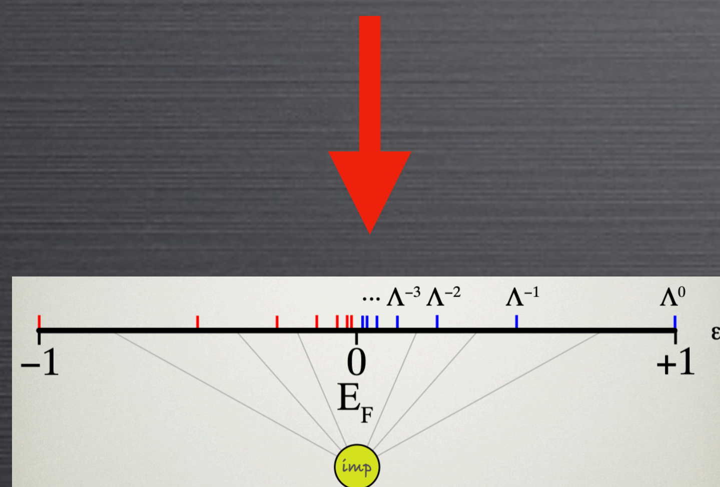
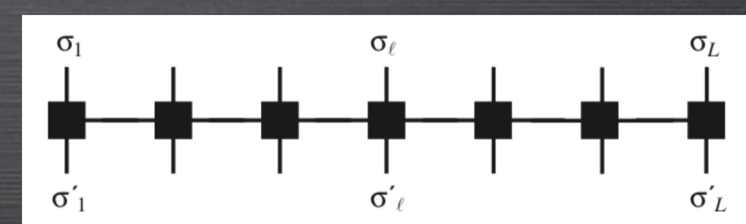
Solvers for quantum impurity problems (with superconducting baths)

Tutorial 2: NRG basics





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University of Copenhagen, Oct 2021

IMPLEMENTATION

SNEG + NRG Ljubljana

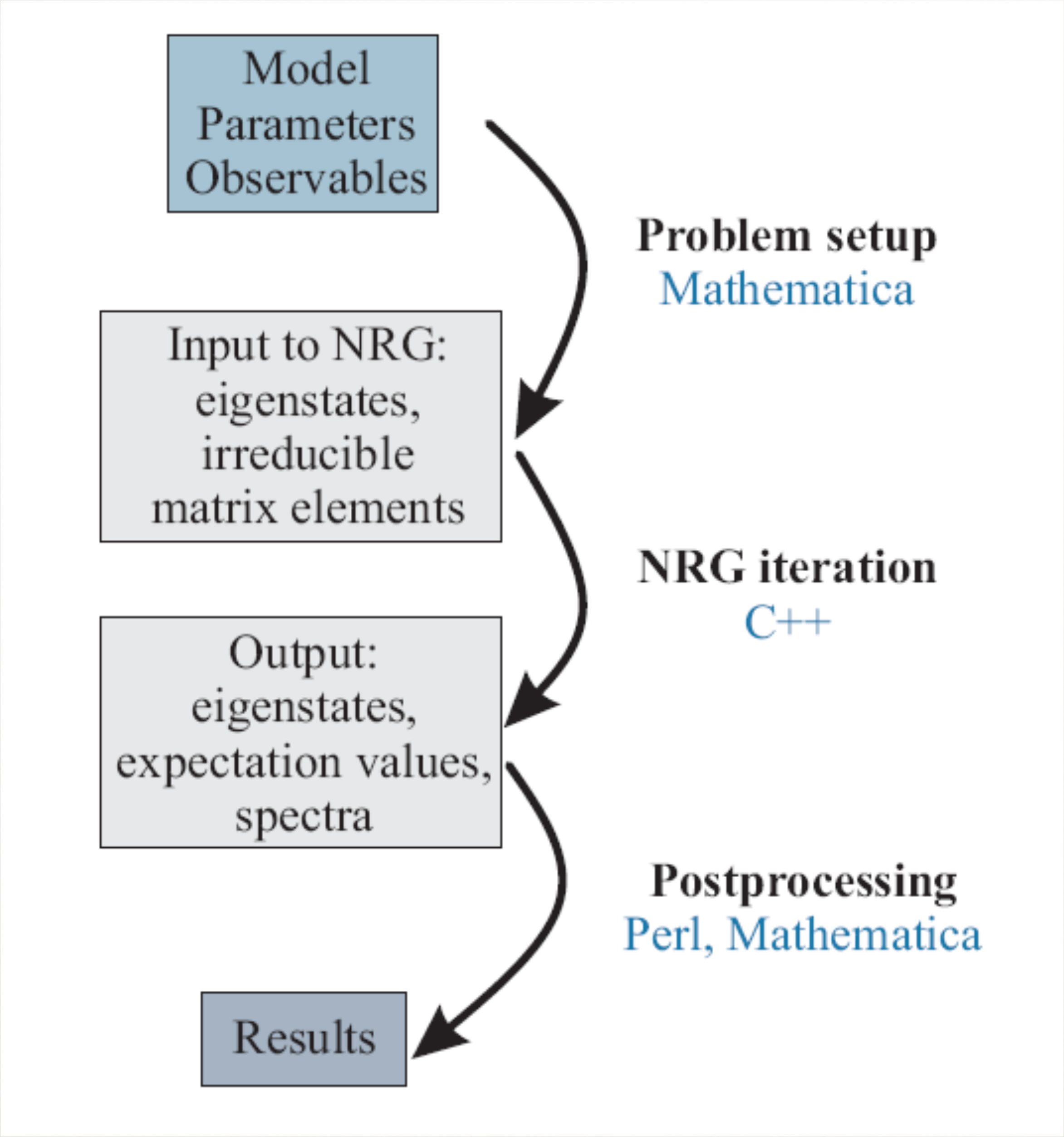
Add-on package for the computer algebra system Mathematica for performing calculations involving non-commuting operators

→

Efficient general purpose numerical renormalization group code

- flexible and adaptable
- highly optimized (partially parallelized)
- easy to use

http://nrgljubljana.ijs.si/



`nrginit`

`nrgrun/nrg`

various scripts

Alternative version: nrgljubljana_interface

https://triqs.github.io/nrgljubljana_interface/latest/

Install | Documentation | Issues | About nrgljubljana_interface

nrgljubljana_interface

NRG Ljubljana -- triqs interface

nrgljubljana_interface

nrgljubljana_iterface provides C++ and Python interfaces between TRIQS and the NRG Ljubljana solver.

nrgljubljana_interface 3.0.0

This is the homepage of nrgljubljana_interface v3.0.0. For changes see the changelog page.

"NRG Ljubljana" is a general-purpose flexible framework for performing large scale numerical renormalization group (NRG) calculations for quantum impurity problems. It is highly extensible without sacrificing numerical efficiency. It supports a great variety of impurity Hamiltonians and symmetry types. More details can be found on the project homepage, while the code itself is hosted on Github.

Learn how to use nrgljubljana_interface in the Documentation.

cea | École Polytechnique, Université Paris-Saclay | cnrs | erc European Research Council, Established by the European Commission | Flatiron Institute | Simons Foundation

Most useful in the context of DMFT.

Example input files

param

```
[extra]
U=0.01
Gamma=0.0007
delta=0

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

model=siam.m
```

siam.m

```
def1ch[1];

H1 = delta (number[d]-1) +
     U/2 pow[number[d]-1, 2];
Hc = gammaPol hop[f[0], d[]];

H = H0 + H1 + Hc;
```

Common symtype settings

- **QS**: conservation of charge and full invariance in spin space
- **QSZ**: external magnetic field (axial spin symmetry)
- **U1**: no spin symmetry
- **SPSU2**, **SPU1**: superconducting case (with full and axial spin symmetry)
- **NONE**: no symmetry at all

Common predefined models

- **KONDO**: single-channel Kondo model
- **SIAM**: single impurity Anderson model
- **CLEAN**: no impurity (just a Wilson chain)

Contents of PARAM file

[extra]	
spin=1/2	
Jkondo=0.2	
[param]	
symtype=QS	symmetry type
discretization=Z	discretization scheme: Y, C, Z
Lambda=2	Λ
Tmin=1e-6	controls the length of chain
keepenergy=8	truncation parameters
keep=5000	
model=kondo.m	

contents of DATA file

```
# Input file for NRG Ljubljana, Rok Zitko, rok.zitko@ijs.si, 2005-2015
# symtype       QS
# Using sneg version    1.250
#!8
# Number of channels, impurities, chain sites, subspaces:
1       0       39      4
# SCALE         1.0201394465967895
# Energies (GS energy subtracted, multiplied by 1/SCALE):
-1      2
1
0.1470387215202821
0       1
1
0.
0       3
1
0.19605162869370946
1       2
1
0.1470387215202821
# Irreducible matrix elements for Wilson chains:
f 0 0
4
1       2       0       3
1.224744871391589
1       2       0       1
0.7071067811865475
0       3       -1      2
1.
0       1       -1      2
-1.
# GS energy in absolute units:
e
-0.15000000000000002
# Irreducible matrix elements for other operators:
# Discretization tables:
z
39
0.54528747084262258072
0.41550946829175445321
0.32189917767609217007
0.24026940945817134999
```

