Numerical renormalization group exercises 1

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http://nrgljubljana.ijs.si/tutorial_2019.tar.gz

First steps

- `cd tutorials_2019`
- `. nrgsetup`
- `cd 00_quick_test`
- `1_run`

```
** Iteration completed.


Total energy:              -2.892022665545651
TKW=1.50877671710845e-05

Memory usage report
===================
  after diag: 68304 kB
after recalc: 68304 kB
 after split: 68304 kB
  after trim: 68304 kB
 after trunc: 68304 kB
      diag_h: 68304 kB

Peak usage: 68304 kB

Timing report
=============
         All: 1 s
        diag: 0 s
    recalc f: 0 s
       Other: 0 s
```

tutorials_2019.tar.gz

Each example directory contains numbered scripts,
e.g., `1_run`, `2_plot`, etc.
Running these scripts should reproduce (overwrite) the results of the calculation, post-process them, produce plots, etc.

Important files:
`param` or `param.loop`: parameters of the calculation
`model.m`: model definition
`data`: input to the C++ part of the code (nrgrun)
`td`, `custom`, `annotated.dat`, `*.dat`: output files

Contents of PARAM file

```
[extra]
spin=1/2
Jkondo=0.2

[param]
symtype=QS
discretization=Z
Lambda=2
Tmin=1e-6
keepenergy=8
keep=5000

model=kondo.m
```

symmetry type

discretization scheme: Y, C, Z

Λ

controls the length of chain

truncation parameters

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
```

Zero-bandwidth approximation to SIAM

Exact diagonalisation of a two-site problem using SNEG

