Homework 3

1 The Fundamental Theorem of MPS

Let A be an injective tensor generating some translationally-invariant matrix product state $|\Psi_A\rangle$. Write down explicitly the overlap, and show — this time without diagrammatic notation — that

$$\langle\Psi_A|\Psi_A\rangle = \mathrm{tr}\left(\begin{array}{c} -\boxed{\bar{A}}- \\ | \\ -\boxed{A}- \end{array}\right)^N = \mathrm{tr}\,\mathbb{E}^N,$$

where $\mathbb{E} = \sum_i \bar{A}^i \otimes A^i$ is the *transfer matrix.* We can associate to it two linear maps, ε, as well as its adjoint ε^* (by looking at the matrix from the other direction)

$$\varepsilon(\sigma) = \sum_i A^i \sigma {A^i}^\dagger, \quad \varepsilon^*(\sigma) = \sum_i {A^i}^\dagger \sigma A^i,$$

Hint You might find the following property useful: $\mathrm{tr}(A\otimes B) = \mathrm{tr}\,A\,\mathrm{tr}\,B$.

Without loss of generality, we can take the spectral radius of the transfer matrix to be unity (we can always achieve that by rescaling A). Let $|r\rangle$ and $\langle\ell|$ be the dominant right and left eigenvectors, respectively, of $\mathbb{E}$. It can be shown that r and ℓ correspond to the fixed points of the associated linear maps ε and ε^*, and they are both positive[1]. Additionally, for injective tensors, r and ℓ are full rank and strictly positive definite. Show that the gauge transformation $\tilde{A}^i = XA^iX^{-1}$, with $X = \sqrt{1/r}$ brings A in its right-canonical form ($\sum_i \tilde{A}^i\tilde{A}^{i\dagger} = \mathbb{1}$), while the gauge $X = \sqrt{\ell}$ gives the left-canonical form[2] ($\sum_i \tilde{A}^{i\dagger}\tilde{A}^i = \mathbb{1}$). Choosing the left-canonical form, we then have $\rho = \ell$, and the fixed points of the maps are

$$\varepsilon(\rho) = \rho, \quad \varepsilon^*(\mathbb{1}) = \mathbb{1}.$$

Write down the diagrammatic expression corresponding to these equations.

Theorem 1.1 (Fundamental theorem of MPS) *Given two MPS characterized by the injective tensors A and B, then $|\Psi_A\rangle = |\Psi_B\rangle$, as $N\to\infty$, if and only if there exists a gauge transform X which relates A and B as $XA^i = B^iX$.*

You shall now prove this theorem. The backwards direction ("$\Leftarrow$") should be immediately clear. Let us now look at the forward direction ("$\Rightarrow$") of the theorem. Assume the states are correctly normalized, hence $|\Psi_A\rangle = |\Psi_B\rangle \Leftrightarrow |\langle\Psi_A|\Psi_B\rangle| = 1$.

Now define the operator

$$\langle\Psi_B|\Psi_A\rangle = \mathrm{tr}\,\mathbb{E}_{\mathrm{rel}}^N$$

Let X be the dominant eigenvector of $\mathbb{E}_{\mathrm{rel}}$ with eigenvalue λ. What are the maximum value of $|\lambda|$? How does it determine the overlap $\langle\Psi_B|\Psi_A\rangle$ in the thermodynamic limit? The eigenvalue equation for its associated linear map reads $\varepsilon^*_{\mathrm{rel}}(X) = \sum_i B^{i\dagger}XA^i = \lambda X$. Now, without loss of generality, we can take A and B to be in canonical form. Use the Cauchy–Schwarz inequality $|\langle u|v\rangle|^2 \le \|u\|^2\|v\|^2$ to show that

$$\left|\lambda\,\mathrm{tr}(X\rho X^\dagger)\right|^2 \le \left(\sum_i \mathrm{tr}(XA^i\rho {A^i}^\dagger X^\dagger)\right)\left(\sum_i \mathrm{tr}(B^iX\rho X^\dagger {B^i}^\dagger)\right) = \left|\mathrm{tr}(X\rho X^\dagger)\right|^2$$

You may use equations, diagrammatic expressions, or a combination of both. When is the Cauchy-Schwarz inequality an equality? In that case, conclude by showing that $XA^i = B^iX$.