contents of TD

# T	<Sz^2>	<Q>	<Q^2>	<E>	<E^2>	C	F	S
1.02014	0.362367	0	0.49907	0.143255	0.0244887	0.00396666	-1.93426	2.07752
0.721348	0.451726	1.19233e-17	0.868445	0.965006	1.43272	0.501484	-2.23124	3.19624
0.51007	0.518769	-6.18407e-18	1.15429	1.22576	2.69395	1.19145	-2.88775	4.11352
0.360674	0.555072	4.43533e-17	1.31488	1.86786	5.57957	2.09068	-2.84544	4.71329
0.255035	0.568245	-4.70206e-16	1.37861	1.85672	6.27727	2.82986	-3.14618	5.0029
0.180337	0.570338	-3.17518e-15	1.39344	2.14041	7.74478	3.1634	-2.94699	5.0874
0.127517	0.569747	-5.90117e-15	1.39626	1.93828	6.96775	3.21083	-3.16169	5.09997
0.0901684	0.568831	-9.71756e-15	1.3971	2.14611	7.82173	3.21593	-2.95621	5.10233
0.0637587	0.567669	-1.3782e-14	1.39783	1.94892	7.01101	3.21272	-3.15444	5.10337
0.0450842	0.566435	-1.66035e-14	1.39796	2.14515	7.81767	3.21598	-2.9585	5.10366
0.0318794	0.56499	-1.77274e-14	1.39833	1.96067	7.05806	3.21384	-3.1431	5.10377
0.0225421	0.563485	-1.92049e-14	1.39826	2.14416	7.81382	3.21641	-2.95913	5.10329
0.0159397	0.561755	-2.05475e-14	1.39852	1.97403	7.1106	3.2138	-3.12879	5.10283
0.0112711	0.559947	-2.23771e-14	1.39838	2.14287	7.8091	3.21722	-2.95919	5.10205
0.00796984	0.557866	-2.34782e-14	1.39852	1.98954	7.17093	3.21265	-3.11135	5.10089

magnetization

heat capacity

entropy

free energy

PLOTTING WITH GNUPLOT

```
#!/bin/bash
gnuplot --persist <<EOF
set termoption enh
set title "Kondo model"
set logscale x
set format x '10^{%L}'
set xlabel 'Temperature'
set xrange [1e-8:1e-1]
set ylabel 'S(T)/k_B'
plot 'td-S.dat' with lp title 'impurity entropy', log(2)
EOF
```

PLOTTING WITH MATPLOTLIB

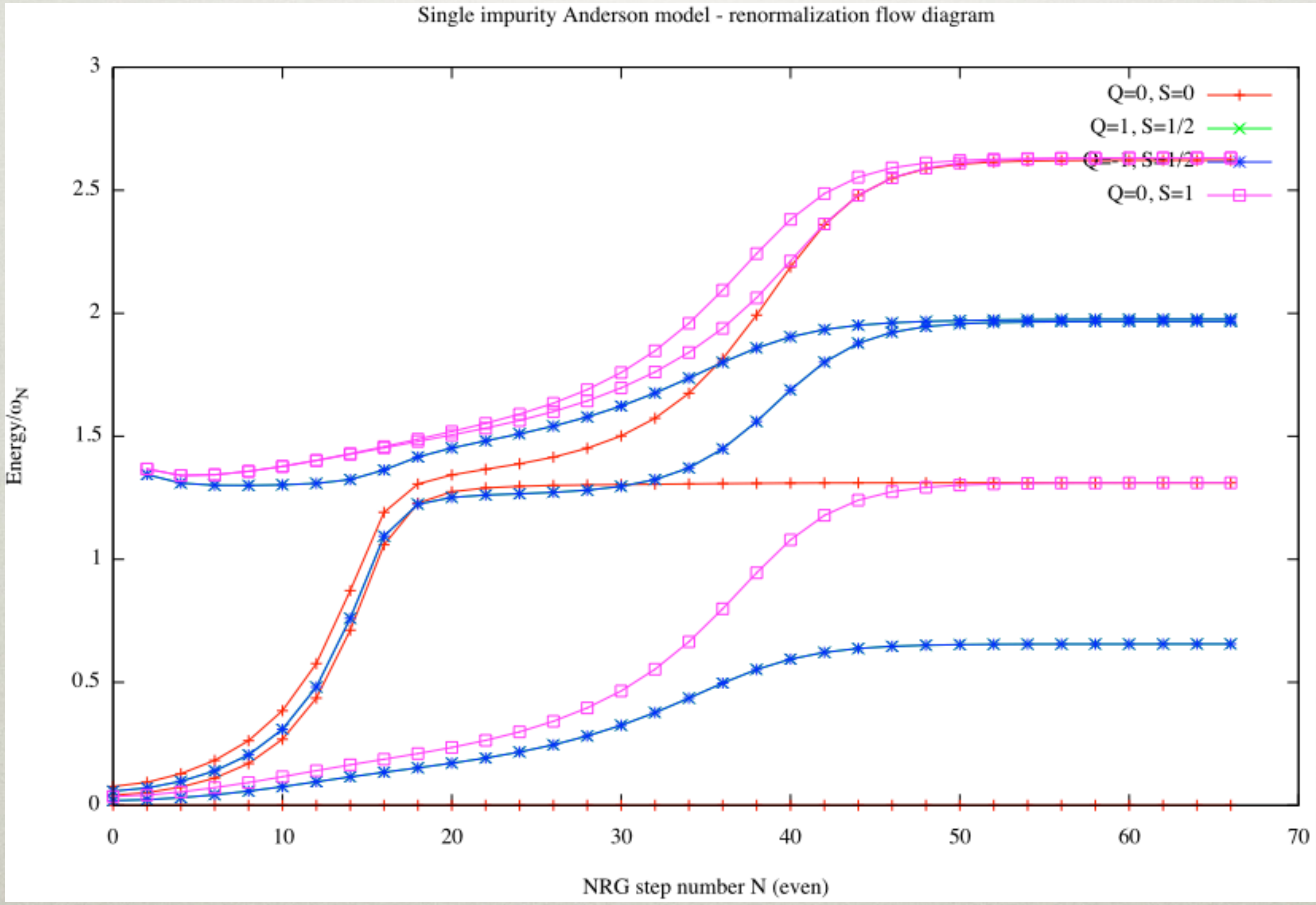
```
#!/bin/sh
python <<EOF
# -*- coding: utf-8 -*-

import matplotlib as mpl
mpl.use('agg')
import matplotlib.pyplot as plt
import numpy as np

f = plt.figure()

plt.title("Kondo model", fontsize=12)
plt.xlabel(r'\$T/D\$', fontsize=12)
plt.ylabel(r'\$S(T)\ [k_B]\$', fontsize=12)
plt.xlim(1e-8,1e-1)
plt.xscale('log')
plt.ylim(bottom=0)
plt.tick_params(labelsize=12)

plt.tight_layout()

x1,y1 = np.loadtxt('td-S.dat', unpack=True)
l1, = plt.plot(x1,y1, color='black', label='Impurity entropy')

plt.legend()
plt.show()
plt.savefig('entropy.pdf')

EOF
```