```
snegfermionoperators
nc
number, hubbard, hop
qsbasisvc
matrixrepresentationvc
```

Schrieffer-Wolff transformation for quantum many-body systems

Sergey Bravyi, David DiVincenzo, Daniel Loss

(Submitted on 3 May 2011)

The Schrieffer-Wolff (SW) method is a version of degenerate perturbation theory in which the low-energy effective Hamiltonian H_{eff} is obtained from the exact Hamiltonian by a unitary transformation decoupling the low-energy and high-energy subspaces. We give a self-contained summary of the SW method with a focus on rigorous results. We begin with an exact definition of the SW transformation in terms of the so-called direct rotation between linear subspaces. From this we obtain elementary proofs of several important properties of H_{eff} such as the linked cluster theorem. We then study the perturbative version of the SW transformation obtained from a Taylor series representation of the direct rotation. Our perturbative approach provides a systematic diagram technique for computing high-order corrections to H_{eff}. We then specialize the SW method to quantum spin lattices with short-range interactions. We establish unitary equivalence between effective low-energy Hamiltonians obtained using two different versions of the SW method studied in the literature. Finally, we derive an upper bound on the precision up to which the ground state energy of the n-th order effective Hamiltonian approximates the exact ground state energy.

Comments:	47 pages, 3 figures
Subjects:	**Quantum Physics (quant-ph)**; Statistical Mechanics (cond-mat.stat-mech); Strongly Correlated Electrons (cond-mat.str-el)
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DOI:	10.1016/j.aop.2011.06.004
Cite as:	**arXiv:1105.0675 [quant-ph]**
	(or **arXiv:1105.0675v1 [quant-ph]** for this version)

Plemelj formula

$$\frac{1}{x - i0^+} = P\frac{1}{x} + i\pi\delta(x)$$

Sokhotski–Plemelj theorem

From Wikipedia, the free encyclopedia

Not to be confused with Casorati–Sokhotski–Weierstrass theorem.

The **Sokhotski–Plemelj theorem** (Polish spelling is *Sochocki*) is a theorem in complex analysis, which helps in evaluating certain integrals. The real-line version of it (see below) is often used in physics, although rarely referred to by name. The theorem is named after Julian Sochocki, who proved it in 1868, and Josip Plemelj, who rediscovered it as a main ingredient of his solution of the Riemann-Hilbert problem in 1908.

Contents [hide]

Let C be a smooth closed simple curve in the plane, and φ an analytic function on C. Then the Cauchy-type integral

$$\frac{1}{2\pi i}\int_C \frac{\varphi(\zeta)\,d\zeta}{\zeta - z},$$

defines two analytic functions of z, ϕ_i inside C and ϕ_e outside.[*clarification needed*] The Sokhotski–Plemelj formulas relate the limiting boundary values of these two analytic functions at a point z on C and the Cauchy principal value $\mathcal{P}$ of the integral:

$$\phi_i(z) = \frac{1}{2\pi i}\mathcal{P}\int_C \frac{\varphi(\zeta)\,d\zeta}{\zeta - z} + \frac{1}{2}\varphi(z),$$

$$\phi_e(z) = \frac{1}{2\pi i}\mathcal{P}\int_C \frac{\varphi(\zeta)\,d\zeta}{\zeta - z} - \frac{1}{2}\varphi(z).$$

Proof of the real version [edit]

A simple proof is as follows.

$$\lim_{\varepsilon\to 0^+}\int_a^b \frac{f(x)}{x\pm i\varepsilon}\,dx = \mp i\pi \lim_{\varepsilon\to 0^+}\int_a^b \frac{\varepsilon}{\pi(x^2+\varepsilon^2)} f(x)\,dx + \lim_{\varepsilon\to 0^+}\int_a^b \frac{x^2}{x^2+\varepsilon^2}\,\frac{f(x)}{x}\,dx.$$

