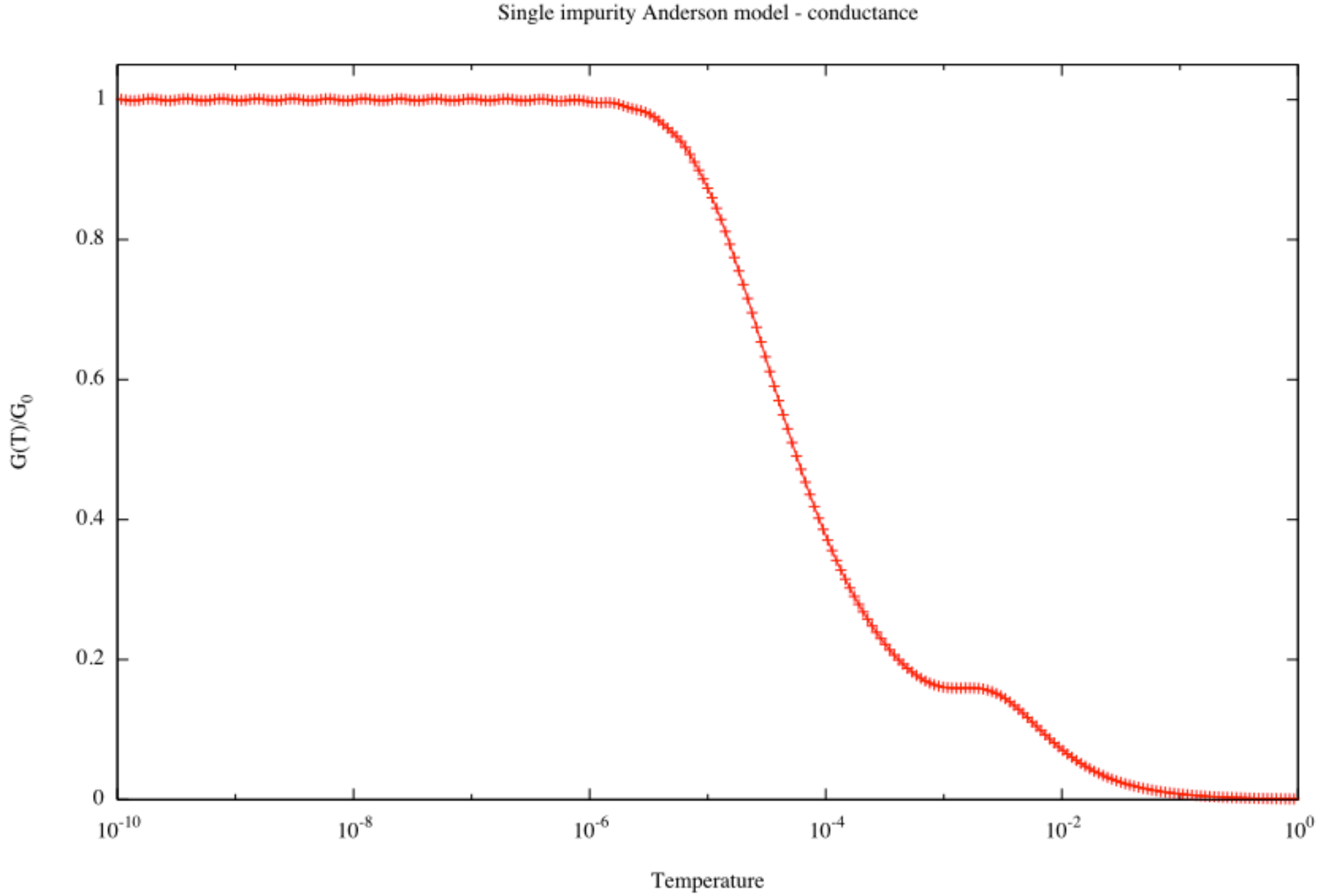
07_cond/1_zloop

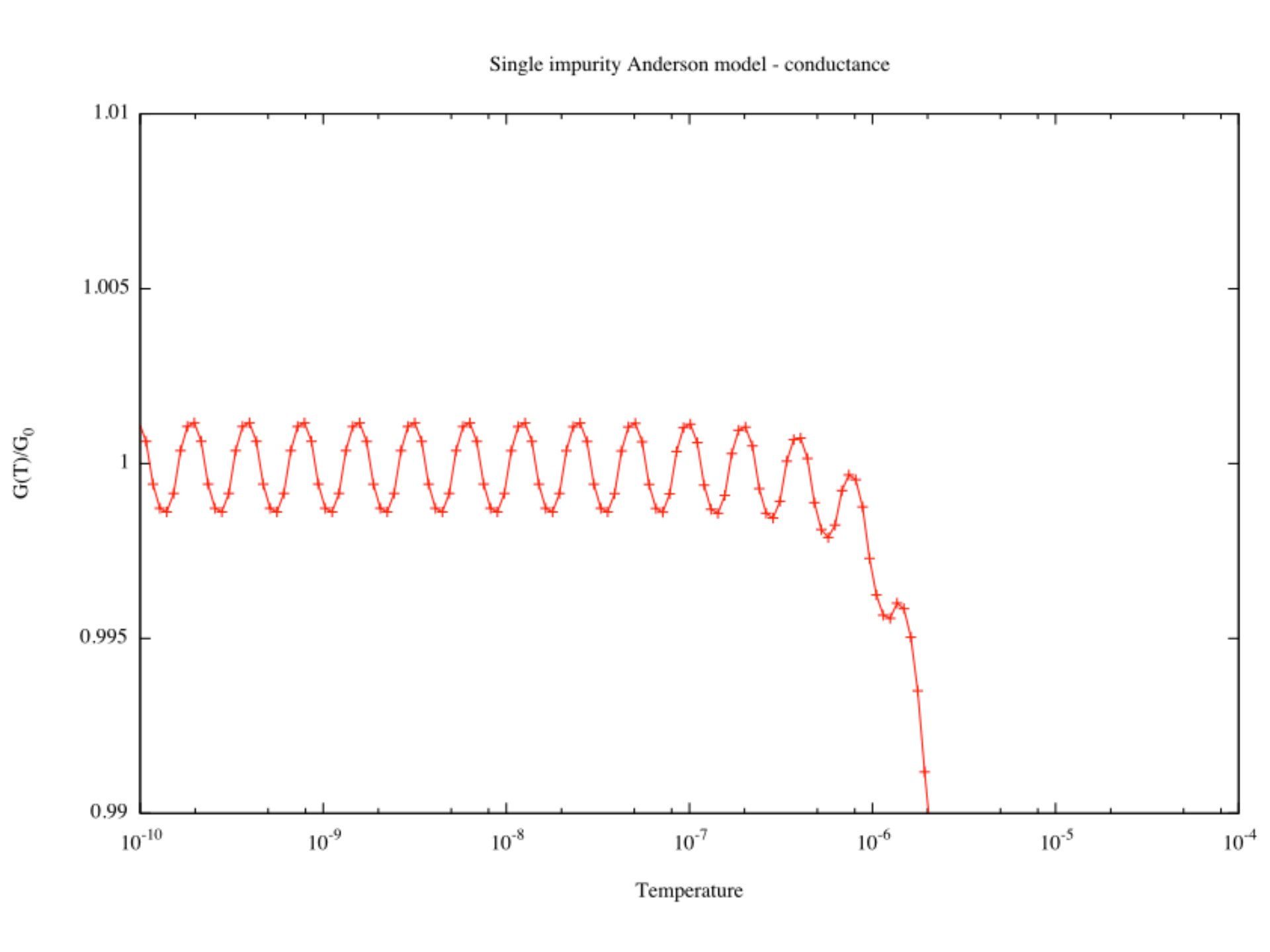
```
#!/usr/bin/env looper
# Conductance calculation for
SIAM
#AUTOLOOP: nrginit ; nrgrun
#OVERWRITE

[param]
symtype=QS
discretization=Z
@$z = 1/8; $z <= 1; $z += 1/8
z=$z
Lambda=2
Tmin=1e-10
keepenergy=10
keep=10000
```

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

```
ops=A_d

specgt=A_d-A_d
speci1t=A_d-A_d
speci2t=A_d-A_d
