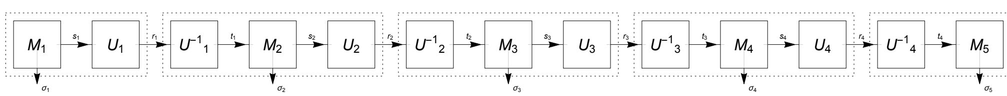
Chapter 4

Canonical Forms

A. Equivalent Representations of Matrix Product States

We are now going to develop some more machinery about matrix product states.

I think it is pretty intuitive that any quantum state can be written as a MPS if one takes the bond dimension high enough. We will shortly present an algorithm for this. The MPS representation of a quantum state is not unique. For example, imagine taking a set of square invertable matrices U and inserting UU^{-1} between each matrix:

$|\psi\rangle =$  (4.1)

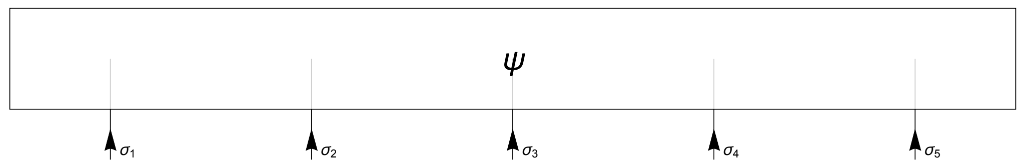
Grouping the matrices as shown by dashed lines:

$$M_j \to U_{j-1}^{-1} M_j U_j, \tag{4.2}$$

one gets a new representation of the same state. This is often referred to as a "Gauge" freedom. We will use it to convert our Matrix Product States into Canonical forms. There are four forms worth considering: the left, right, mixed, and symmetric forms.

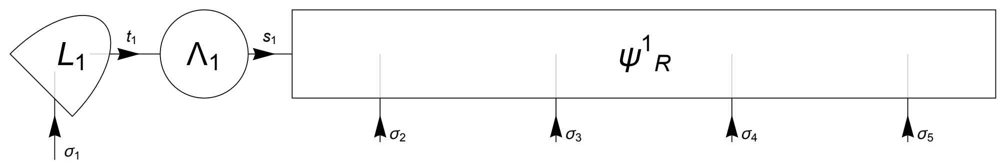
I will introduce the left canonical form, by showing how to convert an arbitrary state $\psi(\sigma_1, \sigma_2, \cdots, \sigma_n)$ into it. We will then convert it to the other canonical forms. Without any loss of generality, I will assume that the state is normalized. I begin at the left, and think of ψ as a matrix with two indices: σ_1 and a composite index $\{\sigma_2, \cdots \sigma_n\}$. I then perform a SVD:

$|\psi\rangle$ =



(4.3)

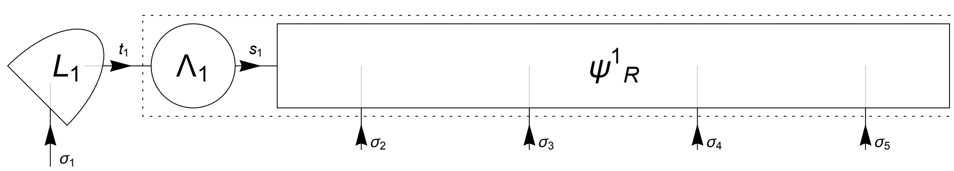
=



(4.4)

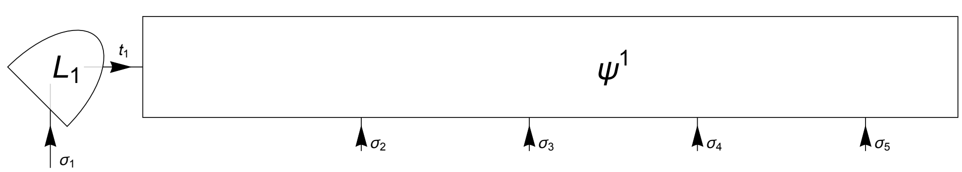
The t'th left Schmidt state is: L^t. The s'th right Schmidt state is $(\psi^1_R)^S$. One can think of L as the matrix which transforms from the Schmidt basis to the left physical basis, and ditto on the right. One then combines Λ with ψ, generating the expression:

$|\psi\rangle$ =



(4.5)

