The DMRG and Matrix Product States

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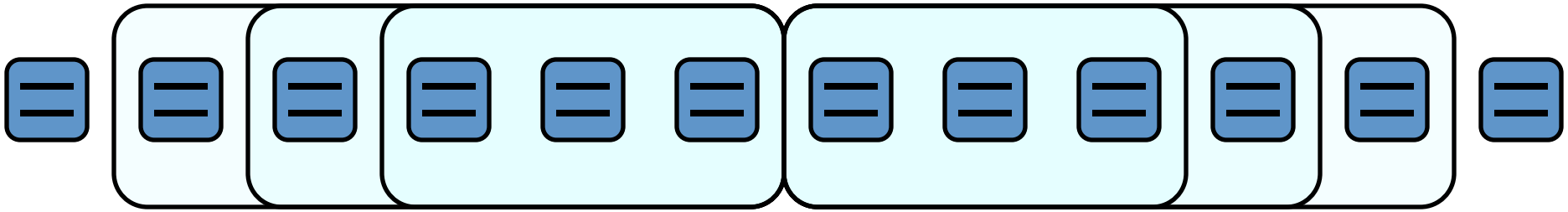
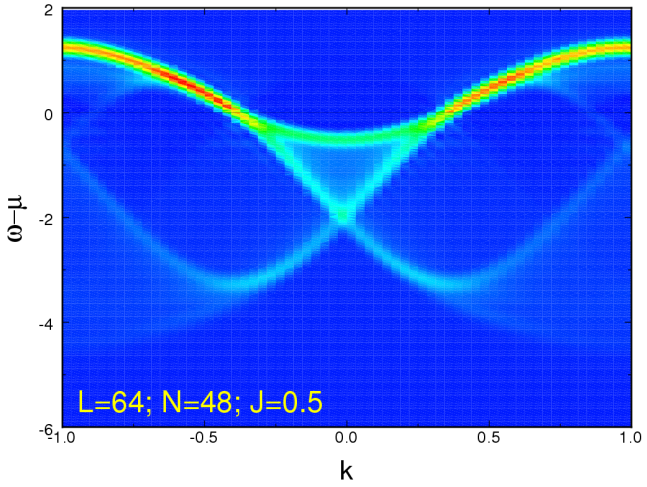
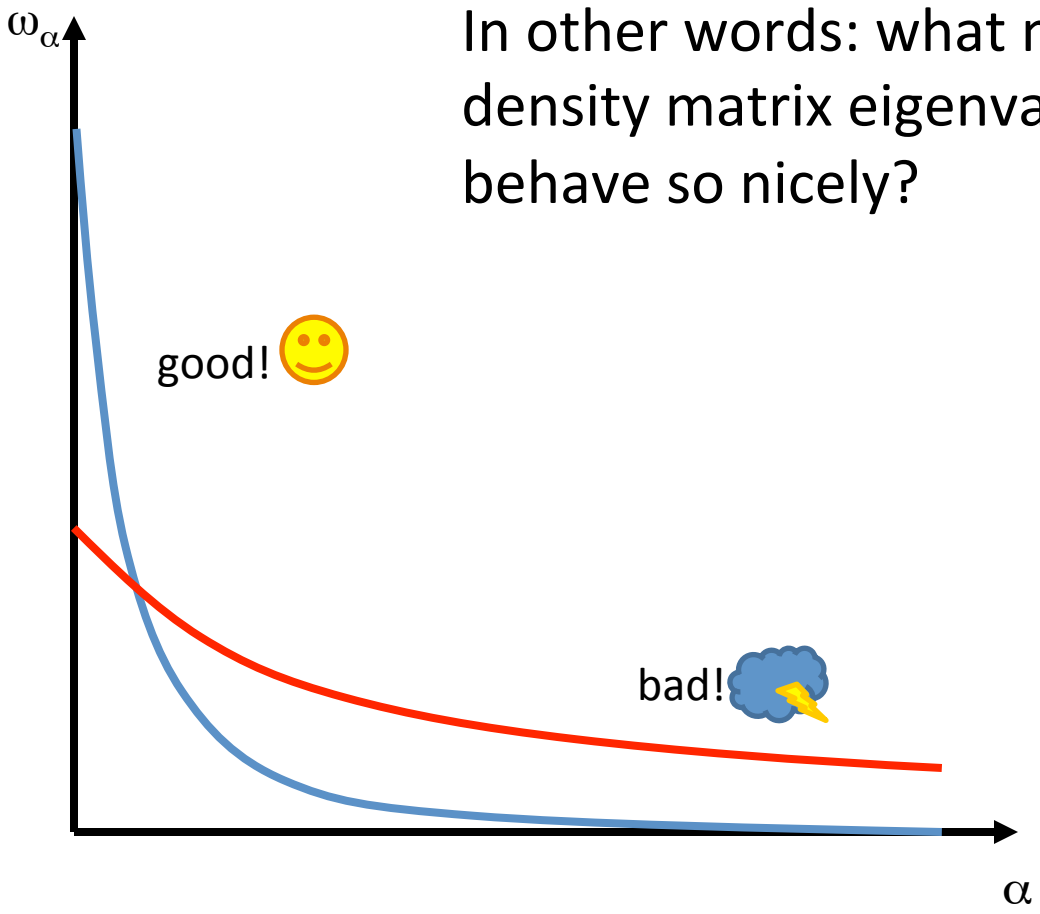