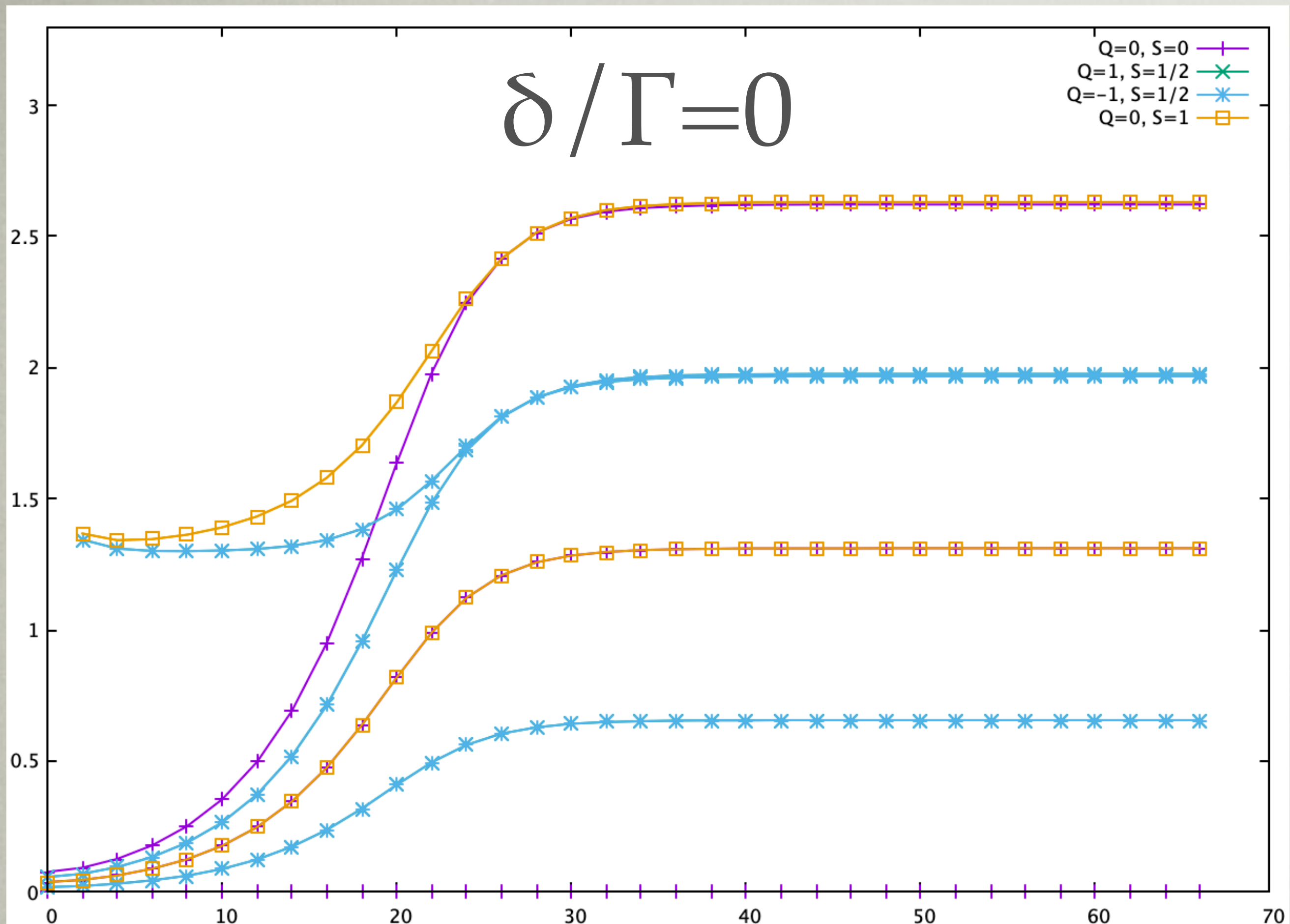
Analysis

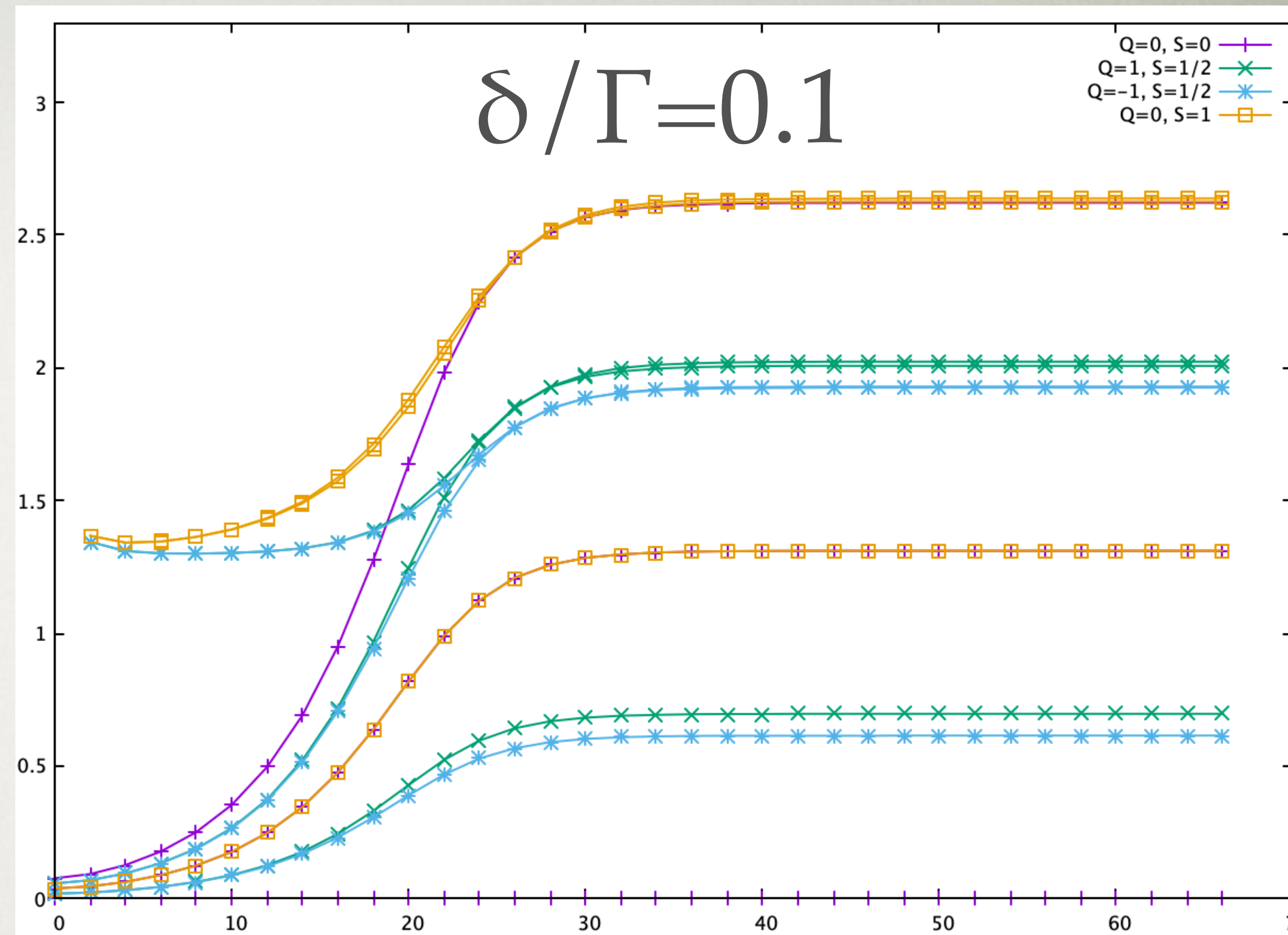
- Renormalization flow & analysis of fixed points and operators
- Thermodynamics properties
- Static quantities (expectation values)
- Dynamics properties (spectra, susceptibilities)
- Real-time evolution