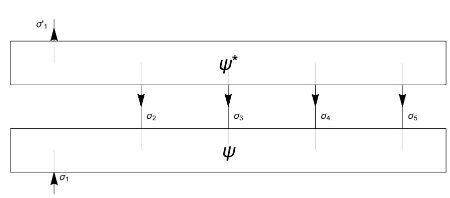
=



.(4.6)

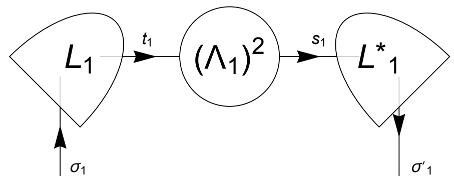
To expand on this, let me give an alternative way to carry out this procedure. Namely first calculate the reduced density matrix of the left hand side of the system,

$\rho_1 =$



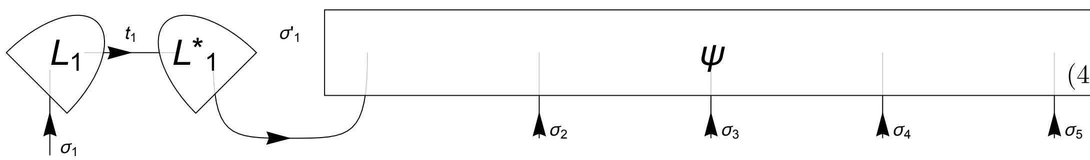
(4.7)

Here ρ_1 is a $d \times d$ matrix, where d is the size of the local Hilbert Space. Diagonalize ρ_1,

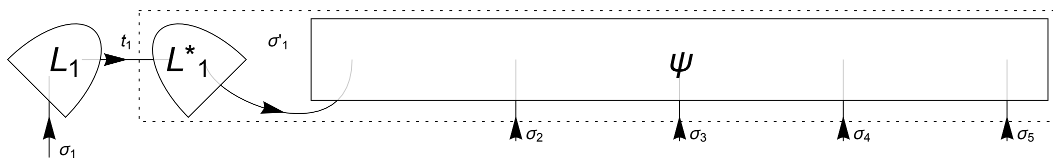
$\rho_1 =$ 

. (4.8)

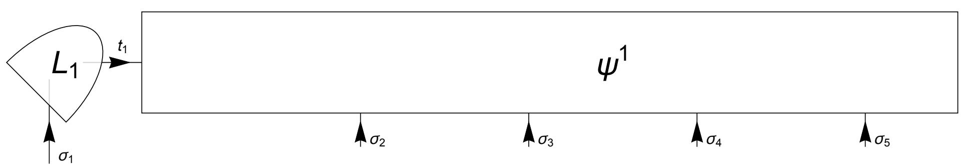
We then use those eigenstates to create a "resolution of the identity" that we insert into the wavefunction

$|\psi\rangle =$ 

(4.9)

$=$ 

(4.10)

$=$ 

, (4.11)

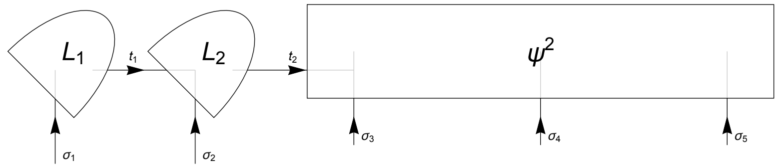
which gives an identical decomposition.

What we see is that we could have put any resolution of the identity in Eq. (4.9). What is special about the Schmidt basis is that its reduced density matrix is diagonal. The other feature is that we make no error in throwing away the zero singular values. So the dimension of t_1 is the number of non-zero Schmidt values.

An important approximation scheme is that we can truncate the decomposition – taking only singular values above some threshold. This compresses the quantum state, and is the basis for the DMRG. I have read that this truncation is *optimal* in the sense that it is the one which minimizes the deviation $\sum_{\{\sigma_j\}} |\psi_{\sigma_1\cdots\sigma_n} - \psi^t_{\sigma_1\cdots\sigma_n}|^2$. IE. If one takes L_1 to be a $d \times m$ left-orthogonal matrix, (with $m < d$ fixed matrix), then the optimal L_1 is the one generated by this scheme.