Hint The trick is to think of the trace as an overlap: $\mathrm{tr}(u^\dagger v) = \langle u|v\rangle$.

[1] D. E. Evans and E. Høegh-Krohn, J. London Math. Soc. 17, 345-355 (1978). See Thm. 2.5.

[2] These forms are possible even without injectivity. It is slightly harder to show, since A needs to be decomposed in blocks. See D. Peréz-García, F. Verstraete, M.M. Wolf and J.I. Cirac, arXiv:0608197 (2006).

2 The AKLT State, Once Again

In the last homework we derived the tensor for the AKLT state $|\Psi\rangle = \sum_{\boldsymbol{\sigma}} \operatorname{tr}\left(A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_L}\right) |\boldsymbol{\sigma}\rangle$, with

$$A^{+} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad A^{0} = \frac{1}{2} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A^{-} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}.$$

Rescale the matrices such that $\sum_\sigma A^{\sigma\dagger} A^{\sigma} = \mathbb{1}$, to obtain the left-canonical form. Compute the transfer matrix and its eigenvalues (numerically, if you want). Check that in the limit $L \to \infty$, $\|\Psi\|^2 = 1$.

3 A Non-Injective MPS

Recall that the GHZ state is generated by the tensor $A^i = \delta_{i,a,b}$, $i = 0, 1$. Show that for any blocking of length L (see the next exercise for a definition), the subspace $\mathcal{S}_L$ of the GHZ state contains only two linearly independent vectors. Deduce that one cannot obtain an injective tensor after blocking for any finite L. Hence A cannot be a so-called *normal* tensor.

Compute the transfer matrix. Notice that there are two distinct dominant eigenvectors, let us call them $|\rho_\uparrow\rangle$ and $|\rho_\downarrow\rangle$. What is $\langle \mathrm{GHZ}|\mathrm{GHZ}\rangle$ as a function of N? Let O_n be a *local* operator acting on site n. Calculate the expectation values

$$\langle \cdot \rangle = \frac{\langle \psi | \cdot | \psi \rangle}{\langle \psi | \psi \rangle}$$

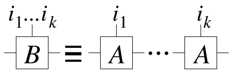
for $\psi = \mathrm{GHZ}$ of the following observables, in terms of the matrix $\mathbb{E}_O = \sum_{i,j} O_{ij} (\bar{A}^i \otimes A^j)$:

- $\langle O_n \rangle$,
- $C_L = \langle O_n O_{L+n} \rangle - \langle O_n \rangle \langle O_{L+n} \rangle$,

Does the correlation go to zero as $L \to \infty$?

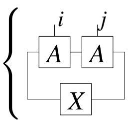
4 Uniqueness of the Ground State for Parent Hamiltonians

Let $|\Psi\rangle$ be an MPS generated by an *injective* tensor A. The *blocking* operation over k sites is the map



Verify the stability of the injectivity condition under blocking — that means, show that the superblock obtained by blocking k tensors still has the injectivity property (modulo a constant). There are a couple ways of doing this, you can use a diagrammatic argument, or you can use the mathematical definition of injectivity, namely that the map $X \mapsto \sum_i \operatorname{tr}(A^i X) |i\rangle$ is injective.

In this exercise we will prove the uniqueness of parent Hamiltonians, for *injective* tensors. To keep thing simple, we will restrict out attention to the one dimension, in the case where the parent Hamiltonian is a sum of *nearest-neighbor* terms $h_{i,i+1}$. Therefore we define the subspace

$$\mathcal{S}_2 = \left\{ \sum_{i,j} \operatorname{tr}(A^i A^j X) |i, j\rangle \middle| X \in \mathbf{L}(\mathbb{C}^{D \times D}) \right\} = \left\{ \right.$$  $$\left. \middle| X \in \mathbf{L}(\mathbb{C}^{D \times D}) \right\}.$$

where $\mathbf{L}(\mathbb{C}^{D \times D})$ is the space of all $D \times D$ matrices over $\mathbb{C}$. This space is just a special case of a series of subspaces