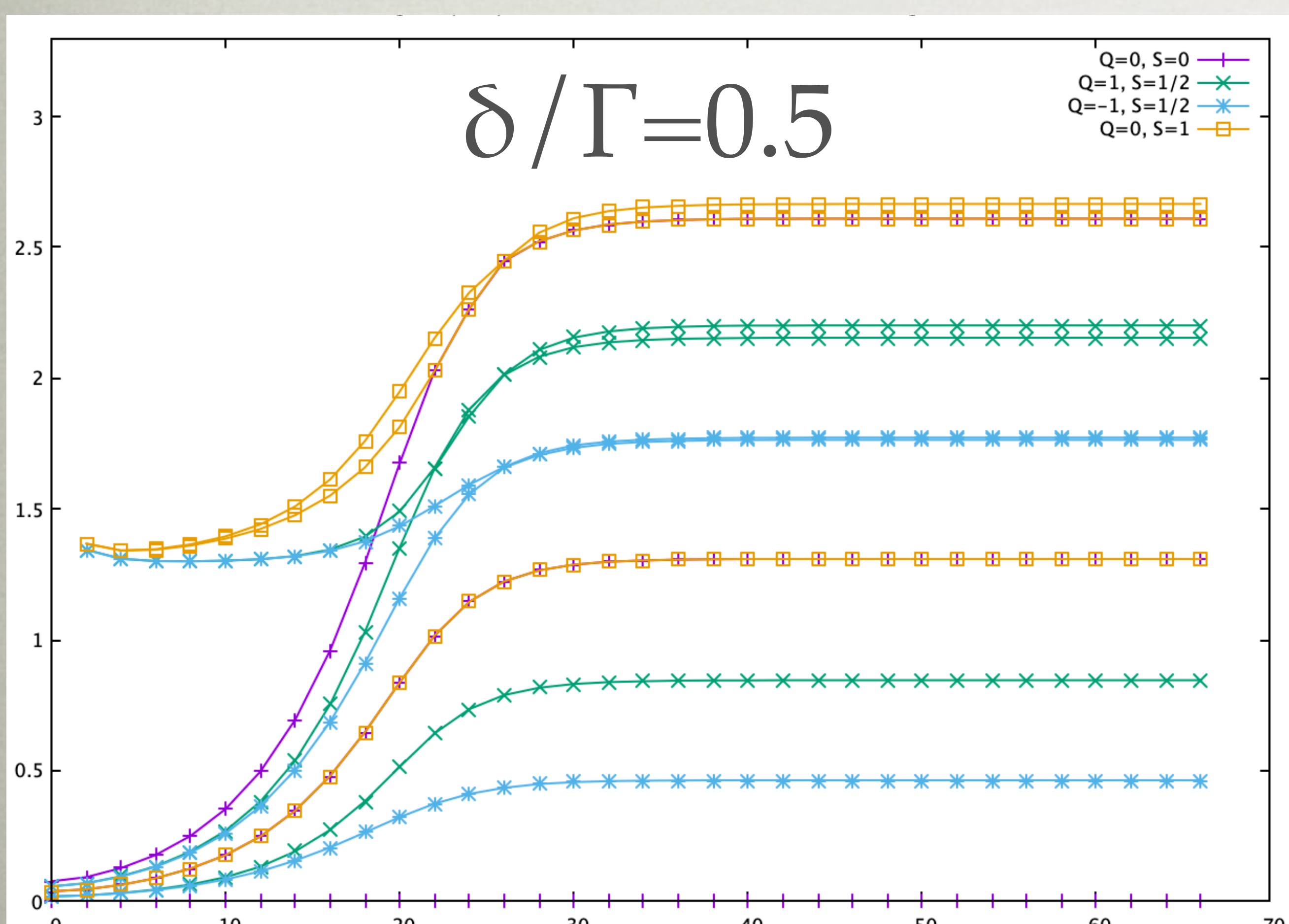
ANALYSIS

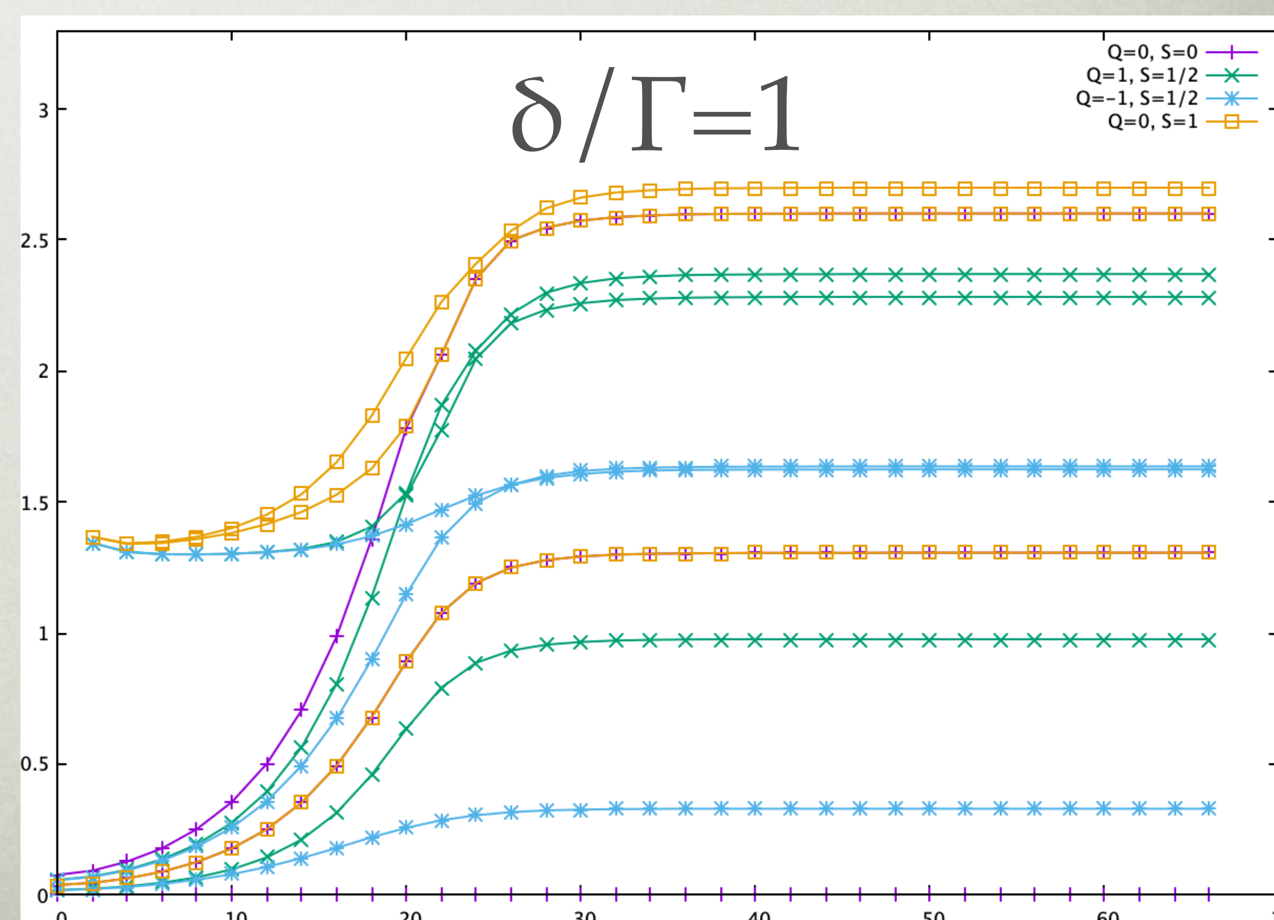
RG flow diagrams (spaghetti plots)