For the first term, we note that $\varepsilon/\pi(x^2+\varepsilon^2)$ is a nascent delta function, and therefore approaches a Dirac delta function in the limit. Therefore, the first term equals $\mp i\pi\, f(0)$.

For the second term, we note that the factor $x^2/(x^2+\varepsilon^2)$ approaches 1 for $|x| \gg \varepsilon$, approaches 0 for $|x| \ll \varepsilon$, and is exactly symmetric about 0. Therefore, in the limit, it turns the integral into a Cauchy principal value integral.

Kramers-kronig transformation

$$G'(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{G''(\omega')}{\omega - \omega'}$$

$$G''(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{G'(\omega')}{\omega - \omega'}$$

causality and the Titchmarsh theorem

Titchmarsh's theorem [edit]

A theorem due to Edward Charles Titchmarsh makes precise the relationship between the boundary values of holomorphic functions in the upper half-plane and the Hilbert transform (Titchmarsh 1948, Theorem 95). It gives necessary and sufficient conditions for a complex-valued square-integrable function $F(x)$ on the real line to be the boundary value of a function in the Hardy space $H^2(U)$ of holomorphic functions in the upper half-plane U.

The theorem states that the following conditions for a complex-valued square-integrable function $F : \mathbf{R} \to \mathbf{C}$ are equivalent:

- $F(x)$ is the limit as $z \to x$ of a holomorphic function $F(z)$ in the upper half-plane such that
$$\int_{-\infty}^{\infty} |F(x+iy)|^2\,dx < K.$$
- $-\mathrm{Im}(F)$ is the Hilbert transform of $\mathrm{Re}(F)$, where $\mathrm{Re}(F)$ and $\mathrm{Im}(F)$ are real-valued functions with $F = \mathrm{Re}(F) + i\,\mathrm{Im}(F)$.
- The Fourier transform $\mathcal{F}(F)(x)$ vanishes for $x < 0$.

Exercise 2: single-impurity Anderson model: impurity Green function, hybridization function, and self energy

(9 points + 5 bonus points)

The impurity Green function of the single-impurity Anderson model can be written in the following general form:

$$G_\sigma(z) = \frac{1}{z - \varepsilon_\mathrm{f} - \Delta(z) - \Sigma^U_\sigma(z)} \,. \tag{2}$$

The idea of this exercise is to explore the possible structures of the impurity Green function using a specific form of the hybridization function and the self energy.

a) Show that any correlation function defined in the upper complex plane can be represented through its spectral function as

$$X(z) = \int_{-\infty}^{\infty} \mathrm{d}\omega' \, \frac{A(\omega')}{z - \omega'} \,.$$

(2 points).

b) The spectral function of the hybridization function, $A_\Delta(\omega)$, is supposed to be of the following form:

$$A_\Delta(\omega) = e^{-(\omega/10)^2} \,.$$

Calculate (numerically) both real and imaginary part of $\Delta(z = \omega + i\delta)$ with $\delta = 0.01$. (4 points).

c) Use the result of b) to calculate the impurity spectral function, $A_\mathrm{imp}(\omega)$, for various values of ε_f and $U = 0$. (3 points).

d) The spectral function of the self energy should take the form

$$A_\Sigma(\omega) = \gamma\omega^2 e^{-\omega^2} \,.$$

Investigate the resulting structures in the impurity Green function for $\varepsilon_\mathrm{f} = 0$ and various values of γ. (5 bonus points).

Exercise 3: Lanczos algorithm

(9 points + 4 bonus points)

We consider a symmetric $(N \times N)$-matrix H with matrix elements $H_{ij} = \sqrt{1+i+j}$. The starting vector of the Lanczos algorithm is given by $|\Phi_0\rangle = (1, 1, \ldots, 1)$.

