

Computational Many-Body Physics

apl. Prof. Dr. R. Bulla, C. Bartel

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Sheet 5: return on: Monday, June 20, 2016, 14:00

Exercise 1: continued fraction representation of Green functions

(10 points + 4 bonus points)

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

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

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 $\delta = 0.05$. (2 points)
- 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 . (5 points)
- c) Now set $a_n = \alpha(-1)^n$ and $b_n = 1$ for $n < N$ and calculate the spectral function for various values of α . (3 points)
- 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 . (4 bonus points)

Exercise 2: logarithmic discretization; broadening

(9 points + 3 bonus points)

Here we consider the semi-elliptic spectral function

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

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). (2 points)
- b) For the broadening function, use Lorentzians with fixed width b to obtain the broadened spectral function $A_{d,b}(\omega)$. (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 $\omega \rightarrow 0$ and $N \rightarrow \infty$? (4 points)
- 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). (3 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 $|\Phi_0\rangle = (1, 1, \dots, 1)$.

- a) Calculate the sequence of vectors $\{|\Phi_0\rangle, |\Phi_1\rangle, \dots, |\Phi_{M-1}\rangle\}$ ($M \leq N$) 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 4: reduced density matrix and entanglement entropy

(11 points + 4 bonus points)

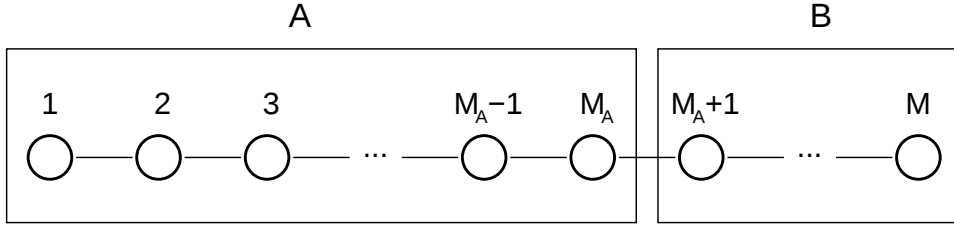
With the definition of the reduced density matrix given in exercise 4 on sheet 4, we can now proceed with calculating the entanglement entropy S_e :

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

with w_{α} 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 $|\psi\rangle_i$. (3 points)

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:



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 is expressed in the standard basis $\{|l\rangle\}$, $l = 1, \dots, 2^M$, with $\{|l\rangle\} = \{|\uparrow\uparrow\dots\uparrow\rangle, |\downarrow\uparrow\dots\uparrow\rangle, \dots\}$:

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

- b) Consider a random state $|\psi\rangle_r$ with $\bar{a}_l$ 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 $M = 10$. (5 points)

- c) The following state has a much simpler structure:

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

Calculate S_e for different values of M_A and $M = 10$. (3 points)

- 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 ($M = 10$)? (4 bonus points)