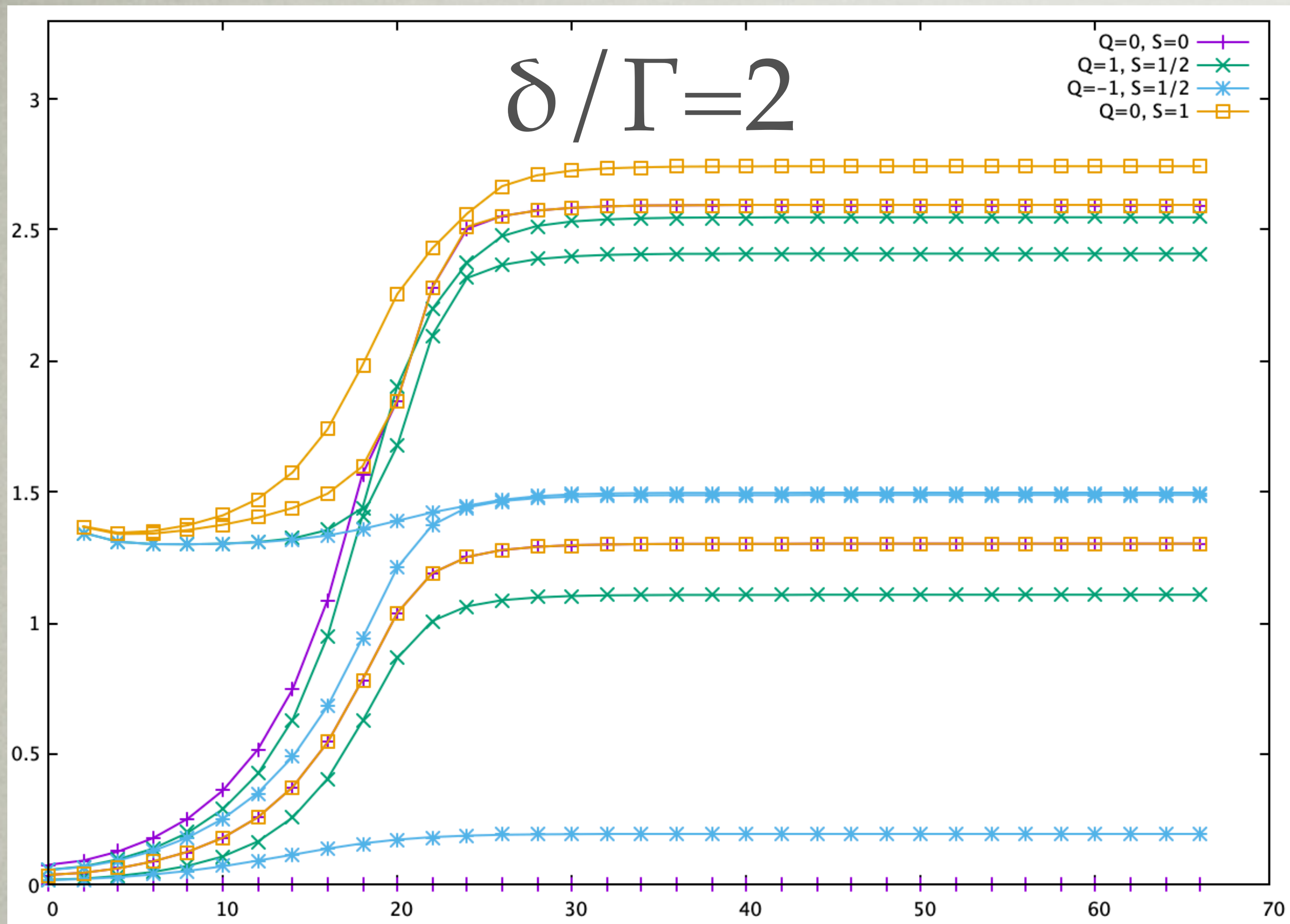


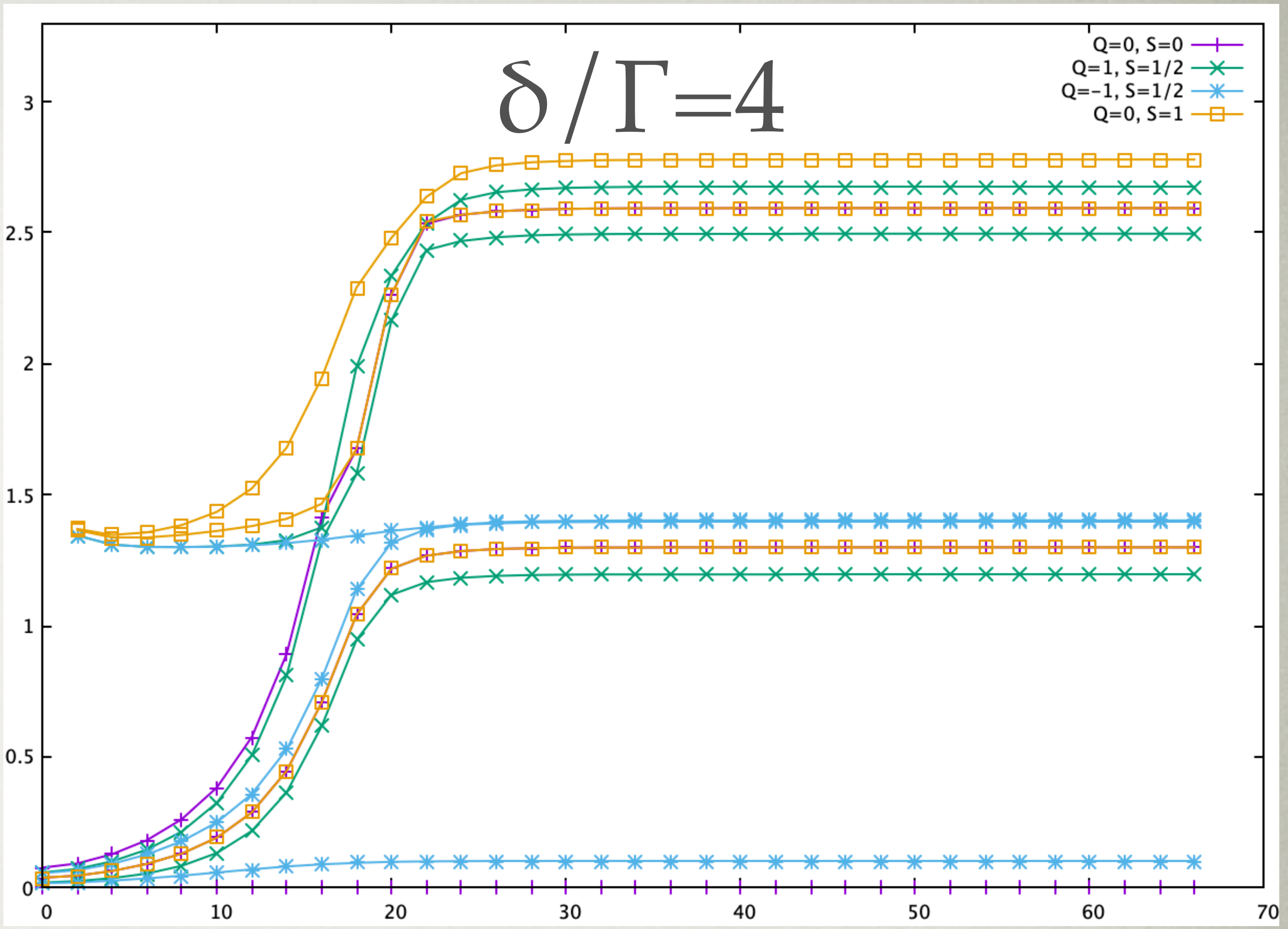

δ/Γ=0
Q=0, S=0
Q=1, S=1/2
Q=-1, S=1/2
Q=0, S=1

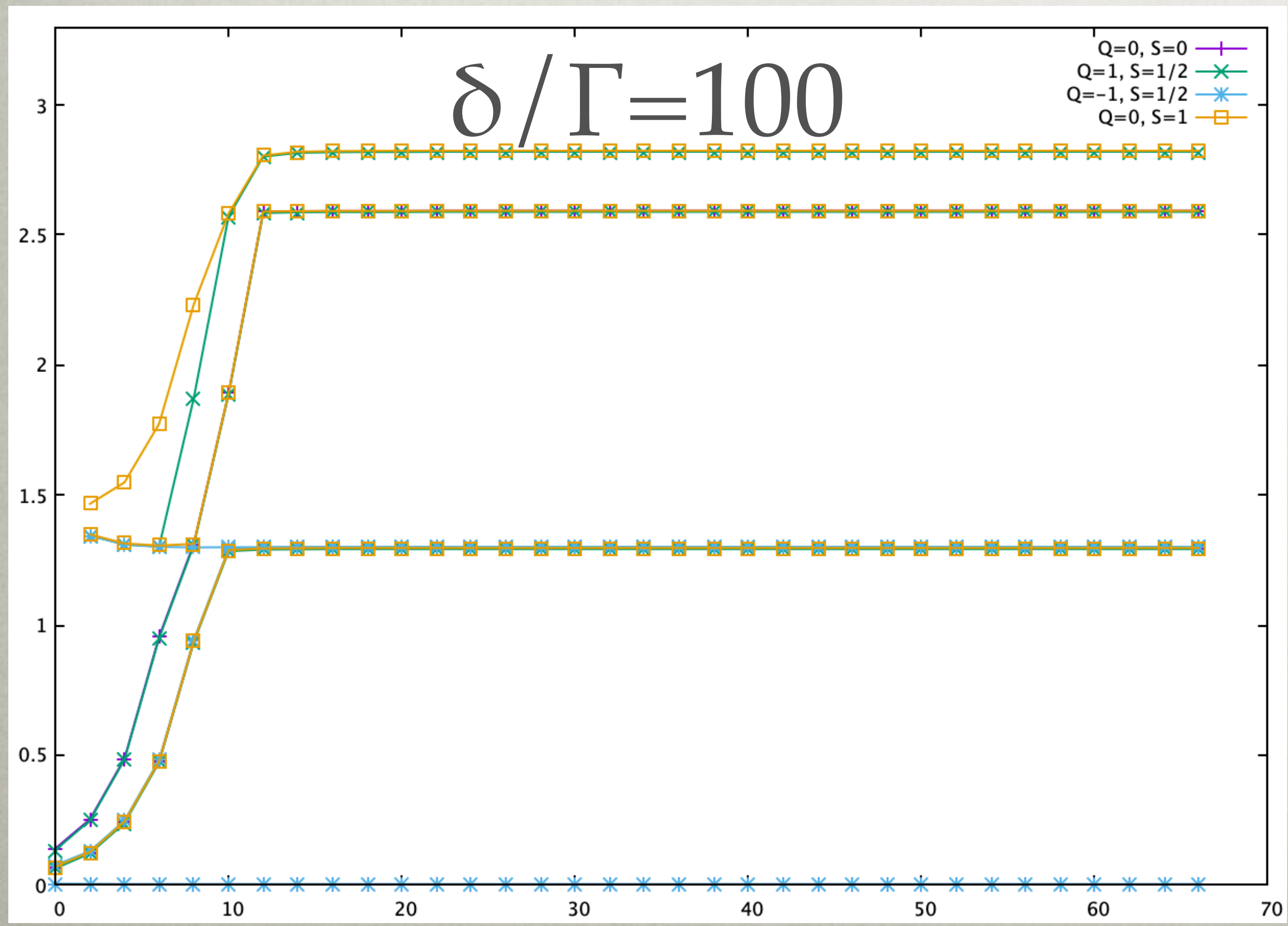

δ/Γ=0.1
Q=0, S=0
Q=1, S=1/2
Q=-1, S=1/2
Q=0, S=1


δ/Γ=0.5
Q=0, S=0
Q=1, S=1/2
Q=-1, S=1/2
Q=0, S=1

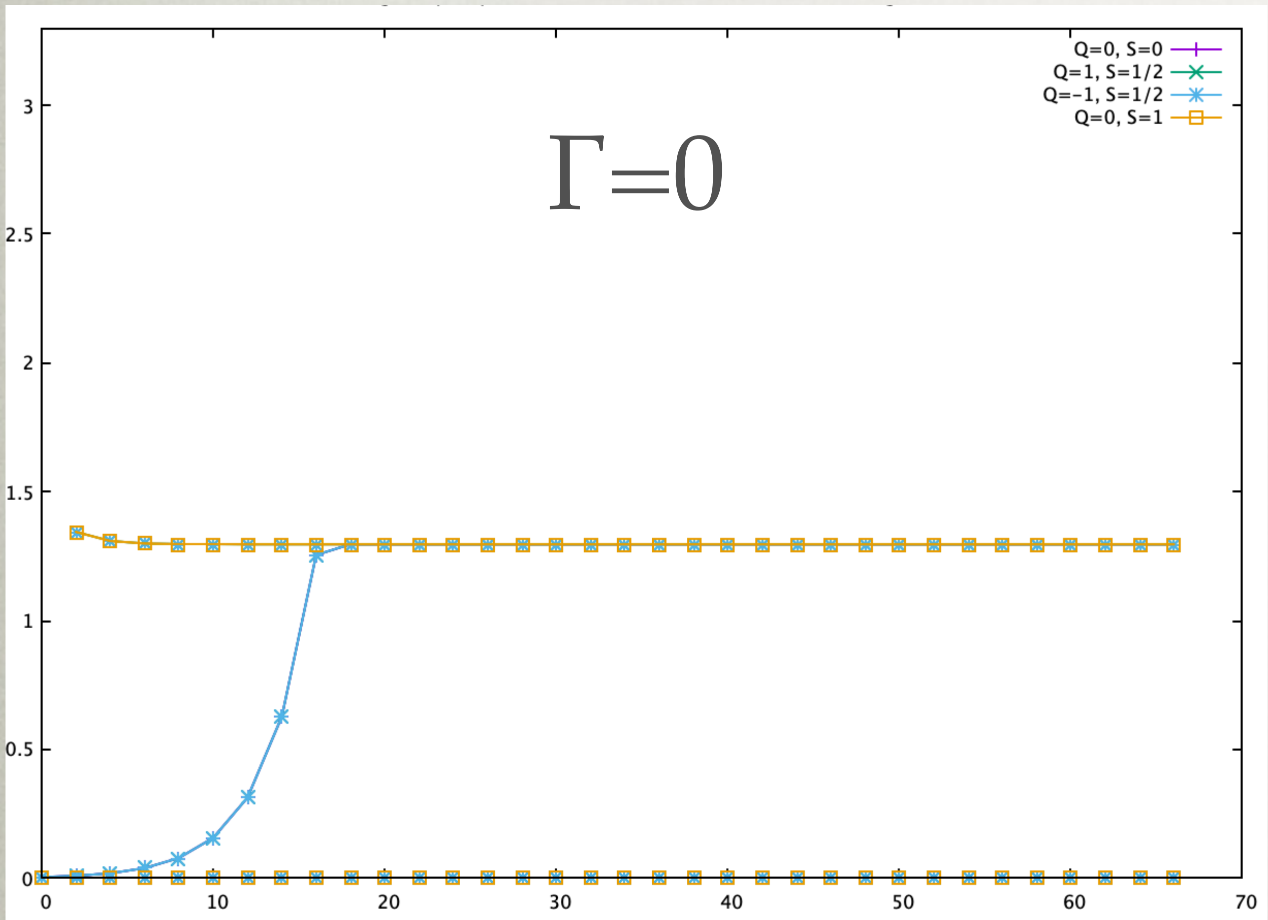

δ/Γ=1
Q=0, S=0
Q=1, S=1/2
Q=-1, S=1/2
Q=0, S=1

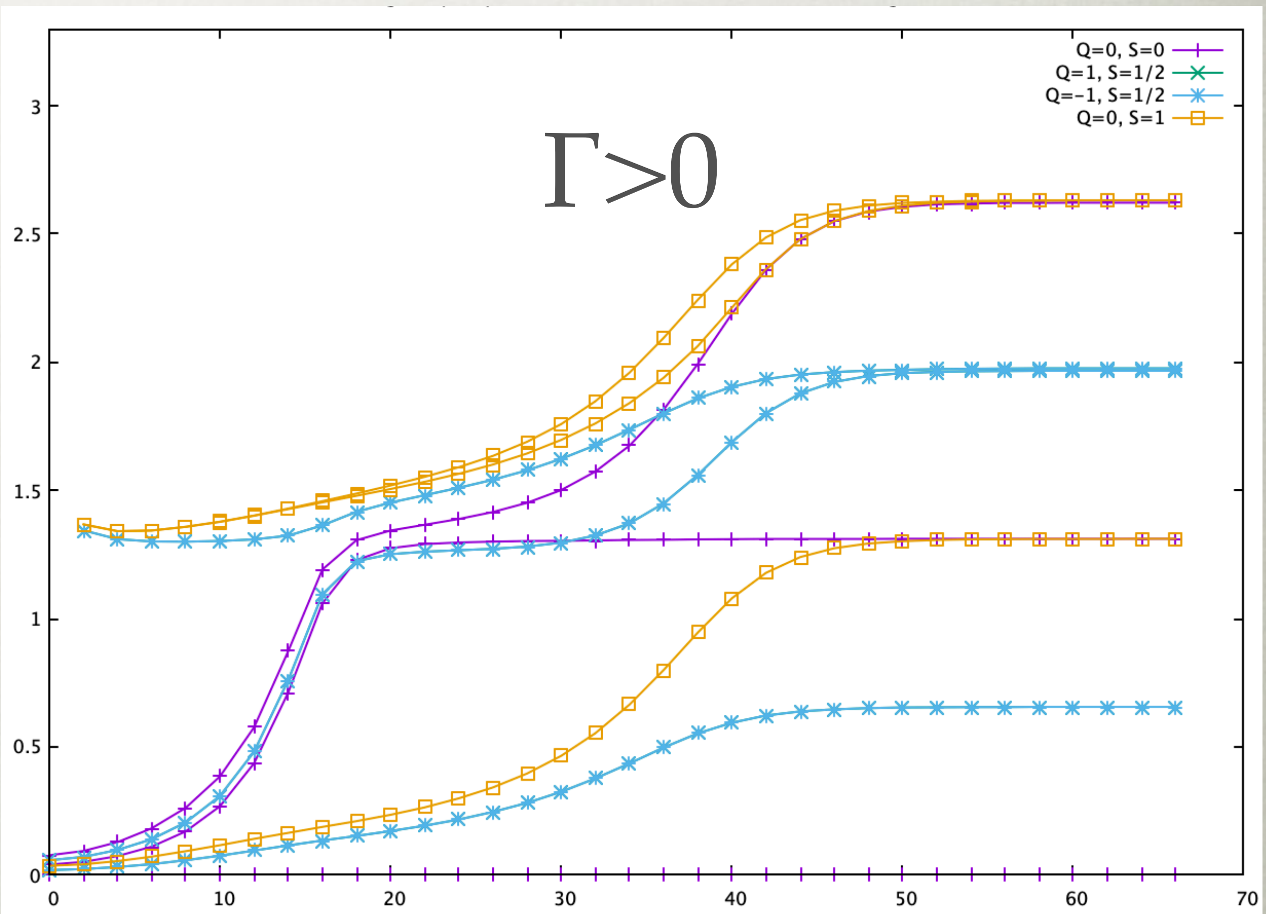

δ / Γ=2
Q=0, S=0
Q=1, S=1/2
Q=−1, S=1/2
Q=0, S=1


δ / Γ=4
Q=0, S=0
Q=1, S=1/2
Q=−1, S=1/2
Q=0, S=1

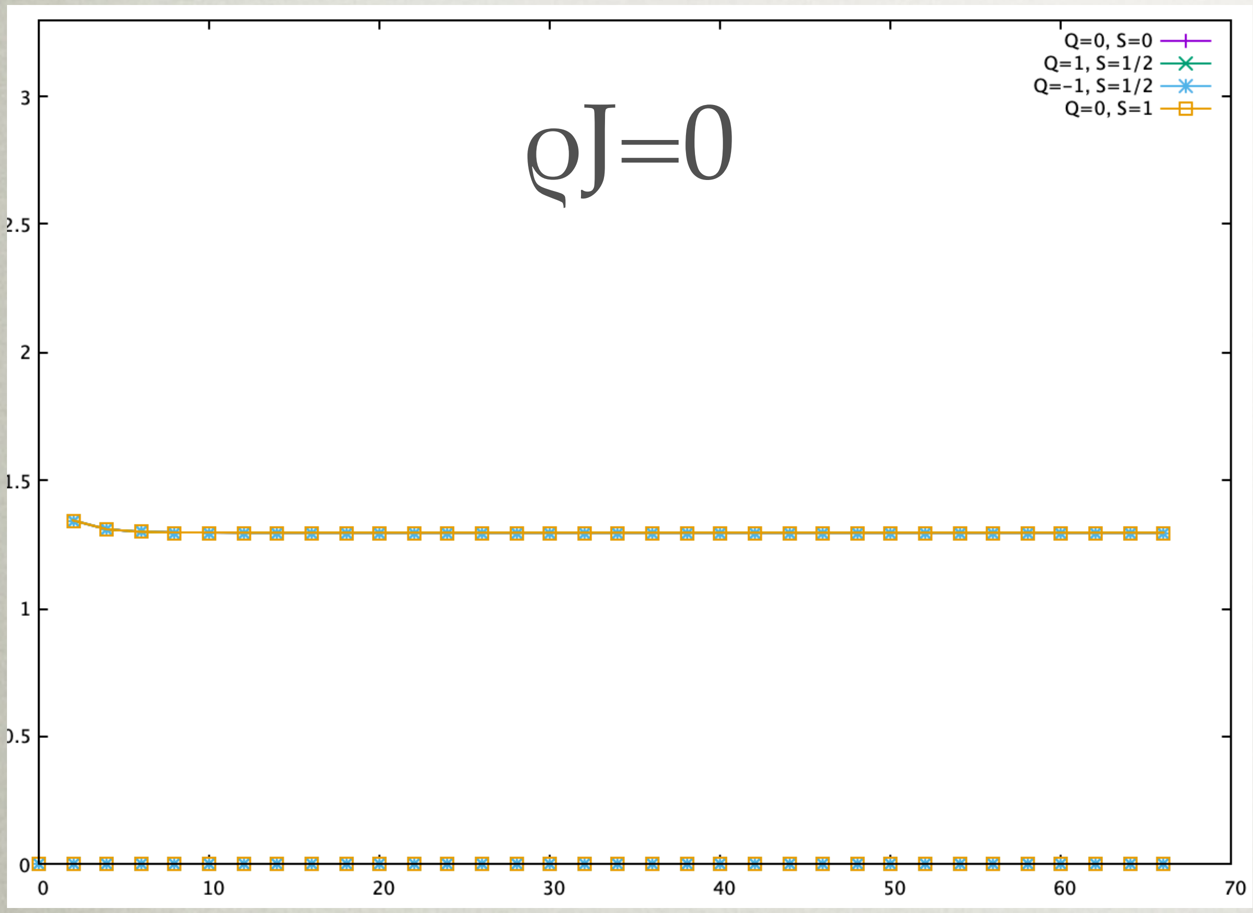

δ / Γ=100
