Exercise 1: continued fraction representation of Green functions

The continued fraction representation of a Green function $G(z)$ is given by

$$G(z) = \frac{1}{z - a_0 - \frac{b_0^2}{z - a_1 - \frac{b_1^2}{z - a_2 - \ldots}}}$$

(1)

with a set of continued fraction coefficients $\{a_n\}$ and $\{b_n\}$. If these coefficients take constant values $a_n = a$, $b_n = b$ for all $n \geq N$, the continued fraction can be terminated via the terminator

$$T_{a,b}(z) = \frac{1}{2b^2} \left( z - a - \sqrt{(z - a)^2 - 4b^2} \right).$$

The following exercise is about calculating $G(z)$ (and the corresponding spectral function $A(\omega)$) for different sets of $\{a_n\}$ and $\{b_n\}$.

a) Calculate real and imaginary part of the terminator $T_{0,1}(z = \omega + i\delta)$ for $\delta = 0.05$.

b) Write a general program for the calculation of $G(z)$ as in eq. (1) with $a_n = 0$ and $b_n = 1$ for all $n \geq N$ and arbitrary $a_n, b_n$ for $n < N$ (use the terminator from part a)). Check the program by setting $a_n = 0$ and $b_n = 1$ for all $n$.

c) Now set $a_n = \alpha (-1)^n$ and $b_n = 1$ for $n < N$ and calculate the spectral function for various values of $\alpha$.

d) With $b_n$ again fixed to 1 for all $n$, the values of the $a_n$ (for $n < N$) are now set to random numbers in the range $[-W, W]$. Investigate the structures appearing in the spectral function for various values of $W$ and $N$. 
Exercise 2: logarithmic discretization; broadening

Here we consider the semi-elliptic spectral function

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

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 \( A_d(\omega) \) for a discretization parameter \( \Lambda = 2 \) (for the notation, see Sec. 2.2.5 in the script).

b) For the broadening function, use Lorentzians with fixed width \( b \) to obtain the broadened spectral function \( A_{d,b}(\omega) \).

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

d) Finally, investigate the structures of the broadened spectral function \( A_{d,b}(\omega) \) 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).

Exercise 3: Lanczos algorithm

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).

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

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

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?
Exercise 4: reduced density matrix and entanglement entropy

With the definition of the reduced density matrix given in exercise 4 on sheet 4, we can now proceed with calculating the entanglement entropy $S_e$:

$$ S_e = -\text{Tr} [\hat{\rho} \ln \hat{\rho}] = -\sum_\alpha w_\alpha \ln w_\alpha , $$

with $w_\alpha$ the eigenvalues of the reduced density matrix. The entanglement entropy is a measure of the entanglement between subsystems $A$ and $B$ of a quantum system; this can now be tested on the three states $|\psi\rangle_i, i = 1, 2, 3$, given in exercise 4 on sheet 4.

a) Calculate the entanglement entropy $S_e$ for the states $|\psi\rangle_i$.

We now extend the analysis to larger systems, in particular one-dimensional spin systems with a bi-partitioning into parts $A$ and $B$ as shown in the figure:

![Diagram of one-dimensional spin system with bi-partitioning into parts A and B](image)

The number of sites in parts $A$ ($B$) is $M_A$ ($M_B$), with $M_A + M_B = M$. The state of the total system in expressed in the standard basis $\{|l\rangle\}$, $l = 1, \ldots, 2^M$, with $\{|l\rangle\} = \{|\uparrow\uparrow\ldots\uparrow\rangle, |\downarrow\uparrow\ldots\rangle, \ldots\}$:

$$ |\psi\rangle = \sum_{l=1}^{2^M} a_l |l\rangle . $$

b) Consider a random state $|\psi\rangle_r$ with $a_l$ random numbers in the range $[-1, 1]$, and $a_l = \bar{a}_l / \sqrt{\sum_l \bar{a}_l^2}$. Calculate $S_e$ for different values of $M_A$ and $M = 10$.

c) The following state has a much simpler structure:

$$ |\psi\rangle_{afm} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\uparrow\downarrow\ldots\rangle - |\downarrow\uparrow\downarrow\uparrow\ldots\rangle) . $$

Calculate $S_e$ for different values of $M_A$ and $M = 10$.

d) In the following state, site 1 is entangled with site 5:

$$ |\psi\rangle_{1-5} = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\downarrow\rangle_5 - |\downarrow\rangle_1 |\uparrow\rangle_5) \prod_{i=2}^4 (|\uparrow\rangle_i + |\downarrow\rangle_i) \prod_{i=6}^M (|\uparrow\rangle_i + |\downarrow\rangle_i) . $$

How does this entanglement show up in the entanglement entropy $S_e$ as a function of $M_A$ ($M = 10$)?