gtp=0.7
```

3a_plot


Single impurity Anderson model - conductance
G(T)/G0
1
0.8
0.6
0.4
0.2
0
10-10
10-8
10-6
10-4
10-2
100
Temperature

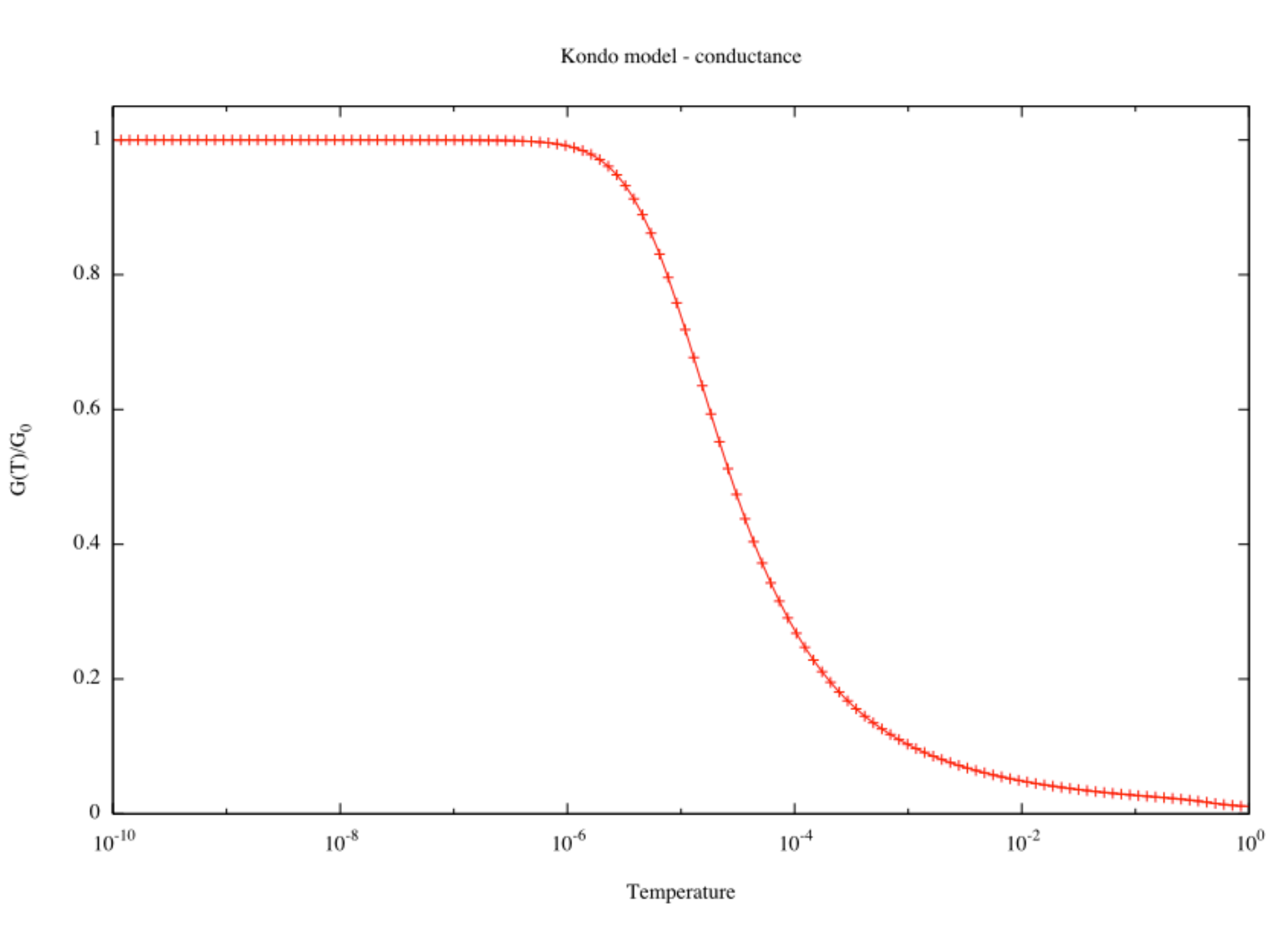

Single impurity Anderson model - conductance
1.01
1.005
1
0.995
0.99
G(T)/G0
10-10
10-9
10-8
10-7
10-6
10-5
10-4
Temperature

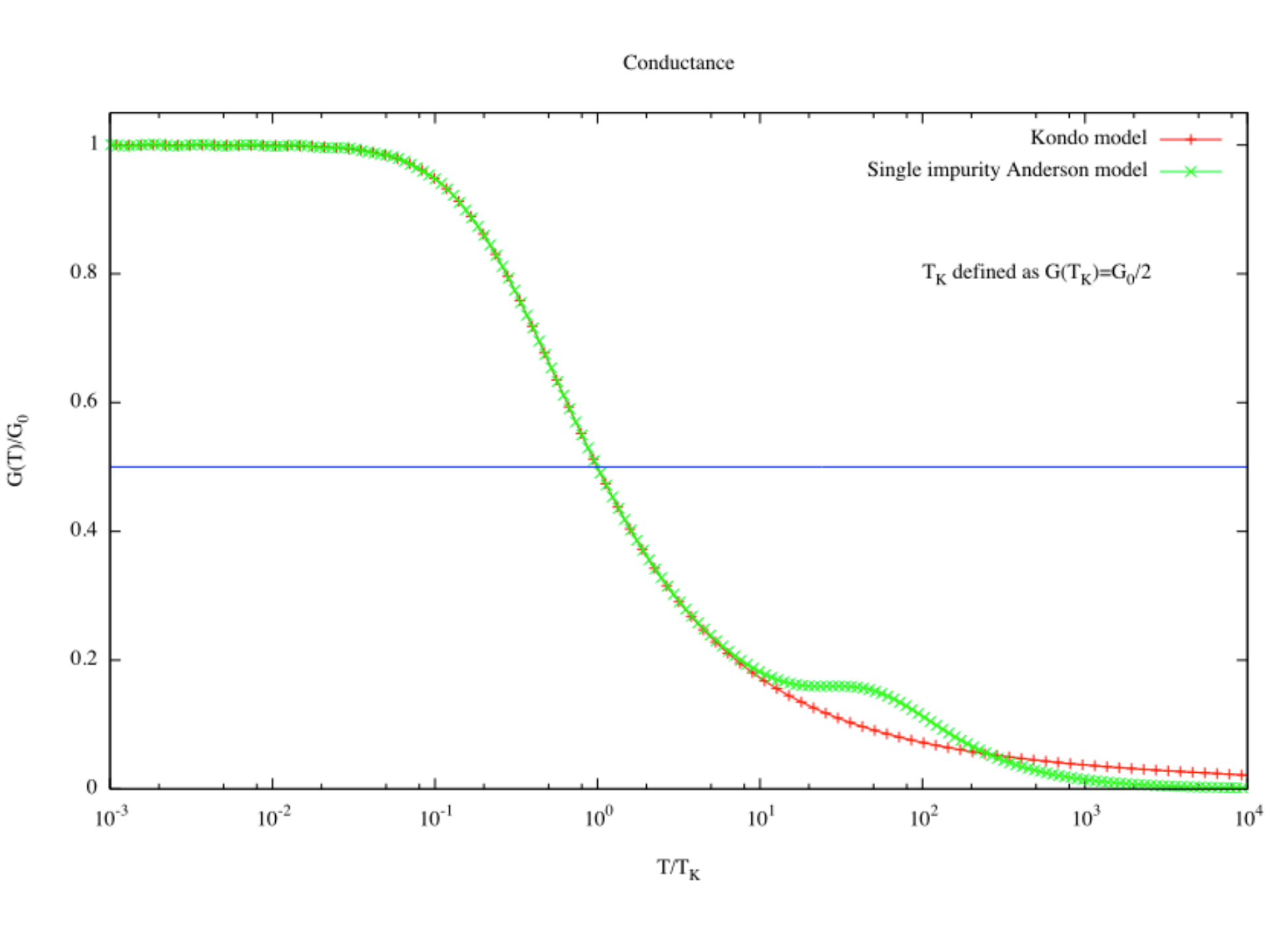
Conductance for the Kondo model

08_cond_kondo/1_zloop

```