Q=0, S=0
Q=1, S=1/2
Q=−1, S=1/2
Q=0, S=1

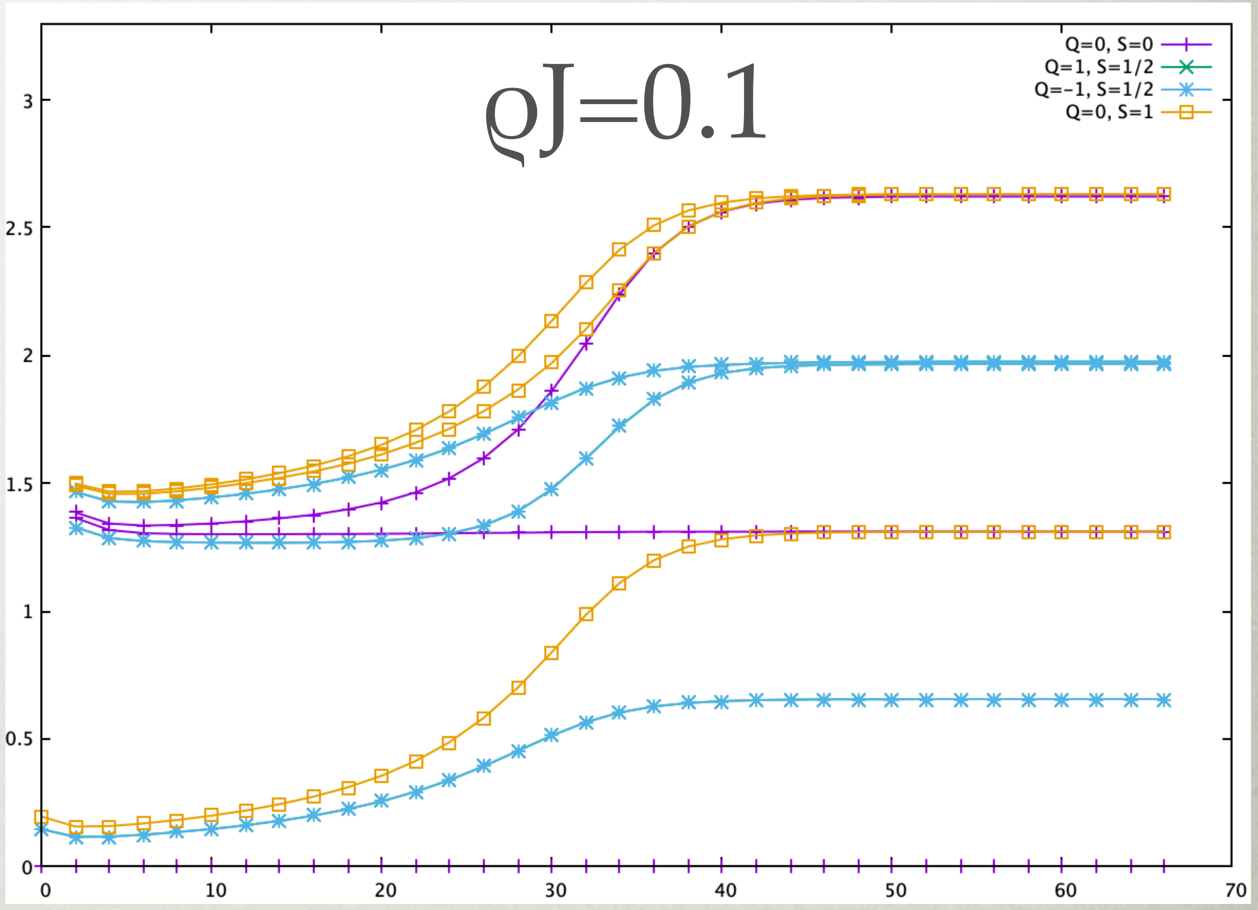
SIAM





Kondo model


ϱJ=0
Q=0, S=0
Q=1, S=1/2
Q=-1, S=1/2
Q=0, S=1
0
10
20
30
40
50
60
70


ϱJ=0.1
Q=0, S=0
Q=1, S=1/2
Q=-1, S=1/2
Q=0, S=1
0
0.5
1
1.5
2
2.5
3
0
10
20
30
40
50
60
70

Calculation of thermodynamic quantities

$$\rho = \frac{1}{Z} e^{-\beta H} \qquad Z = \mathrm{Tr}[e^{-\beta H}]$$

$$E = \langle H \rangle = \mathrm{Tr}[\rho H] = \frac{\mathrm{Tr}[H e^{-\beta H}]}{\mathrm{Tr}[e^{-\beta H}]}$$

$$F = -k_B T \ln Z$$

$$S = -\frac{\partial F}{\partial T} \qquad C = \frac{\partial E}{\partial T}$$