We can now repeat this scheme on ψ^1. This time we treat t_1 and σ_2 as one index, and $\sigma_3 \cdots \sigma_5$ as the other. This gives

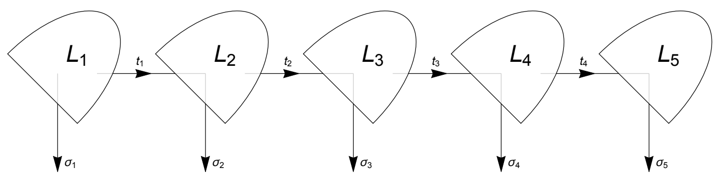
$$|\psi\rangle \quad =$$



. (4.12)

Again t_2 has the meaning of indexing the Schmidt vectors: L_2 converts this index into a wavefunction on the first two sites. Again we can compress the wavefunction by keeping only the larges Schmidt values. Repeating several more times gives a Matrix Product State in the "Left Normal Form"

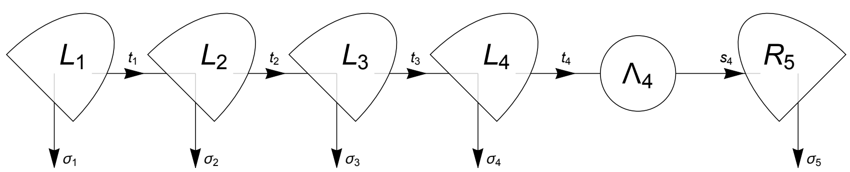
$$|\psi\rangle \quad =$$



. (4.13)

We can now go through the same procedure from the right. After the first step we have

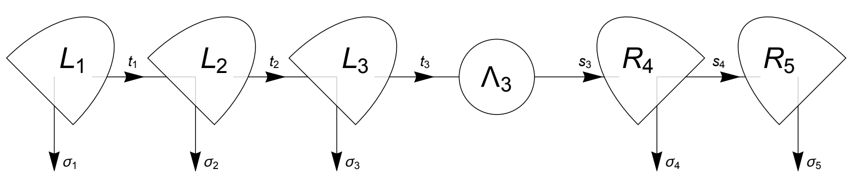
$$|\psi\rangle \quad =$$



, (4.14)

which is one way of expressing the "Mixed Canonical Form." Recall Λ_4 is a diagonal matrix containing the Schmidt values. The squares of the elements are the eigenvalues of the reduced density matrix if you trace over all the sites to the left or the right. We can repeat to move the boundary:

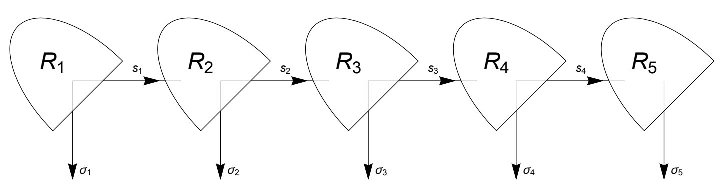
$$|\psi\rangle \quad =$$



, (4.15)

until we get to the right canonical form,

$$|\psi\rangle \quad =$$



. (4.16)

Comparing the various steps of the mixed canonical form, it is clear that

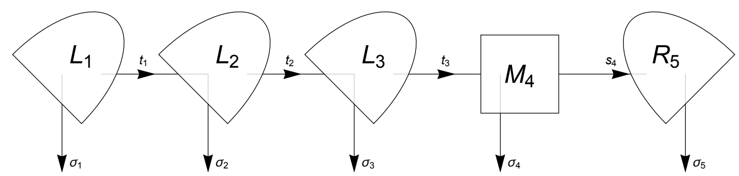
$$L_j \Lambda_j = \Lambda_{j-1} R_j, \tag{4.17}$$

so converting between the forms is as easy as rescaling the rows or columns. An alternative description of the mixed canonical form is to introduce

$$M_j = L_j \Lambda_j = \Lambda_{j-1} R_j, \tag{4.18}$$

so that

$$|\psi\rangle \quad =$$



. (4.19)

Another common representation involves introducing Γ_j given by

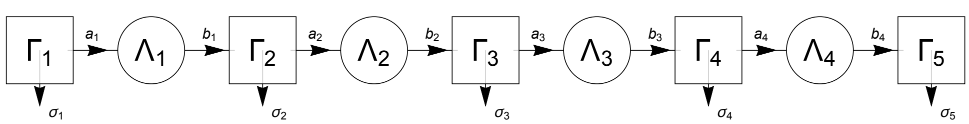
$$\Gamma_j = \Lambda_{j-1}^{-1} L_j = R_j \Lambda_j^{-1}, \tag{4.20}$$

or equivalently

$$\begin{aligned} \Lambda_{j-1}\Gamma_j &= L_j && (4.21) \\ \Gamma_j \Lambda_j &= R_j. && (4.22) \end{aligned}$$