a) Calculate the sequence of vectors $\{|\Phi_0\rangle, |\Phi_1\rangle, \ldots, |\Phi_{M-1}\rangle\}$ $(M \leq N)$ with the Lanczos algorithm as defined in the lecture (N can be set to 10). (5 points)

b) Show numerically that the vectors $|\Phi_i\rangle$ obtained in this way are orthogonal. To this end, calculate the matrix $D_{ij} = \langle\Phi_i|\Phi_j\rangle$. (2 points)

c) Calculate (numerically) the matrix H_Φ in the basis $\{|\Phi_i\rangle\}$: $(H_\Phi)_{ij} = \langle\Phi_i|H|\Phi_j\rangle$. (2 points)

d) Calculate the matrix elements $a_n = \langle\psi_0|\tilde{\Phi}_n\rangle$, with the normalized vectors $|\tilde{\Phi}_n\rangle = |\Phi_n\rangle/\langle\Phi_n|\Phi_n\rangle$ and $|\psi_0\rangle$ the actual ground state of H (the eigenvector with the lowest eigenvalue). Can one tell, from the n-dependence of a_n, whether the Lanczos algorithm converges quickly to the ground state? (4 bonus points)

Exercise 2: Hamilton matrix of the two-site Anderson model

(6 points)

Consider again (see exercise 2 on sheet 2) the single-impurity Anderson model with a single bath site only:

$$H_{\mathrm{ts}} = \sum_{\sigma} \varepsilon_{\mathrm{f}} f_{\sigma}^{\dagger} f_{\sigma} + U f_{\uparrow}^{\dagger} f_{\uparrow} f_{\downarrow}^{\dagger} f_{\downarrow} + V \sum_{\sigma} \left(f_{\sigma}^{\dagger} c_{\sigma} + c_{\sigma}^{\dagger} f_{\sigma} \right) + \sum_{\sigma} \varepsilon_{\mathrm{c}} c_{\sigma}^{\dagger} c_{\sigma} \ , \qquad (2)$$

The basis of the Hilbert space of H_{ts} can be written as:

$$\{|0\rangle_f, |\uparrow\rangle_f, |\downarrow\rangle_f, |\uparrow\downarrow\rangle_f\} \otimes \{|0\rangle_c, |\uparrow\rangle_c, |\downarrow\rangle_c, |\uparrow\downarrow\rangle_c\} \ .$$

a) Due to the conservation of the total particle number N and the z-component of the total spin S_z, the Hilbert space can be decomposed into subspaces (N, S_z). Determine the dimensions of these subspaces. (2 points)

b) Calculate (analytically) the matrix elements of the Hamilton matrix for the subspace $(N = 2, S_z = 0)$. (4 points)

Exercise 2: Symmetries

Consider the following two-site model:

$$H_{\rm ts} = \sum_\sigma \varepsilon_{\rm f} f^\dagger_\sigma f_\sigma + U f^\dagger_\uparrow f_\uparrow f^\dagger_\downarrow f_\downarrow + V \sum_\sigma \left(f^\dagger_\sigma c_\sigma + c^\dagger_\sigma f_\sigma \right) + \sum_\sigma \varepsilon_{\rm c} c^\dagger_\sigma c_\sigma \ , \qquad (1)$$

which corresponds to a single-impurity Anderson model with only a single bath site.

a) Show that, for the model eq. (1), the total particle number is conserved, i.e. $[H_{\rm ts}, \hat{N}]_- = 0$, with $\hat{N} = \sum_\sigma \left(f^\dagger_\sigma f_\sigma + c^\dagger_\sigma c_\sigma \right)$. (3 points)

b) Show that, for the model eq. (1), the z-component of the total spin is conserved, i.e. $[H_{\rm ts}, \hat{S}_z]_- = 0$, with $\hat{S}_z = f^\dagger_\uparrow f_\uparrow - f^\dagger_\downarrow f_\downarrow + c^\dagger_\uparrow c_\uparrow - c^\dagger_\downarrow c_\downarrow$. (3 points)

Now consider a tight-binding model on a finite chain with periodic boundary conditions:

$$H_{\rm tb} = \sum_{i=1}^{N} \epsilon_i c^\dagger_i c_i + \sum_{i=1}^{N-1} t_i \left(c^\dagger_i c_{i+1} + c^\dagger_{i+1} c_i \right) + t_N \left(c^\dagger_N c_1 + c^\dagger_1 c_N \right) \ . \qquad (2)$$

c) Perform the following two transformations:

$$\begin{aligned} H'_{\rm tb} &= H_{\rm tb}(c^\dagger_i \to c_i, c_i \to c^\dagger_i) \ , \\ H''_{\rm tb} &= H'_{\rm tb}(c^\dagger_i \to -c^\dagger_i, c_i \to -c_i, i \text{ even}) \ . \end{aligned}$$

Under which conditions do we have $H''_{\rm tb} = H_{\rm tb}$? (3 points)

Exercise 1: single-particle and many-particle spectra

We consider a Hamiltonian of the form

$$H = \sum_{i=1}^{N} \varepsilon_i c_i^\dagger c_i \ , \tag{1}$$

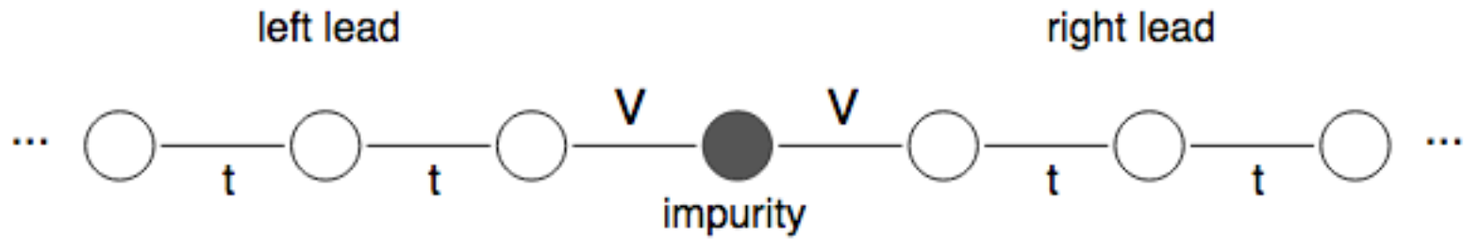
with $N = 6$ and energies $\varepsilon_i = 0.1 \cdot (i - 3.5)$. The many-particle energies of this system are given by $E = \sum_{i=1}^{N} n_i \varepsilon_i$, with $n_i = 0, 1$.

a) Write a program which translates the integer $j = 0, \ldots, 2^N - 1$ into the bit pattern $(n_1, n_2, \ldots, n_N)$, with $j = \sum_{i=1}^{N} n_i 2^{i-1}$. (3 points)

b) With the algorithm of part a), write a program which calculates the many-particle spectrum $\{E_l\}$ of the Hamiltonian eq. (1). (3 points)

Exercise 3: single-impurity Anderson model: even/odd basis

(5 points)



The figure shows a sketch of the single-impurity Anderson model, with coupling of the impurity to left and right 'leads', both represented by tight-binding chains. The Hamiltonian is of the form

$$H = H_{\rm imp} + H_{\rm imp-bath} + H_{\rm bath} \ ,$$

with the individual parts given by

$$\begin{aligned} H_{\rm imp} &= \sum_\sigma \varepsilon_{\rm f} f^\dagger_\sigma f_\sigma + U f^\dagger_\uparrow f_\uparrow f^\dagger_\downarrow f_\downarrow \ , \\ H_{\rm imp-bath} &= V \sum_{\alpha=l,r} \sum_\sigma \left(f^\dagger_\sigma c_{\alpha 1\sigma} + c^\dagger_{\alpha 1\sigma} f_\sigma \right) \ , \\ H_{\rm bath} &= t \sum_{\alpha=l,r} \sum_{i=1}^{\infty} \sum_\sigma \left(c^\dagger_{\alpha i\sigma} c_{\alpha i+1\sigma} + c^\dagger_{\alpha i+1\sigma} c_{\alpha i\sigma} \right) \ . \end{aligned}$$

The impurity in this model seems to couple to two 'channels'. Show that with the following transformation to an even/odd basis, the impurity only couples to a single channel (the even channel), with the odd channel decoupled from the impurity:

$$\begin{aligned} c^e_{i\sigma} &= \frac{1}{\sqrt{2}} \left(c_{li\sigma} + c_{ri\sigma} \right) \ , \\ c^o_{i\sigma} &= \frac{1}{\sqrt{2}} \left(c_{li\sigma} - c_{ri\sigma} \right) \ . \end{aligned}$$

Exercise 1: single-particle and many-particle spectra

(10 bonus points)

For a given single-particle spectrum $\{\varepsilon_i\}$, the many-particle energies can be simply calculated via $E = \sum_{i=1}^{N} n_i \varepsilon_i$, with $n_i = 0, 1$. In this project, you are supposed to solve the *reverse* problem: for a given set of many-particle energies $\{E_l\}$:

- find out whether the many-particle spectrum can be represented at all by a single-particle spectrum;
- if this is possible, calculate the single-particle spectrum $\{\varepsilon_i\}$.

As a specific example, consider the following two sets of many-particle energies:

$$\begin{aligned} \{E_l\}_1 &= -2, -1, 0(2), 1(2), 2, 3, \\ \{E_l\}_2 &= -2, -1(2), 0, 1, 2(2), 3 \end{aligned}$$

(The number in brackets indicate the degeneracies). To simplify the calculation, you can assume that the ε_i take integer values only.

Exercise 2: logarithmic discretization; broadening

(9 points + 3 bonus points)

Here we consider the semi-elliptic spectral function

$$A(\omega) = \begin{cases} \frac{2}{\pi}\sqrt{1-\omega^2} & : \quad |\omega| \leq 1 \,, \\ 0 & : \quad |\omega| > 1 \,. \end{cases}$$