Why does the DMRG work???



In other words: what makes the density matrix eigenvalues behave so nicely?

Entanglement

We say that a two quantum systems A and B are "entangled" when we cannot describe the wave function as a product state of a wave function for system A, and a wave function for a system B

For instance, let us assume we have two spins, and write a state such as:

$$|\psi\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$$

We can readily see that this is equivalent to:

$$|\psi\rangle = (|\uparrow\rangle + |\downarrow\rangle) \otimes (|\uparrow\rangle + |\downarrow\rangle) = |\uparrow\rangle_x \otimes |\downarrow\rangle_x$$

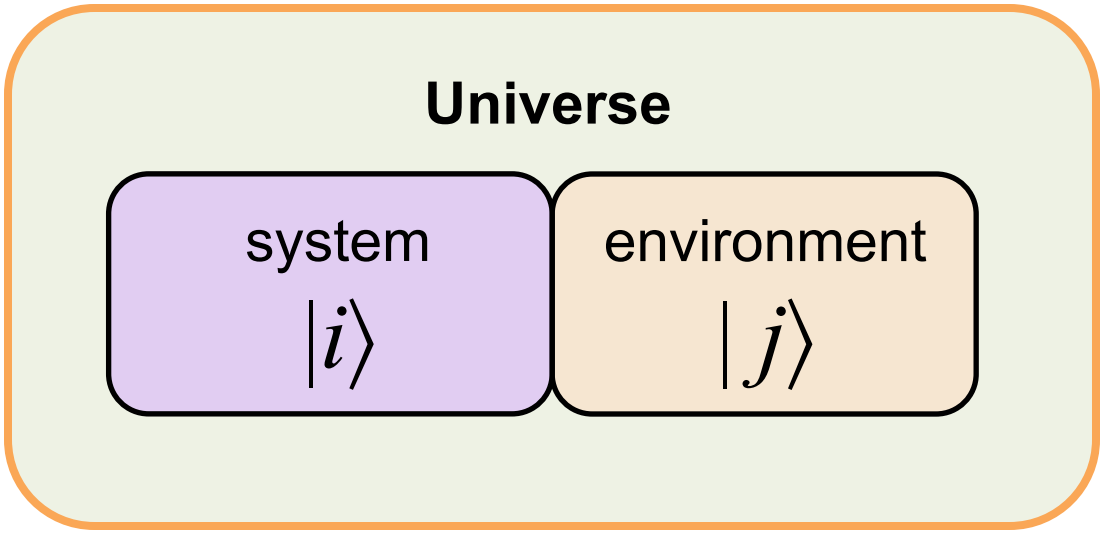
-> The two spins are not entangled! The two subsystems carry information independently

Instead, this state:

$$|\psi\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$$

is "maximally entangled". The state of subsystem A has ALL the information about the state of subsystem B

The Schmidt decomposition



$$|\psi\rangle_{AB} = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B$$

We assume the basis for the left subsystem has dimension $\dim_A$, and the right, $\dim_B$. That means that we have $\dim_A$ x $\dim_B$ coefficients.
We go back to the original DMRG premise: Can we simplify this state by changing to a new basis? (what do we mean with “simplifying”, anyway?)

