Computational Many-Body Physics

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Sheet 3 - tutorial of Monday, May 20, 14:00

Exercise 1: Reduced density matrix and entanglement entropy

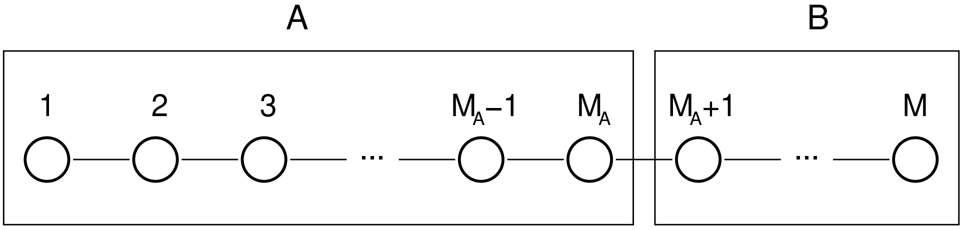
With the definition of the reduced density matrix given in exercise 4 on sheet 2, we can now proceed with calculating the entanglement entropy S_{e}:

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

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 2.

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 $\{|l\rangle\} = \{|\downarrow\downarrow\ldots\downarrow\rangle, |\uparrow\downarrow\ldots\downarrow\rangle, \ldots\}$:

$$|\psi\rangle = \sum_{l=0}^{2^M-1} a_l |l\rangle \ .$$

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:

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

How does this entanglement show up in the entanglement entropy S_{e} as a function of M_{A} ($M = 10$)?

Exercise 2: Entanglement entropy for one-dimensional spin models

The entanglement entropy S_{e} has been introduced in the previous exercise and applied to various states $|\psi\rangle$ for a system of M spins, with a bi-partitioning into parts A (with M_{A} sites) and B. In this exercise, the state $|\psi\rangle$ is taken as the ground state of the spin models defined via

$$H = -\sum_{i=1}^{M-1} \sum_{\alpha} J_i^\alpha S_i^\alpha S_{i+1}^\alpha \ ,$$

and different choices for the J_i^α.

Calculate S_{e} as a function of M_{A} ($M_{\mathrm{A}} = 1, 2, \ldots, M-1$) for fixed M and the state $|\psi\rangle$ given as the ground state of the following three models:

a) $J_i^\alpha = J\delta_{\alpha z}$,

b) $J_i^\alpha = J$,

c) $J_i^\alpha = \begin{cases} J\delta_{\alpha x} & : i \text{ even}, \\ J\delta_{\alpha z} & : i \text{ odd}. \end{cases}$

The total number of sites can be fixed to $M = 8$; consider both $J = +1$ and $J = -1$. If the ground state happens to be degenerate, the calculations should be performed for one of the ground states.

Exercise 3: tight-binding chain

The tight-binding model on a finite chain with periodic boundary conditions is defined as:

$$H_{\mathrm{tb}} = \sum_{i=1}^{N} \epsilon c_i^\dagger c_i + \sum_{i=1}^{N-1} t \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + t \left(c_N^\dagger c_1 + c_1^\dagger c_N \right) \ . \tag{1}$$

a) Show that the single-particle spectrum of this Hamiltonian can be obtained analytically via the following unitary transformation of the operators c_l:

$$c_l = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{i\frac{2\pi}{N}ml} d_m \ .$$

(The resulting single-particle energies are given by $\varepsilon_m = \epsilon + 2t\cos(\frac{2\pi}{N}m)$).

b) Compare the analytical values for the ε_m obtained in a) with the eigenvalues obtained from a numerical diagonalization of the matrix T. For the definition of T, see Sec. 2.1E in the script (summer term 2017).

Exercise 4: Hamilton matrix of the tight-binding chain

The idea of this exercise is to calculate the many-particle spectrum of the tight-binding chain via diagonalization of the *full* Hamilton matrix, and to check whether the result agrees with the many-particle spectrum constructed from the single-particle levels. The model is the tight-binding chain with open boundary conditions:

$$H_{\rm tb} = \sum_{i=1}^{N-1} t \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) \ . \tag{2}$$

a) Set up a program which calculates the full $2^N \times 2^N$-matrix $H_{lm} = \langle l | H_{\rm tb} | m \rangle$. One option here, which is not required, is to split up the Hilbert space into subspaces with different particle numbers.

b) Show that the eigenvalues of the Hamilton matrix agree with the many-particle energies constructed from the single-particle levels. ($N = 3, 4$ and 5 is sufficient.)

Exercise 5: Symmetries

Consider the following two-site model:

$$H_{\rm ts} = \sum_\sigma \varepsilon_{\rm f} f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow + V \sum_\sigma \left(f_\sigma^\dagger c_\sigma + c_\sigma^\dagger f_\sigma \right) + \sum_\sigma \varepsilon_{\rm c} c_\sigma^\dagger c_\sigma \ , \tag{3}$$

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 $\hat{N} = \sum_\sigma \left(f_\sigma^\dagger f_\sigma + c_\sigma^\dagger c_\sigma \right)$.

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 $\hat{S}_z = f_\uparrow^\dagger f_\uparrow - f_\downarrow^\dagger f_\downarrow + c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow$.

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

$$H_{\rm tb} = \sum_{i=1}^{N} \epsilon_i c_i^\dagger c_i + \sum_{i=1}^{N-1} t_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + t_N \left(c_N^\dagger c_1 + c_1^\dagger c_N \right) \ . \tag{4}$$

c) Perform the following two transformations:

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

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