For notational simplicity we treat Γ_0 and Γ_{n+1} as identity operators. That is $\Gamma_1 = L_1$ and $\Gamma_n = R_n$. In terms of these Γ matrices, the matrix product state looks more symmetrical

$$|\psi\rangle =$$

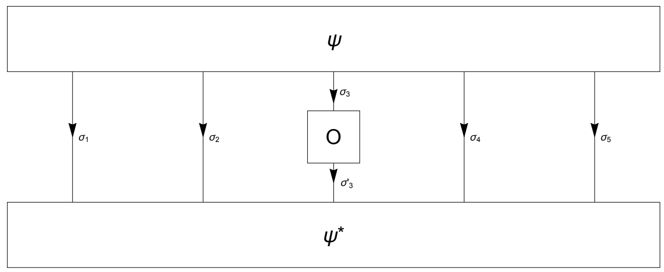


. (4.23)

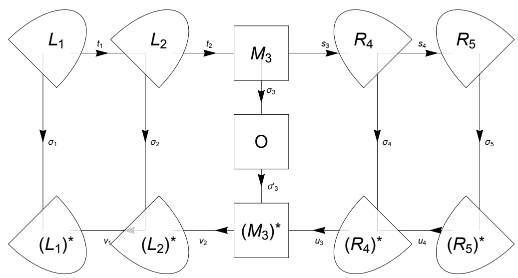
I have nice physical pictures for the L and R matrices – they are just basis changes. The Λ's are the Schmidt values. I don't have a really good physical intuition about the Γ's.

These canonical forms are useful for many reasons. The first property is that expectation values are simple. Because of the left and right orthogonality,

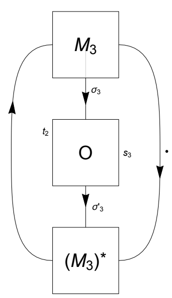
$$\langle\psi|O|\psi\rangle \quad = \tag{4.24}$$



$$= \tag{4.25}$$



$$= \tag{4.26}$$



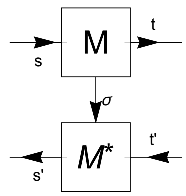
Draw the diagram expressing the expectation value of a local operator on site j, O_j in terms of L_j (the left canonical matrix on site j) and the diagonal matrix of singular values, Λ_j.

Draw the diagram expressing the expectation value $\langle A_j B_{j+1}\rangle$ in terms of L_j, R_{j+1} and Λ_j.

Complete the fourth tensor intro notebook.

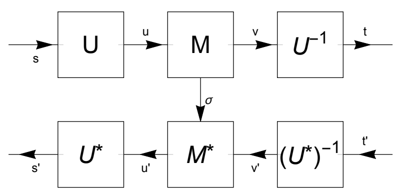
B. Canonical Forms for Infinite Matrix Product States

The same reasoning can can clearly be applied to infinite matrix product states – and the same Canonical forms can be defined. What is less clear is how to transform an arbitrary state into the form. Here we are going to focus on transforming a given Matrix Product State into the canonical forms. As in our previous class, the key is to work with the transfer matrix,

$E_I^0 =$ 

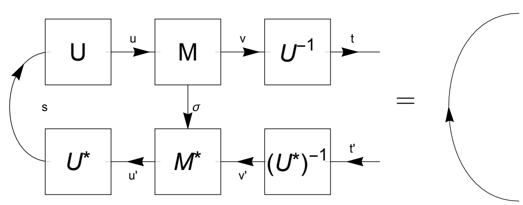
. (4.27)

The superscript 0 denotes that it is given. We can assume that the largest eigenvalue of E_I^0 is 1. If not we divide M by $\sqrt{\lambda}$. The quantum state is unchanged if we transform this to

$E_I^L =$ 

. (4.28)

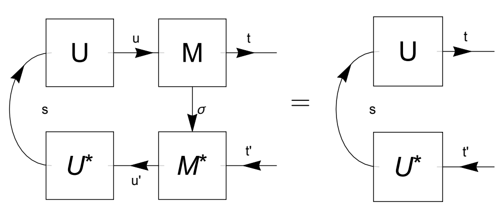
If we want the new $M_L = UMU^{-1}$ to be left normalized, we require



(4.29)

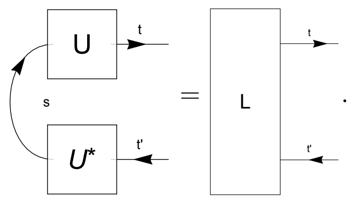
That is, the identity matrix is a left-eigenvector of the transfer matrix with eigenvalue 1. Note: despite the bad notation, U is not unitary.