The Schmidt decomposition

We have seen that through a SVD decomposition, we can rewire the state as:

$$|\psi\rangle_{AB} = \sum_{\alpha}^{r} \lambda_\alpha |\alpha\rangle_A |\alpha\rangle_B$$

Where

$$r = \min(\dim_A, \dim_B);\ \lambda_\alpha \geq 0 \quad \text{and} \quad |\alpha\rangle_A ; |\alpha\rangle_B \quad \text{are orthonormal}$$

Notice that if the Schmidt rank *r*=1, then the wave-function reduces to a product state, and we have "disentangled" the two subsystems.

After the Schmidt decomposition, the reduced density matrices for the two subsystems read:

$$\rho_{A/B} = \sum_{\alpha}^{r} \lambda_\alpha^2 |\alpha\rangle_{A/B}\ {}_{A/B}\langle\alpha|$$

The Schmidt decomposition, entanglement and DMRG

It is clear that the efficiency of DMRG will be determined by the spectrum of the density matrices (the "entanglement spectrum"), which are related to the Schmidt coefficients:

- If the coefficients decay very fast (exponentially, for instance), then we introduce very little error by discarding the smaller ones.
- Few coefficients mean less entanglement. In the extreme case of a single non-zero coefficient, the wave function is a product state and it completely disentangled.
- NRG minimizes the energy…DMRG concentrates entanglement in a few states. The trick is to disentangle the quantum many body state!

Quantifying entanglement

In general, we write the state of a bipartite system as:

$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle$$

We saw previously that we can pick and orthonormal basis for "left" and "right" systems such that

$$|\psi\rangle = \sum_{\alpha} \lambda_{\alpha} |\alpha_L\rangle |\alpha_R\rangle$$

We define the "von Neumann entanglement entropy" as:

$$S = -\sum_{\alpha} \lambda_{\alpha}^2 \log \lambda_{\alpha}^2$$

Or, in terms of the reduced density matrix:

$$\rho_L = \sum_{\alpha} \lambda_{\alpha}^2 |\alpha_L\rangle\langle\alpha_L| \rightarrow S = -\mathrm{Tr}\left(\rho_L \log \rho_L\right)$$

Entanglement entropy

Let us go back to the state:

$$|\psi\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$$

We obtain the reduced density matrix for the first spin, by tracing over the second spin (and after normalizing):

$$\rho_L = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

We say that the state is "maximally entangled" when the reduced density matrix is proportional to the identity.

$$S = -\frac{1}{2}\log\frac{1}{2} - \frac{1}{2}\log\frac{1}{2} = \log 2$$

Entanglement entropy

- If the state is a product state:

$$|\psi\rangle = |\alpha_L\rangle|\alpha_R\rangle \rightarrow w_\alpha = \{1,0,0,\ldots\} \rightarrow S = 0$$

- If the state maximally entangled, all the w_α are equal

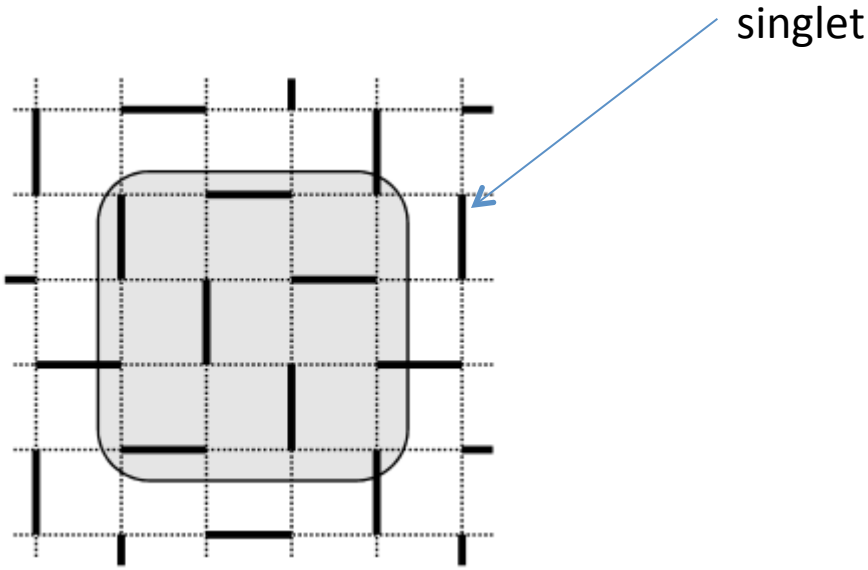
$$\rightarrow w_\alpha = \left\{1/D, 1/D, 1/D, \ldots\right\} \rightarrow S = \log D$$