#!/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
specgt=hyb_f-hyb_f
speci1t=hyb_f-hyb_f
speci2t=hyb_f-hyb_f

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

fdm=true
T=1e-15

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


Kondo model - conductance
G(T)/G0
1
0.8
0.6
0.4
0.2
0
10-10
10-8
10-6
10-4
10-2
100
Temperature


Conductance
Kondo model
Single impurity Anderson model
T_K defined as $G(T_K)=G_0/2$
$G(T)/G_0$
T/T_K
0
0.2
0.4
0.6
0.8
1
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}

Different definitions of T_K

Wilson's definition

$$\chi(T \ll T_{\mathrm{KW}}) = \frac{0.1032 \pm 0.0005}{T_{\mathrm{KW}}} \qquad T_{\mathrm{KW}}\chi(T_{\mathrm{KW}}) = 0.701$$

$$W = \frac{e^{C+1/4}}{\sqrt{\pi}} \approx 1.29026 \qquad W/4\pi = 0.102676\ldots \approx 0.1032 \pm 0.0005$$

"Fermi-liquid definition"

$$R(T)/R(0) = 1 - c\left(T/T_{\mathrm{K}}^{(0)}\right)^2 \qquad \chi(T=0) = \frac{(g\mu_B)^2}{4k_B T_{\mathrm{K}}^{(0)}}$$

Hamann definition

$$R(T = T_{\mathrm{KH}}) = R(0)/2$$

$$T_{\mathrm{KW}} = 0.4128 T_{\mathrm{K}}^{(0)}$$

$$T_{\mathrm{KH}} = 0.91 T_{\mathrm{K}}^{(0)} = 2.2 T_{\mathrm{KW}}$$

(Charge and spin) thermopower

$$\mathcal{I}_{n\sigma} = \int \mathrm{d}\omega\, \omega^n [-f'(\omega)] \mathcal{T}_\sigma(\omega)$$

B=0