If we multiply this equation on the right by UU^*, we get



. (4.30)

This can only be true if (up to an un-important multiplicative constant)



(4.31)

That is, considering the left eigenvector of M as a matrix, we want U to be the square root of that matrix. The best way I know of constructing the square root of a matrix is to do an eigenvalue decomposition:

$$L = S^{\dagger} D S, \tag{4.32}$$

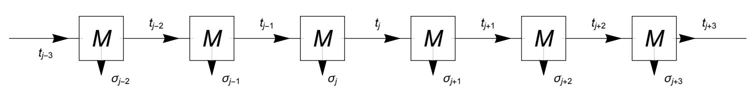
where S is unitary. We can therefore clearly write

$$U = W D^{1/2} S, \tag{4.33}$$

where W is an arbitrary unitary matrix – which we will choose shortly. For arbitrary W, the tensor $M_L = UMU^{-1}$ can be interpreted as a basis change: The left normalized condition is that the states are orthonormal. The unitary matrix W simply rotates this basis. We will choose W so that it is the Schmidt basis.

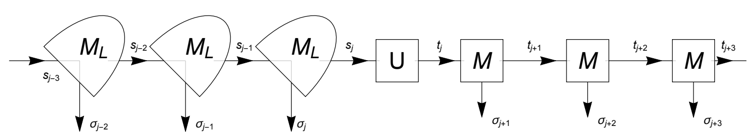
To proceed, we write our wavefunction as

$|\psi\rangle \;=\; \cdots$



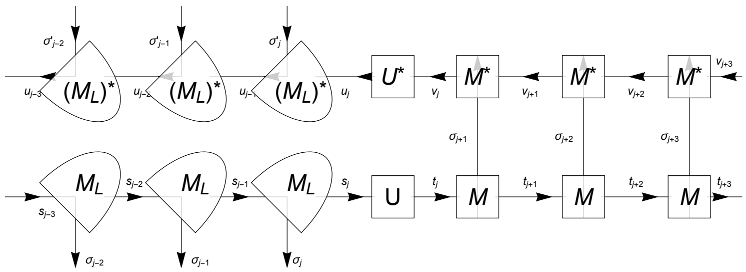
$\cdots$ (4.34)

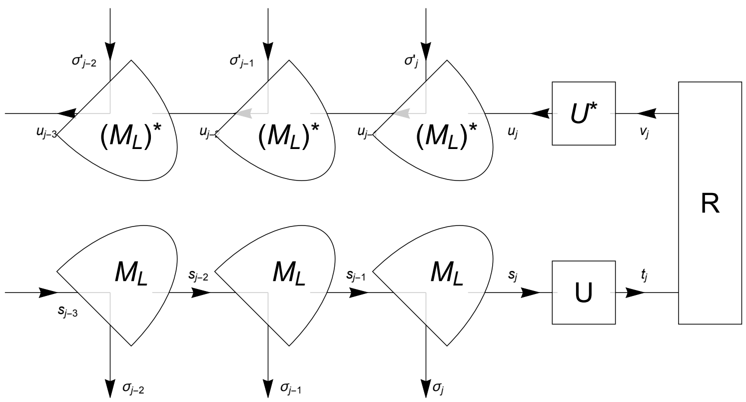
$= \;\cdots$



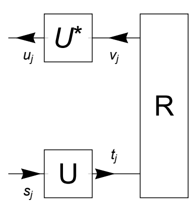
$\cdots\,.$ (4.35)

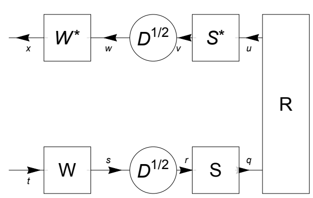
We then create the reduced density matrix, where we trace over all the spins whose index is bigger than j,

$\rho \quad = \quad \cdots$  $\cdots$ (4.36)

$= \quad \cdots$  (4.37)

But since M_L is just a basis change (also referred to as an isometry), I can look at the reduced density matrix in that basis

$\bar{\rho} \quad =$  (4.38)

$=$  . (4.39)

We now choose W so that it diagonalizes $D^{1/2}S^{\dagger}RSD^{1/2}$, in order to turn the wavefunction into the Canonical form. IE.