where *D* is

$$D = \min\{\dim H_L, \dim H_R\}$$

Area law: Intuitive picture

Consider a valence bond solid in 2D



$$S = \log 2 \times (\#\text{of bonds cut}) \approx L \log 2$$

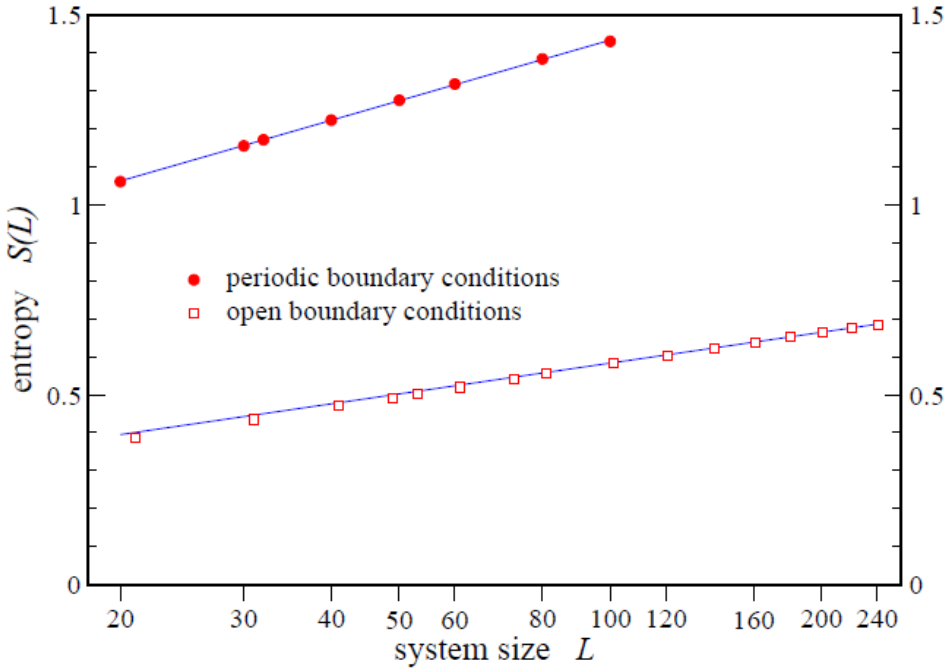
The entanglement entropy is proportional to the area of the boundary separating both regions. This is the prototypical behavior in gapped systems. Notice that this implies that the entropy in 1D is independent of the size of the partition

Critical systems in 1D

$$S_{PBC} = \frac{c}{3} \log(L),$$

$$S_{OBC} = \frac{c}{6} \log(L),$$

c is the "central charge" of the system, a measure of the number of gapless modes



Entropy and DMRG

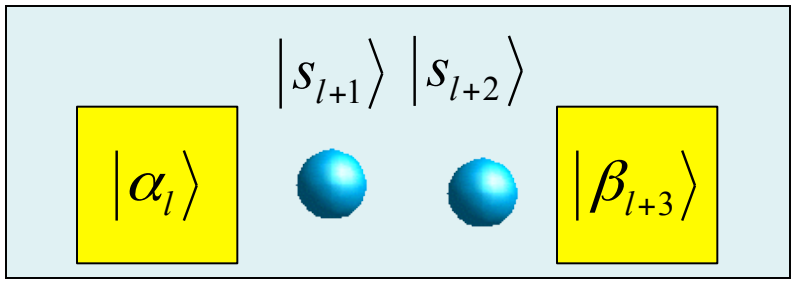
The number of states that we need to keep is related to the entanglement entropy:

$$m \approx \exp S$$

- Gapped system in 1D: m=const.
- Critical system in 1D: $m=L^{\alpha}$
- Gapped system in 2D: m=exp(L)
- In 2D in general, most systems obey the area law (not free fermions, or fermionic systems with a 1D Fermi surface, for instance)…
- Periodic boundary conditions in 1D: twice the area -> m^2