Trick: avoid numerical differentiation!

ISOTHERMAL SUSCEPTIBILITY

$$H' = BS_z$$

$$\chi(T) = \frac{\partial \langle S_z \rangle}{\partial B}$$

Kubo, linear response theory:

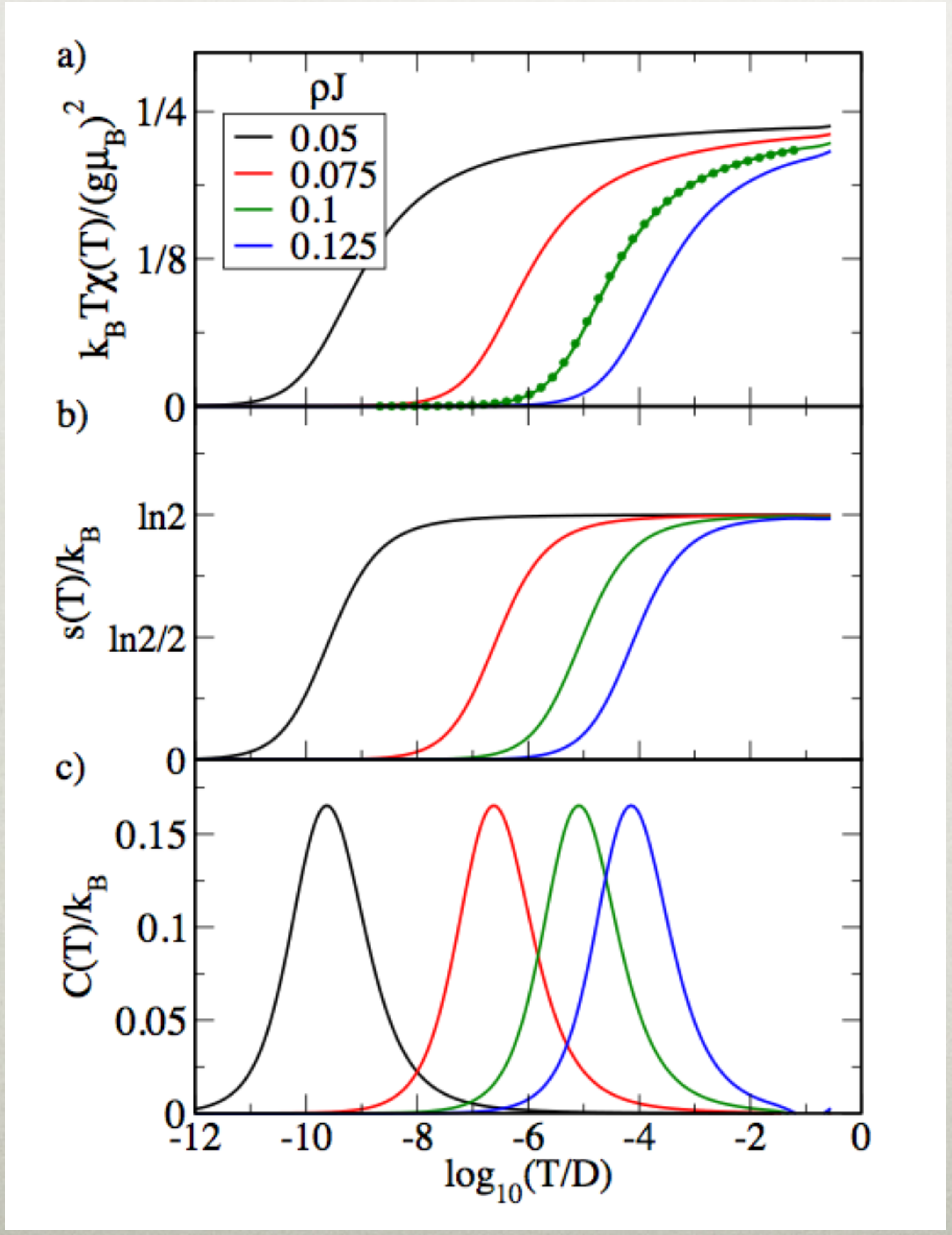
$$\chi(T) = \int_0^\beta \mathrm{d}\tau \, \langle S_z(\tau) S_z \rangle - \beta \langle S_z \rangle^2$$

Impurity contribution to...

$$S_{\mathrm{imp}}(T) = \frac{(E-F)}{T} - \frac{(E-F)_0}{T}$$

$$\chi_{\mathrm{imp}}(T) = \frac{(g\mu_B)^2}{k_B T}\Big(\langle S_z^2\rangle - \langle S_z^2\rangle_0\Big)$$