$$S = -\frac{eV}{\Delta T}\Big|_{I=0} = \frac{1}{T}\frac{\mathcal{I}_1}{\mathcal{I}_0}$$

(charge) Seebeck coefficient

δ=0 (particle-hole symmetric point)

$$S_s = -\frac{eV_s}{\Delta T}\Big|_{I_s=0} = \frac{2}{T}\frac{\mathcal{I}_1}{\mathcal{I}_0}$$

spin Seebeck coefficient

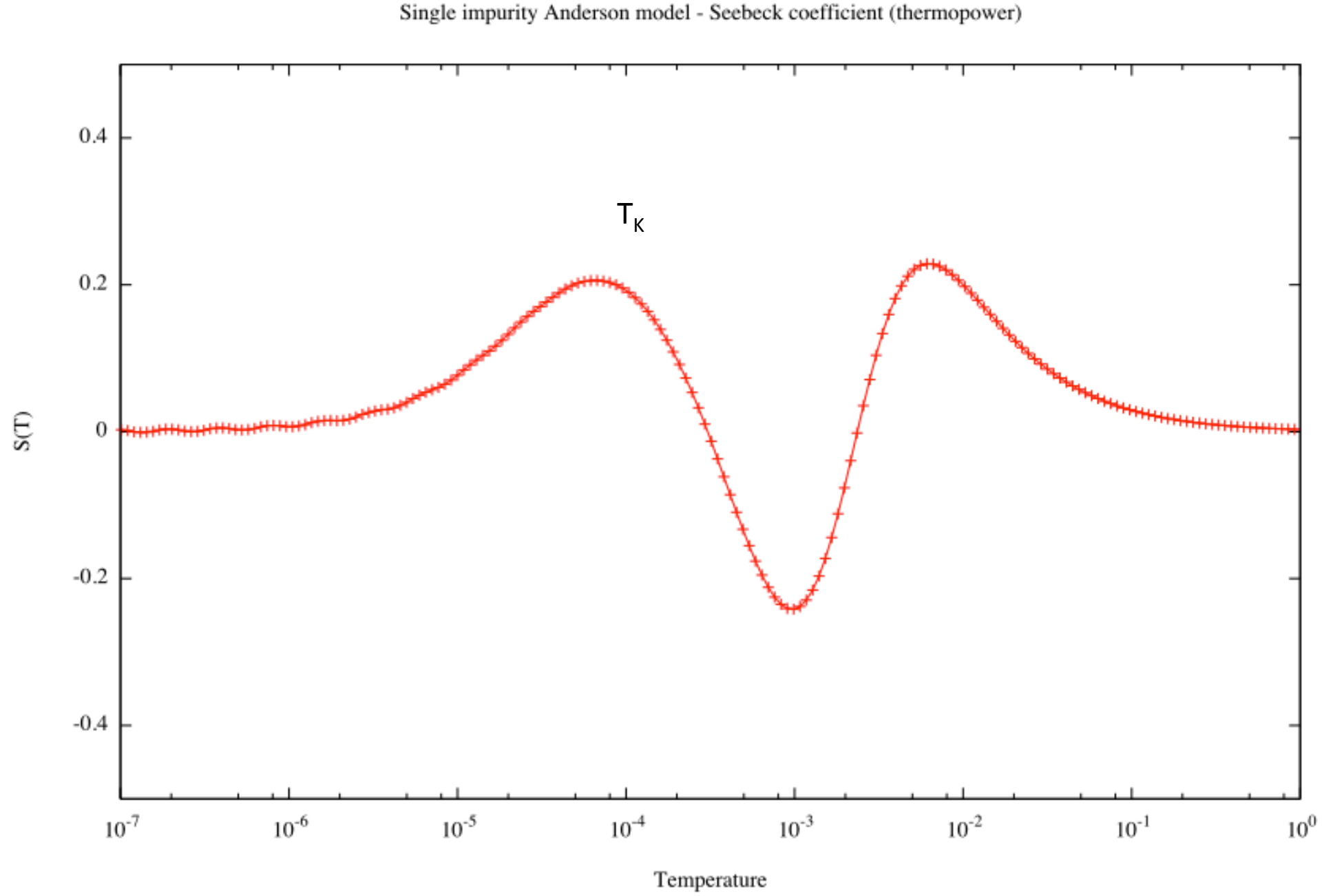
Charge thermopower in SIAM

```
#!/usr/bin/env perl

use warnings;

$Nz = 4;

$file = "gt_GT_dens_A_d-A_d.dat";
system "intavg $file $Nz";