The wave-function transformation

Before the transformation, the superblock state is written as:



$$|\psi\rangle = \sum_{\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3}} \langle \alpha_l s_{l+1} s_{l+2} \beta_{l+3} | \psi \rangle | \alpha_l \rangle \otimes | s_{l+1} \rangle \otimes | s_{l+2} \rangle \otimes | \beta_{l+3} \rangle$$

After the transformation, we add a site to the left block, and we "spit out" one from the right block

$$|\psi\rangle = \sum_{\alpha_{l+1}, s_{l+2}, s_{l+3}, \beta_{l+4}} \langle \alpha_{l+1} s_{l+2} s_{l+3} \beta_{l+4} | \psi \rangle | \alpha_{l+1} \rangle \otimes | s_{l+2} \rangle \otimes | s_{l+3} \rangle \otimes | \beta_{l+4} \rangle$$

After some algebra, and assuming $\sum_{\alpha_l} |\alpha_l\rangle\langle\alpha_l| \approx 1$, one readily obtains:

$$\langle \alpha_{l+1} s_{l+2} s_{l+3} \beta_{l+4} | \psi \rangle \approx \sum_{\alpha_l, s_{l+1}, \beta_{l+3}} \langle \alpha_{l+1} \| \alpha_l s_{l+1} \rangle \langle \alpha_l s_{l+1} s_{l+2} \beta_{l+3} | \psi \rangle \langle s_{l+3} \beta_{l+4} \| \beta_{l+3} \rangle$$

The DMRG transformation

When we add a site to the block we obtain the wave function for the larger block as:

$$\left|\alpha_l\right\rangle = \sum_{s_l,\alpha_{l-1}} \left\langle \alpha_l \left| U_L^l \right| \alpha_{l-1} s_l \right\rangle \left|\alpha_{l-1}\right\rangle \otimes \left| s_l \right\rangle$$

Let's change the notation…

$$A\left[s_l\right]_{\alpha_l,\alpha_{l-1}} \equiv \left\langle \alpha_l \left| U_L^l \right| \alpha_{l-1} s_l \right\rangle$$

$$\rightarrow \left|\alpha_l\right\rangle = \sum_{s_l,\alpha_{l-1}} A\left[s_l\right]_{\alpha_l,\alpha_{l-1}} \left|\alpha_{l-1}\right\rangle \otimes \left| s_l \right\rangle$$

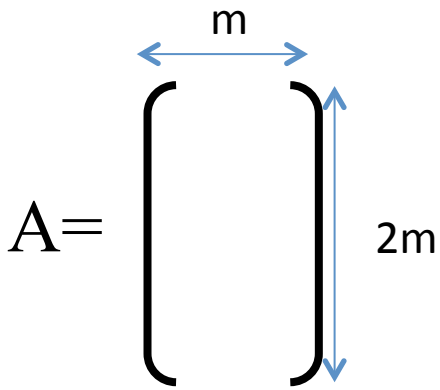
We can repeat this transformation for each l, and recursively we find

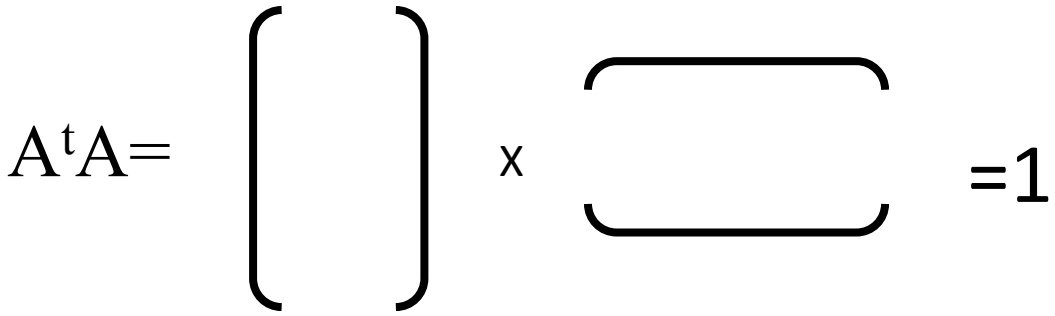
$$\left|\alpha_l\right\rangle = \sum_{\{s\}} A[s_1]_{\alpha_1} A[s_2]_{\alpha_1,\alpha_2} \ldots A[s_l]_{\alpha_{l-1}\alpha_l} \left| s_1 \ldots s_l \right\rangle$$

Notice the single index. The matrix corresponding to the open end is actually a vector!