The idea of this exercise is to perform a logarithmic discretization on $A(\omega)$ and then apply different broadening schemes to see how well the original spectral function is recovered.

a) Calculate the weights $a_n^{\pm}$ and frequencies $\omega_n^{\pm}$ of the discretized spectral function $A_\mathrm{d}(\omega)$ for a discretization parameter $\Lambda = 2$ (for the notation, see Sec. 2.2.5 in the script). (2 points)

b) For the broadening function, use Lorentzians with fixed width b to obtain the broadenend spectral function $A_{\mathrm{d,b}}(\omega)$. (3 points)

c) Now set the b of the Lorentzians to $b_n = \alpha|\omega_n^{\pm}|$, with α of the order of 0.5. What happens in the limit $\omega \to 0$ and $N \to \infty$? (4 points)

d) Finally, investigate the structures of the broadened spectral function $A_{\mathrm{d,b}}(\omega)$ using logarithmic Gaussians as broadening functions with $b = 0.3, 0.4, 0.5, 0.6$ (as above, see Sec. 2.2.5 in the script for the notation). (3 bonus points)

Exercise 3: logarithmic discretization of the single-impurity Anderson model

(4 points)

The conduction electron part of the Hamiltonian, $H_{\rm bath}$ (see eq. (2) in exercise 2), can be written in the form

$$\begin{aligned} H_{\rm bath} &= \sum_{np\sigma} \left(\xi_n^+ a_{np\sigma}^\dagger a_{np\sigma} + \xi_n^- b_{np\sigma}^\dagger b_{np\sigma} \right) \\ &+ \sum_{n,p\neq p',\sigma} \left(\alpha_n^+(p,p') a_{np\sigma}^\dagger a_{np'\sigma} - \alpha_n^-(p,p') b_{np\sigma}^\dagger b_{np'\sigma} \right) , \end{aligned} \tag{5}$$

with the definitions of the operators $a_{np\sigma}$ and $b_{np\sigma}$ given in the lecture. For a constant hybridization function $\Delta(\omega) = \Delta$ we can simply set the dispersion as $g(\varepsilon) = \varepsilon$. Show that in this case the quantities $\xi_n^\pm$ and $\alpha_n^\pm$ are given by:

$$\xi_n^\pm = \pm \frac{1}{2} \Lambda^{-n} (1 + \Lambda^{-1}) ,$$

$$\alpha_n^\pm(p,p') = \frac{1-\Lambda^{-1}}{2\pi i} \frac{\Lambda^{-n}}{p'-p} \exp\left[\frac{2\pi i (p'-p)}{1-\Lambda^{-1}} \right] .$$

Exercise 4: flow diagrams for the tight-binding model

(5 points + 3 bonus points)

Consider the following quantum impurity model defined on a chain with $N+1$ sites:

$$H = \varepsilon f^\dagger f + V\left(f^\dagger c_1 + c_1^\dagger f\right) + \sum_{n=1}^{N-1} t_n \left(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n\right) \ . \tag{6}$$

This model corresponds to a tight-binding model of spinless fermions with a special choice of parameters, in particular, the hoppings t_n are assumed to fall off exponentially: $t_n = \Lambda^{-n/2}$ with $\Lambda = 2$. As the Hamiltonian eq. (6) is non-interacting, it can be diagonalized via an orthogonal transformation (see Sec. 2.1 in the lecture). This gives the single-particle spectrum from which the many-particle energies can be constructed.

The lowest-lying many-particle energies $E_N(r)$ ($r = 1, \ldots, r_{\max}$ and we assume $E_N(r) \leq E_N(r+1)$) for a chain with N bath sites can now be used to plot the energy-level flow diagram, i.e. $\Lambda^{N/2} E_N(r)$ as a function of N.

a) Plot the five ($r_{\max} = 5$) lowest-lying many-particle energies in this way for $\varepsilon = 0$, $V = 0.1$, and N in the range $N = 3, \ldots, 20$. (5 points).

b) Investigate the effect of the value of ε on the flow diagram by varying ε in the range [-2,2]. (3 bonus points).