Lecture 260070 "Entanglement in quantum many-body systems" – SS 2021

— Exercise Sheet #4 —

Problem 6: Transfer matrix I – unitary degree of freedom

Consider an MPS

$$|\Psi\rangle = \sum_{i_1,\dots,i_N} \mathrm{tr}[A^{i_1,(1)}A^{i_2,(2)}\dots A^{i_N,(N)}]\,|i_1,i_2,\dots,i_N\rangle\ . \tag{1}$$

1. Consider the state

$$|\Psi'\rangle = (U^{(1)}\otimes U^{(2)}\otimes\cdots\otimes U^{(N)})|\Psi\rangle\ , \tag{2}$$

where each $U^{(N)}$ acts on the Nth spin. Show that $|\Psi'\rangle$ can be written as an MPS with tensors

$$B^{i,(k)} = \sum_j U^{(k)}_{ij}A^{j,(k)}\ . \tag{3}$$

Now consider the transfer operators obtained from A and B,

$$\mathbb{E}^{(k)} = \sum_i A^{i,(k)}\otimes \bar{A}^{i,(k)} \text{ and } \mathbb{F}^{(k)} = \sum_i B^{i,(k)}\otimes \bar{B}^{i,(k)}\ . \tag{4}$$

2. Show that if $A^{(k)}$ and $B^{(k)}$ are related by (3) with $U^{(k)}$ unitary, then $\mathbb{E}^{(k)} = \mathbb{F}^{(k)}$. (That is, $|\Psi\rangle$ and $|\Psi'\rangle = (U^{(1)}\otimes U^{(2)}\otimes\cdots\otimes U^{(N)})|\Psi\rangle$ have the same transfer operator.)
3. Show that if $\mathbb{E}^{(k)} = \mathbb{F}^{(k)}$, then (3) holds with $U^{(k)}$ unitary. (That is, two MPS with the same transfer operators are the same up to local unitaries.)

Problem 7: Transfer matrix II – optimal contraction

1. Consider an MPS

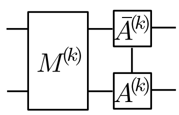
$$|\Psi\rangle = \sum_{i_1,\dots,i_N} \mathrm{tr}[A^{i_1,(1)}A^{i_2,(2)}\dots A^{i_N,(N)}]\,|i_1,i_2,\dots,i_N\rangle \tag{5}$$

with a bond dimension D. Consider the normalization $\langle\Psi|\Psi\rangle$. Express it explicitly in terms of the MPS above, and show that by rearranging terms, this can be transformed to

$$\langle\Psi|\Psi\rangle = \mathrm{tr}[\mathbb{E}^{(1)}\mathbb{E}^{(2)}\cdots\mathbb{E}^{(N)}]\ , \tag{6}$$

with $\mathbb{E}^{(k)} = \sum_i A^{i,(k)}\otimes\bar{A}^{i,(k)}$.
(*Note:* You can do this either by expressing the matrix multiplication in terms of indices as well, or by using properties of the tensor product, such as e.g. suitable manipulations of $\mathrm{tr}[A\otimes B]$ or $(AB)\otimes(CD)$.)

2. In order to numerically evaluate the expression (6) starting from the MPS tensors $A^{(k)}$, three things have to be done:
   (a) First, the matrix $M^{(1)} := \mathbb{E}^{(1)}$ has to be computed from $A^{(1)}$. Determine the computational cost (number of elementary operations) of this operation.
   (b) Second, the operation $M^{(k)}\mapsto M^{(k+1)} := M^{(k)}\mathbb{E}^{(k)}$ has to be applied (using the definition of $\mathbb{E}^{(k)}$ in terms of $A^{(k)}$!),

$M^{(k+1)} =$ 

(7)

This step involves a total of three contractions, which can be carried out in different orders. This includes the possibility of carrying out two contractions at the same time. List all these possible contraction orders, and determine the computational cost for each of them.

(c) Third, the trace of $M^{(N)}$ has to be computed. Determine the computational cost of this step as well.

(d) How does the total computational cost of computing the normalization $\langle\Psi|\Psi\rangle$ scale?

Note: You can assume a constant bond dimension D throughout the MPS if you want.

3. Repeat the preceding point for the case of an OBC MPS, where the $M^{(k)}$ are vectors rather than matrices.
(*Note:* If you solved the preceding problem for *general* bond dimensions D_k, you should already have the solution.)