Some properties the A matrices

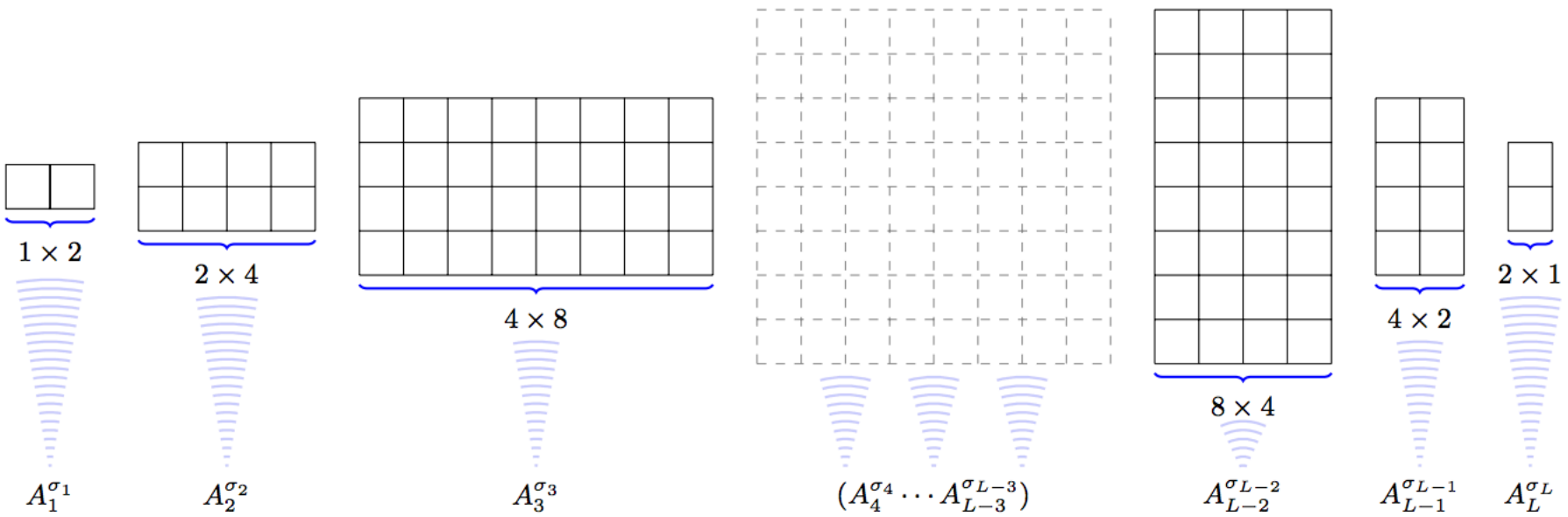
Recall that the matrices A in our case come from the rotation matrices U





This is not necessarily the case for arbitrary MPS's, and normalization is usually a big issue!

Left canonical representation



The DMRG wave-function in more detail…

We can repeat the previous recursion from left to right…

$$|\beta_l\rangle = \sum_{\{s\}} B[s_l]_{\beta_l,\beta_{l+1}} B[s_{l+2}]_{\beta_{l+2},\beta_{l+3}} \ldots B[s_L]_{\beta_L} \, | s_l \ldots s_L \rangle$$

At a given point we may have

$$|\psi\rangle = \sum_{\alpha_l,\beta_l} \langle \alpha_l \beta_{l+1} | \psi \rangle \, | \alpha_l \rangle \, | \beta_{l+1} \rangle =$$

$$\sum_{\{s\}} A[s_1]_{\alpha_1} A[s_2]_{\alpha_1,\alpha_2} \ldots A[s_l]_{\alpha_{l-1}\alpha_l} \langle \alpha_l \beta_{l+1} | \psi \rangle B[s_{l+1}]_{\beta_{l+1},\beta_{l+2}} B[s_{l+2}]_{\beta_{l+2},\beta_{l+3}} \ldots B[s_L]_{\beta_L} \, | s_1 \ldots s_L \rangle$$

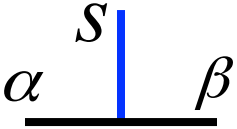
Without loss of generality, we can rewrite it:

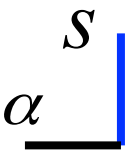
$$|\psi\rangle = \sum_{\{s\}} M[s_1]_{\alpha_1} M[s_2]_{\alpha_1,\alpha_2} \ldots M[s_2]_{\alpha_{L-1},\alpha_L} M[s_L]_{\alpha_L} \, | s_1 \ldots s_L \rangle$$

MPS wave-function for open boundary conditions

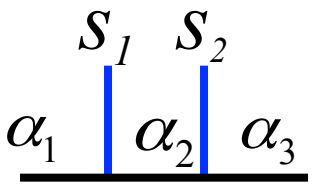
Diagrammatic representation of MPS

The matrices can be represented diagrammatically as

$A[s]_{\alpha\beta} \equiv$ 

$A[s]_{\alpha} \equiv$ 

And the contractions, as:



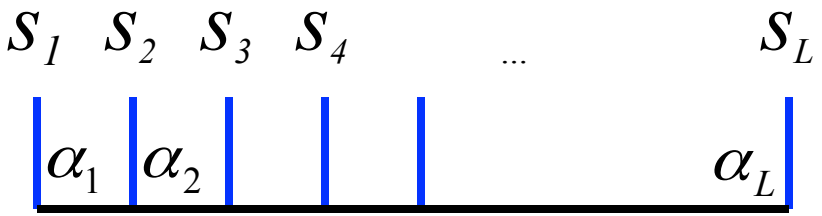
The dimension D of the left and right indices is called the "bond dimension"

MPS for open boundary conditions

$$|\psi\rangle = \sum_{\{s\}} M[s_1]_{\alpha_1} M[s_2]_{\alpha_1,\alpha_2} \ldots M[s_2]_{\alpha_{L-1},\alpha_L} M[s_L]_{\alpha_L} \, | s_1 \ldots s_L \rangle$$

$$= \sum_{\{s\}} M[s_1] M[s_2] \ldots M[s_L] \, | s_1 \ldots s_L \rangle$$

$$= \sum_{\{s\}} \prod_{l=1}^{L} M[s_l] \, | s_1 \ldots s_L \rangle$$

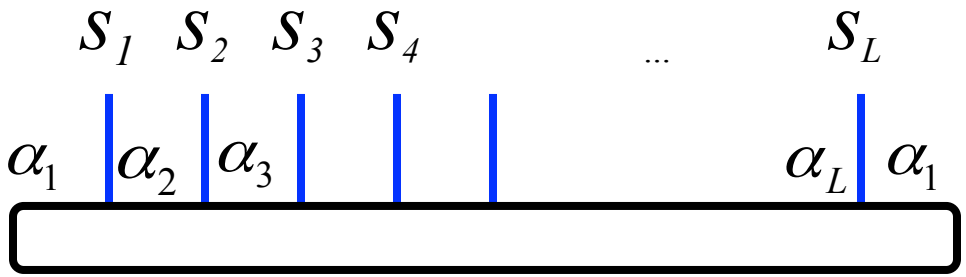


MPS for periodic boundary conditions

$$|\psi\rangle = \sum_{\{s\}} M[s_1]_{\alpha_L \alpha_1} M[s_2]_{\alpha_1,\alpha_2} \ldots M[s_2]_{\alpha_{L-1},\alpha_L} M[s_L]_{\alpha_L,\alpha_1} \, | \, s_1 \ldots s_L \rangle$$

$$= \sum_{\{s\}} \mathrm{Tr}\left(M[s_1] M[s_2] \ldots M[s_L] \right) | \, s_1 \ldots s_L \rangle$$

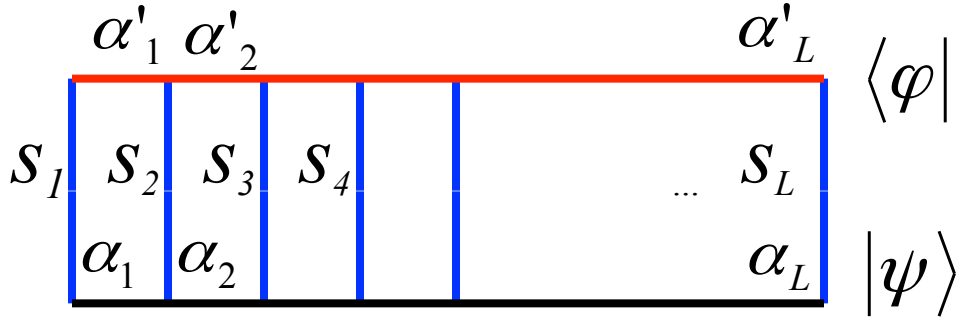
$$= \sum_{\{s\}} \mathrm{Tr}\left(\prod_{l=1}^{L} M[s_l] \right) | \, s_1 \ldots s_L \rangle$$