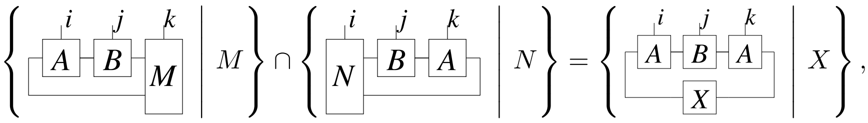
$$\mathcal{S}_k = \left\{ \sum_{i_1, \dots, i_k} \operatorname{tr}(A^{i_1} \dots A^{i_k} X) |i_1, \dots, i_k\rangle \middle| X \in \mathbf{L}(\mathbb{C}^{D \times D}) \right\}.$$

Show that $\mathcal{S}_k$ is the range of the k-sites reduced density matrix ρ_k.

Let me remind you of how you obtain the parent Hamiltonian: by defining the projector onto the space orthogonal to $\mathcal{S}_2$, we can construct the local term $h_{i,i+1}$. The parent Hamiltonian is then simply the sum of these local terms, $H = \sum_i h_{i,i+1}$.

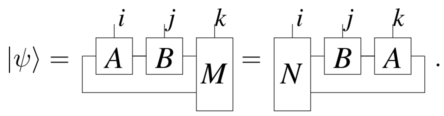
In order to prove the uniqueness, we will start by considering a chain with open boundary conditions, and show that the ground state subspace is $\mathcal{S}_2$. We will then close the boundaries, and show that the only state remaining is $|\Psi\rangle$. We can formalize this with two theorems.

Theorem 4.1 (Intersection property) *Let A and B be injective tensors. Then,*



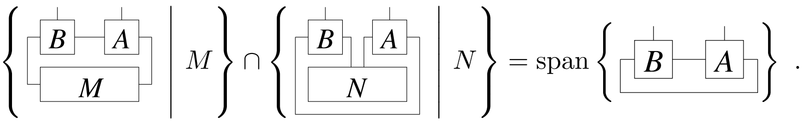
with M, N, $X \in \mathbf{L}(\mathbb{C}^{D\times D})$.

We shall prove this theorem by showing inclusion in both directions. Construct a state in the right hand side that belongs in both of the other two sets on the left hand side. Conversely, for any state $|\psi\rangle$ in the l.h.s., there exists M, N such that



Apply the inverse of A and B to find a relationship between M and N. Use this relationship to show that $|\psi\rangle$ is contained in the r.h.s., proving inclusion both ways.

Theorem 4.2 (Closure property) *For injective A and B,*



with M, $N \in \mathbf{L}(\mathbb{C}^{D\times D})$.

As for Theorem **??**, show that the r.h.s. is included in the intersection by choosing M and N appropriately. To prove inclusion the other way around, take a state belonging to the intersection, apply the inverses, and find that $M \propto \mathbb{1}$, concluding the proof.

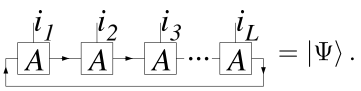
We define the operator $h_{i,i+1}$ acting on site $(i, i+1)$

$$h_{i,i+1} = \mathbb{1} \otimes (\mathbb{1} - P_{\mathcal{S}_2}) \otimes \mathbb{1},$$

where $P_{\mathcal{S}_2}$ is the projector on $\mathcal{S}_2$. Notice that $\mathcal{S}_2$ is the *ground space* of $h_{i,i+1}$. Conclude by proving the following theorem.

Theorem 4.3 (Parent Hamiltonian) *Let A be an injective tensor generating an MPS $|\Psi\rangle$. There exists a self-adjoint operator H, such that $|\Psi\rangle$ is its unique and frustration-free ground state.*

By induction, use Theorem **??** to prove that the intersection between acting with $h_{i,i+1}$ on every two-body pair $(1,2), (2,3), \dots (L-1, L)$ gives the support of $\mathcal{S}_L$. Finally, use Theorem **??** to prove that acting with the last term $h_{L,1}$ necessarily implies that the only remaining state is



Note This theorem is valid for any injective tensor network.