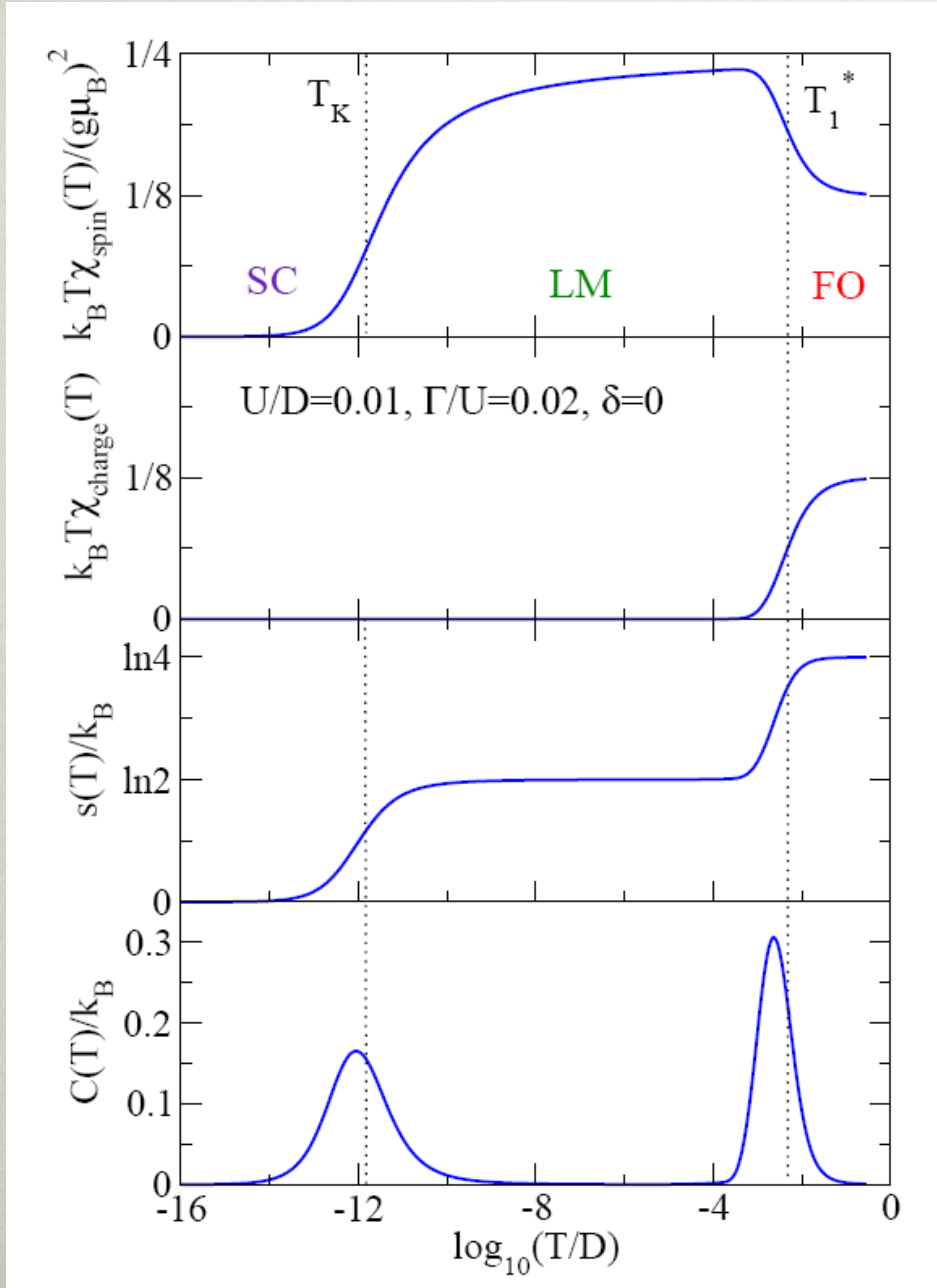
Thermodynamics of the Kondo model



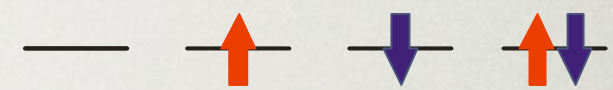
$$T_K\,\chi(T_K) = 0.07$$

Wilson's definition of the Kondo temperature

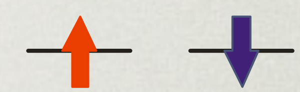
Single impurity Anderson model



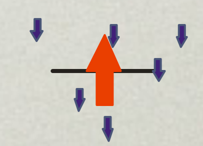
FO: free orbital

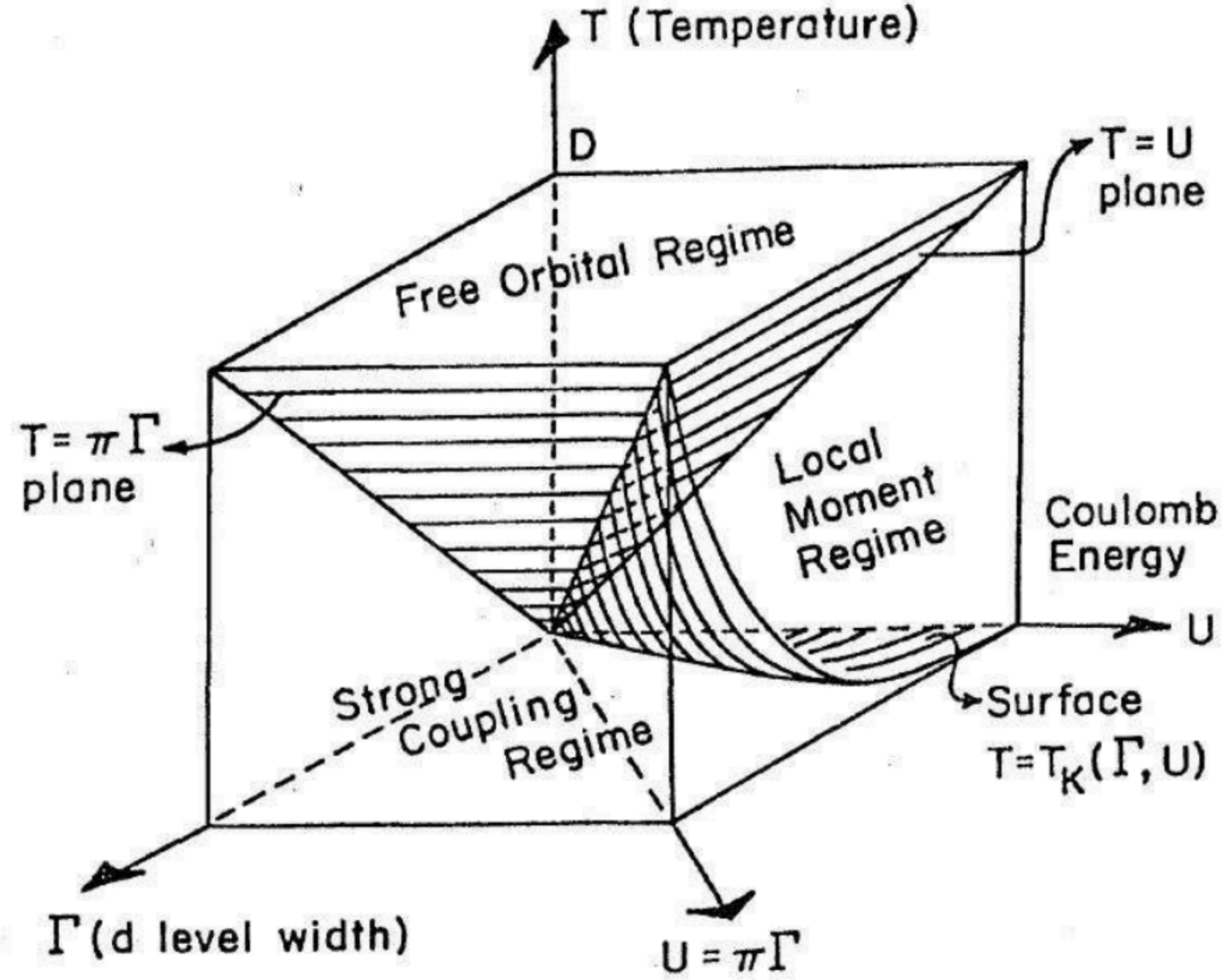


LM: local moment

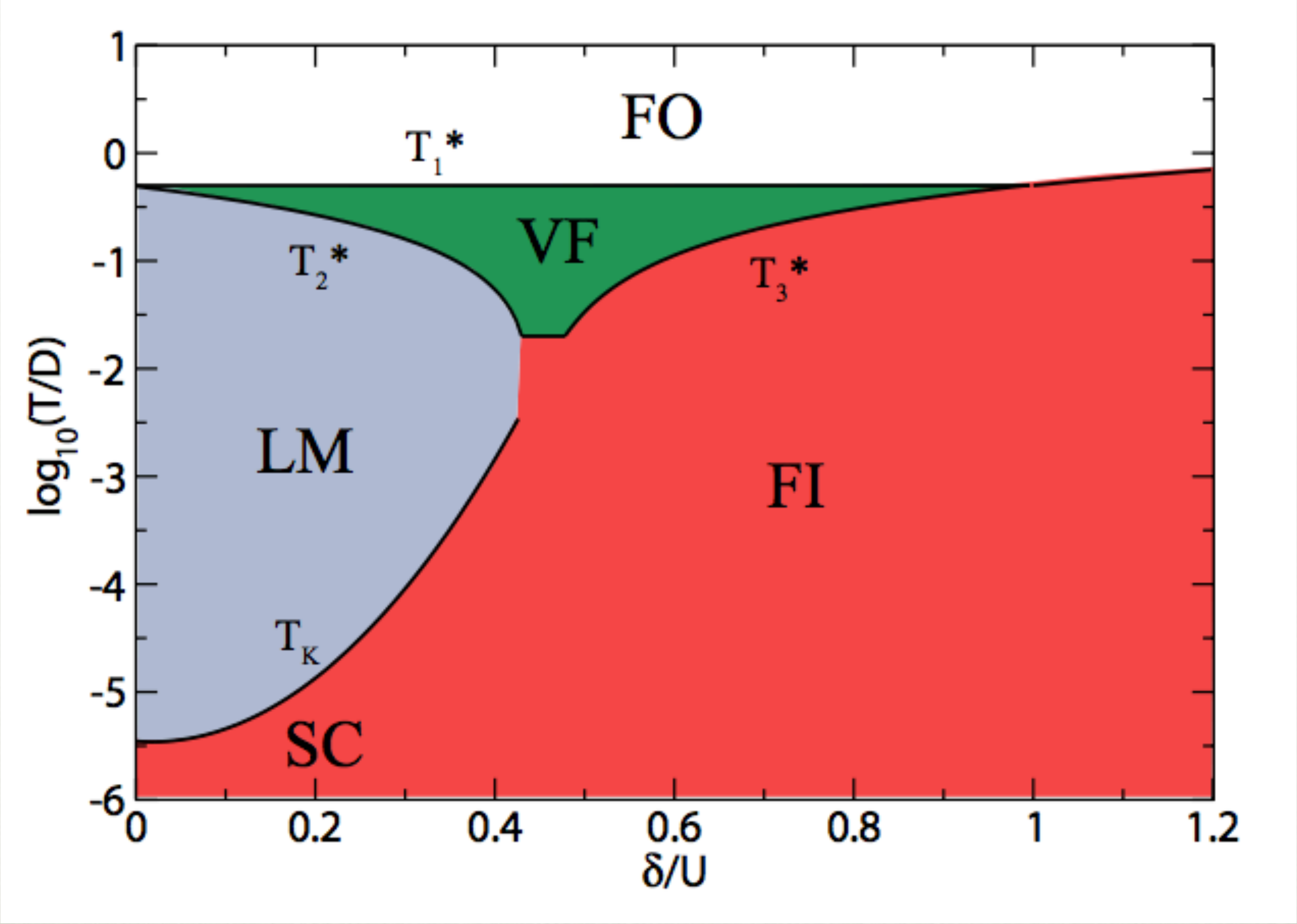


SC: strong coupling




T (Temperature)
D
T = U
plane
Free Orbital Regime
T= πΓ
plane
Local
Moment
Regime
Coulomb
Energy
U
Strong
Coupling
Regime
Surface
T=T_K(Γ, U)
Γ (d level width)
U = πΓ

Phase diagram of SIAM



Problems

1. Study runtime dependence vs. "keepenergy"
2. Plot the amplitude of oscillations in entropy (between neighbouring T points) vs. Lambda for a single-z calculation
3. Plot the thermodynamic properties of SIAM for a range of delta from 0 to ~U. Follow the evolution of fixed points.
4. Study the thermodynamic properties of SIAM for U decreasing towards 0. What is happening with the local-moment regime?
5. Verify the scaling of the Kondo temperature, exp(-pi U/8 Gamma), at fixed U and variable Gamma.
6. Analyse a finite-size spectrum in terms of single-particle energies.
7. How do the finite-size spectra (RG flow diagrams) depend on Lambda?
8. Calculate S_z vs. B dependence at T=0 for different J in the Kondo model.