system "mv $file i0.dat";

$file = "i1t_I1T_dens_A_d-A_d.dat";
system "intavg $file $Nz";
system "mv $file i1.dat";

system "divy i1.dat i0.dat >tmp";
system "divybyx tmp >S_charge.dat";
unlink "tmp";
```

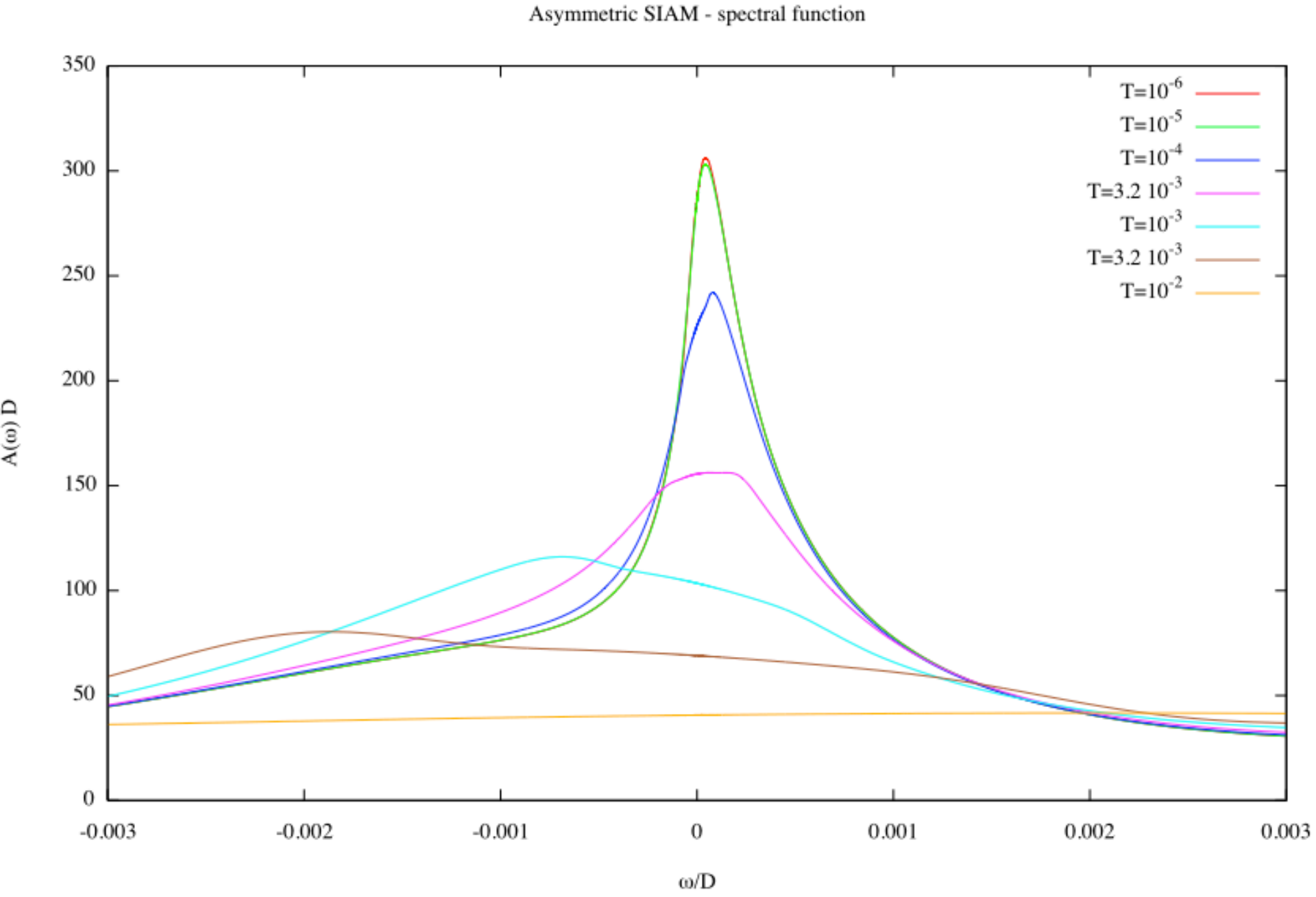
I1/I0

(I1/I0)/T

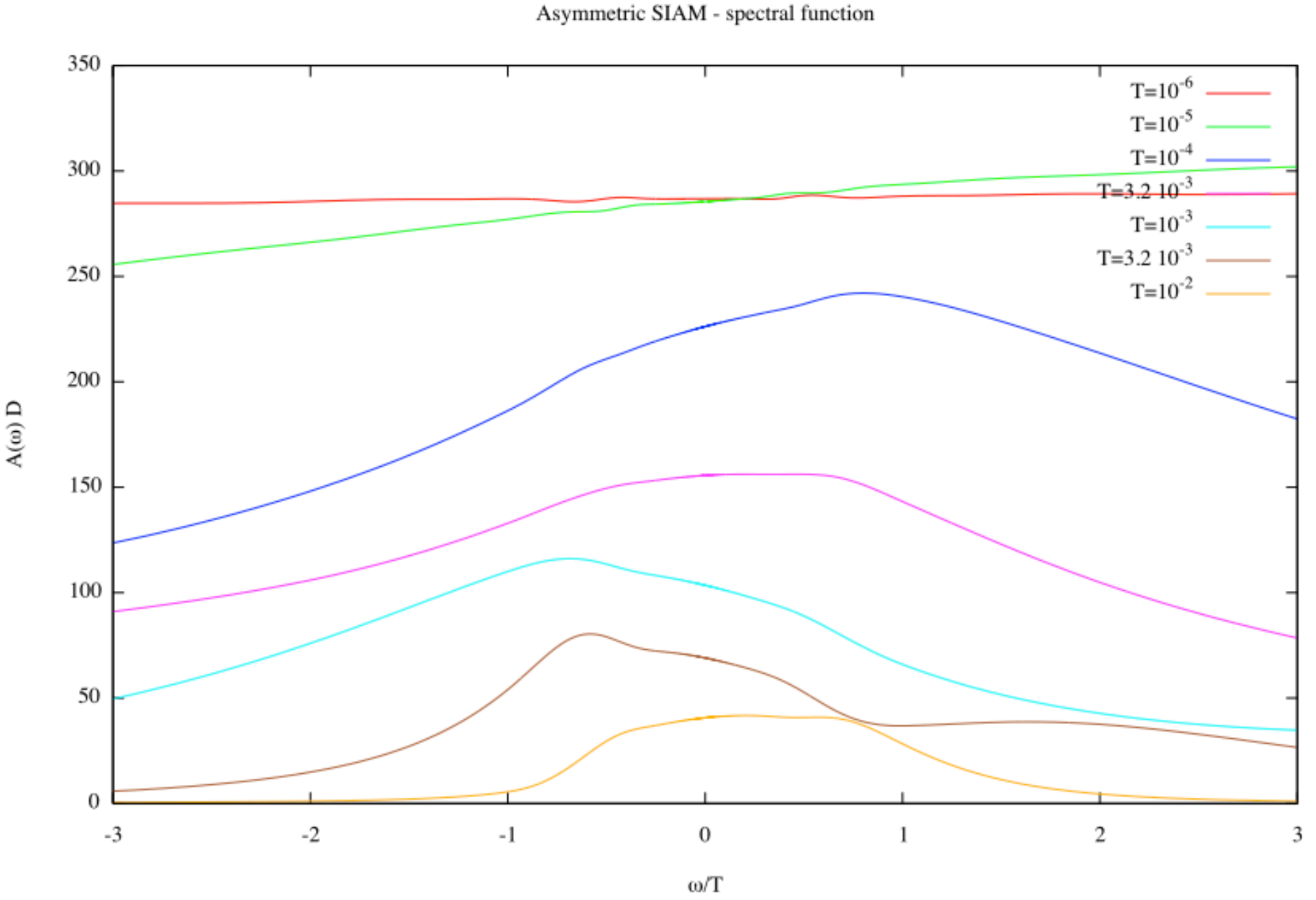
07_tp/3_plot


Single impurity Anderson model - Seebeck coefficient (thermopower)
T_K
S(T)
0.4
0.2
0
-0.2
-0.4
10^{-7}
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
Temperature

07_tp_spec


Asymmetric SIAM - spectral function
A(ω) D
ω/D
350
300
250
200
150
100
50
0
-0.003
-0.002
-0.001
0
0.001
0.002
0.003
T=10-6
T=10-5
T=10-4
T=3.2 10-3
T=10-3
T=3.2 10-3
T=10-2

07_tp_spec


Asymmetric SIAM - spectral function
A(ω) D
ω/T
T=10^-6
T=10^-5
T=10^-4
T=3.2 10^-3
T=10^-3
T=3.2 10^-3
T=10^-2
350
300
250
200
150
100
50
0
-3
-2
-1
0
1
2
3