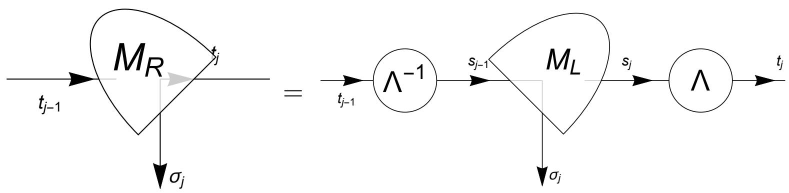
$$\rho = W^{\dagger}D^{1/2}S^{\dagger}RSD^{1/2}W = \Lambda^2 \tag{4.40}$$

is a diagonal matrix. The entanglement entropy is

$$S = -\sum_j \lambda_j \log(\lambda_j) \tag{4.41}$$

where λ_j are the elements of Λ.

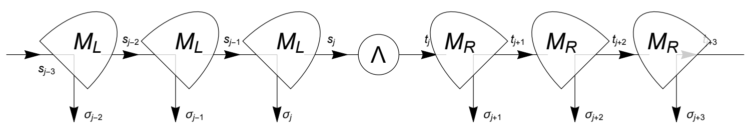
I will leave it as an exercise to show that M_R is right normalized, where



(4.42)

and that the wavefunction can be expressed in the mixed cannonical form

$|\psi\rangle = \cdots$



$\cdots$ (4.43)

To summarize, if you want to convert M to canonical form. You first find the left and right eigenvectors L and R of the transfer matrix. You re-express these as matrices. You diagonalize $L = S^\dagger D S$. You then diagonalize $D^{1/2} S^\dagger R S D^{1/2} = W^\dagger \Lambda^2 W$. The entries of Λ are the Schmidt coefficients. The canonical tensors are

$$M_L = W D^{1/2} S M S^\dagger D^{-1/2} W^\dagger \tag{4.44}$$

$$M_R = \Lambda^{-1} M_L \Lambda \tag{4.45}$$

$$\Gamma = \Lambda^{-1} M_L. \tag{4.46}$$

Note, if you look in the literature, you will see mathematically equivalent varieats on this procedure – for example you can do it with SVD's. The original work was [Orus and Vidal, PRB 78, 155117 (2008)] but there is also a nice discussion by McCulloch from around the same time [arXiv:0804.2509].

C. Homework 4 – Due Feb 7

Problem 16. For Credit Consider the matrix product state defined by Eq. (1.1).

16.1. Show that the following corresponds to that wavefunction in the left canonical form,

$$|\psi\rangle = \begin{pmatrix} |0\rangle & a|1\rangle \end{pmatrix} \begin{pmatrix} |0\rangle & b|1\rangle \\ & c|0\rangle \end{pmatrix} \begin{pmatrix} |0\rangle & d|1\rangle \\ & e|0\rangle \end{pmatrix} \begin{pmatrix} |0\rangle & f|1\rangle \\ & g|0\rangle \end{pmatrix} \begin{pmatrix} h|1\rangle \\ i|0\rangle \end{pmatrix} \tag{4.47}$$

where

$$a = \frac{\psi_1}{|\psi_1|} \tag{4.48}$$

$$b = \frac{\psi_2}{\sqrt{|\psi_1|^2 + |\psi_2|^2}} \tag{4.49}$$

$$c = \sqrt{1 - |b|^2} \tag{4.50}$$

$$d = \frac{\psi_3}{\sqrt{|\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2}} \tag{4.51}$$

$$e = \sqrt{1 - |d|^2} \tag{4.52}$$

$$f = \frac{\psi_4}{\sqrt{|\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2}} \tag{4.53}$$

$$g = \sqrt{1 - |f|^2} \tag{4.54}$$

$$h = \frac{\psi_5}{\sqrt{|\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2 + |\psi_5|^2}} \tag{4.55}$$

$$i = \sqrt{1 - |h|^2} \tag{4.56}$$

Problem 16. cont...

16.2. Find the Schmidt values corresponding to dividing the wavefunction in Eq. (4.47) between sites 1 and 2, between sites 2 and 3, between sites 3 and 4, and between sites 4 and 5.

