Computational Many-Body Physics

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Sheet 5

Exercise 1: continued fraction representation of Green functions

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

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

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 follwing 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 α.

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 $A_{\mathrm{d}}(\omega)$ 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 broadenend spectral function $A_{\mathrm{d,b}}(\omega)$.

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 $N \to \infty$?

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).

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_Φ 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

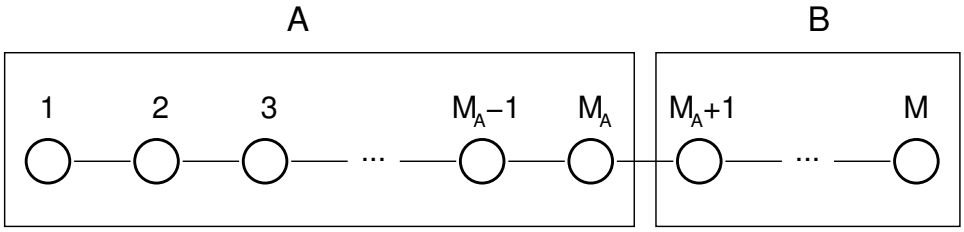
With the definition of the reduced density matrix given in exercise 4 on sheet 4, we can now proceed with calculating the entanglement entropy S_e:

$$S_\mathrm{e} = -\mathrm{Tr}\left[\hat{\rho}\ln\hat{\rho}\right] = -\sum_\alpha w_\alpha \ln w_\alpha \ ,$$

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 $|\psi\rangle_i$.

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 $M_\mathrm{A} + M_\mathrm{B} = M$. The state of the total system in expressed in the standard basis $\{|l\rangle\}$, $l = 1, \ldots, 2^M$, with $\{|l\rangle\} = \{|\uparrow\uparrow\ldots\uparrow\rangle, |\downarrow\uparrow\ldots\uparrow\rangle, \ldots\}$:

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

b) Consider a random state $|\psi\rangle_\mathrm{r}$ 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 $M = 10$.

c) The following state has a much simpler structure:

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

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

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

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

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