Problem 17. For Credit Complete the exercise in the notebook "TensorIntro4.nb." I know the figures don't show up for everyone – it should be Eq. (4.15).

Problem 18. Bonus For a chain of spin-1 objects with nearest-neighbor interactions, the most general Hamiltonian which is invariant under rotating all spins:

$$H = \sum_j c_0 P^0_{j,j+1} + c_1 P^1_{j,j+1} + c_2 P^2_{j,j+1}, \tag{4.57}$$

where P^S is the projector of two neighboring sites into total spin S. Actually, this is redundant, since $P^0 + P^1 + P^2$ is the identity matrix – so up to an unimportant constant,

$$H = \sum_j c_1 P^1_{j,j+1} + c_2 P^2_{j,j+1}. \tag{4.58}$$

It turns out that as you vary the parameters, there are different sectors with gapped ground states – some of which have broken symmetries that distinguish them. There are also ones with no local order parameter which are topologically distinct (at least under the condition that the rotational symmetry is maintained). To understand some of this physics we need to construct the projectors. We can use Clebsch-Gordan coefficients, but a more elegant approach is to use the fact that they projector into the eigenspaces of the operator $S^2_{ij} = |\mathbf{S_i} + \mathbf{S_j}|^2$, with eigenvalues $0, 2,$ and 6. Therefore

$$P^0_{ij} = \frac{(S^2_{ij} - 2)(S^2_{ij} - 6)}{(0-2)(0-6)} \tag{4.59}$$

$$P^1_{ij} = \frac{S^2_{ij}(S^2_{ij} - 6)}{(2)(2-6)} \tag{4.60}$$

$$P^2_{ij} = \frac{S^2_{ij}(S^2_{ij} - 2)}{(6)(6-2)}. \tag{4.61}$$

18.1. Write these projectors in terms of $\mathbf{S_i} \cdot \mathbf{S_j}$. [which is how these Hamiltonians are typically written]. Because of this structure, Eq (4.57) can described as the spin-1 bilinear-biquadratic model.

Problem 18. cont...

18.2. One special case is the AKLT (Affleck, Kennedy, Tasaki, and Lieb) Hamiltonian

$$H = \sum_j P^2_{j,j+1}, \tag{4.62}$$

which is in a symmetry-protected topological phase. AKLT found an exact solution to this model, which was central to the development of the concept of topological order, and forshadowed the development of matrix product states.

The construction used by AKLT was elegant, and a future homework will likely walk you through it – it gives one story about how to construct matrix product states. Right now we are just going to explore some of the properties of the ground state:

$$|\psi\rangle = \begin{pmatrix} |0\rangle & |+\rangle \end{pmatrix} \begin{pmatrix} \frac{-1}{\sqrt{3}}|0\rangle & \sqrt{\frac{2}{3}}|+\rangle \\ -\sqrt{\frac{2}{3}}|-\rangle & \frac{1}{\sqrt{3}}|0\rangle \end{pmatrix} \begin{pmatrix} \frac{-1}{\sqrt{3}}|0\rangle & \sqrt{\frac{2}{3}}|+\rangle \\ -\sqrt{\frac{2}{3}}|-\rangle & \frac{1}{\sqrt{3}}|0\rangle \end{pmatrix} \begin{pmatrix} \frac{-1}{\sqrt{3}}|0\rangle & \sqrt{\frac{2}{3}}|+\rangle \\ -\sqrt{\frac{2}{3}}|-\rangle & \frac{1}{\sqrt{3}}|0\rangle \end{pmatrix} \begin{pmatrix} \frac{-1}{\sqrt{3}}|0\rangle \\ -\sqrt{\frac{2}{3}}|-\rangle \end{pmatrix}. \tag{4.63}$$

The generalization to more sites is obvious.

Show that this state is left-normalized.

Problem 18. cont...

18.3. Convert this state to the mixed canonical form, where the third site is the orthogonality center.

Problem 18. cont...

18.4. Find the entanglement spectrum if you split this state between the third and fourth state.

Problem 19. Bonus Consider the matrix product state defined by Eq. (2.1). Find the tensors M_L, M_R and Λ used to represent this state in the left, right, and mixed canonical forms.

Problem 20. Bonus Consider a system described by an infinite matrix product state. Write the expectation value of a local operator in terms of the canonical matrices M_L and Λ.

Problem 21. Bonus Prove Eqs. (4.42) and (4.43).