Properties of Matrix Product States

Inner product:

$$\langle \varphi | \psi \rangle$$



Addition:

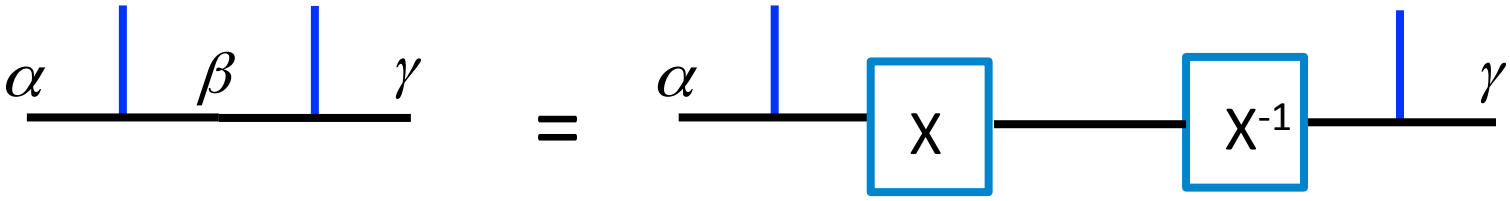
$$|\psi\rangle = \sum_{\{s\}} M_1 M_2 \ldots M_L \,|\, s_1 \ldots s_L\rangle; |\varphi\rangle = \sum_{\{s\}} \tilde{M}_1 \tilde{M}_2 \ldots \tilde{M}_L \,|\, s_1 \ldots s_L\rangle$$

$$\rightarrow |\psi\rangle + |\varphi\rangle = \sum_{\{s\}} N_1 N_2 \ldots N_L \,|\, s_1 \ldots s_L\rangle$$

$$\text{with } N = \begin{pmatrix} M & 0 \\ 0 & \tilde{M} \end{pmatrix}$$

$$\rightarrow N_1 N_2 \ldots N_L = \begin{pmatrix} M_1 M_2 \ldots M_L & \\ & \tilde{M}_1 \tilde{M}_2 \ldots \tilde{M}_L \end{pmatrix}$$

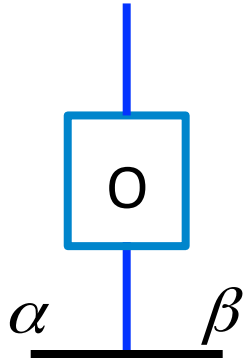
Gauge Transformation



There are more than one way to write the same MPS.
This gives you a tool to othonormalize the MPS basis

Operators

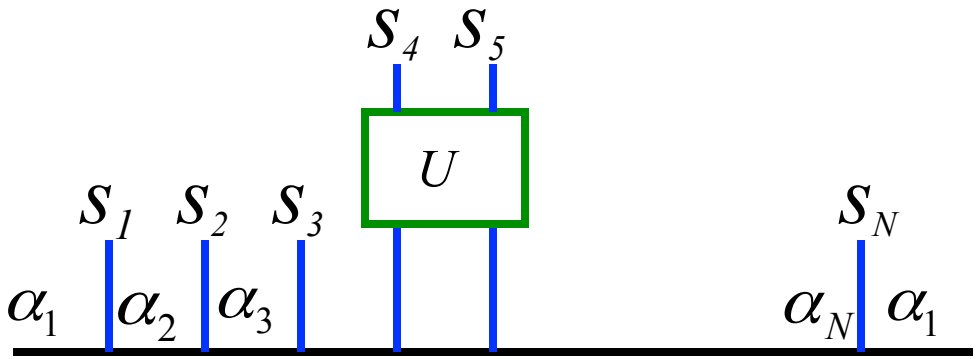
O is a matrix with elements $\langle s|O|s'\rangle$



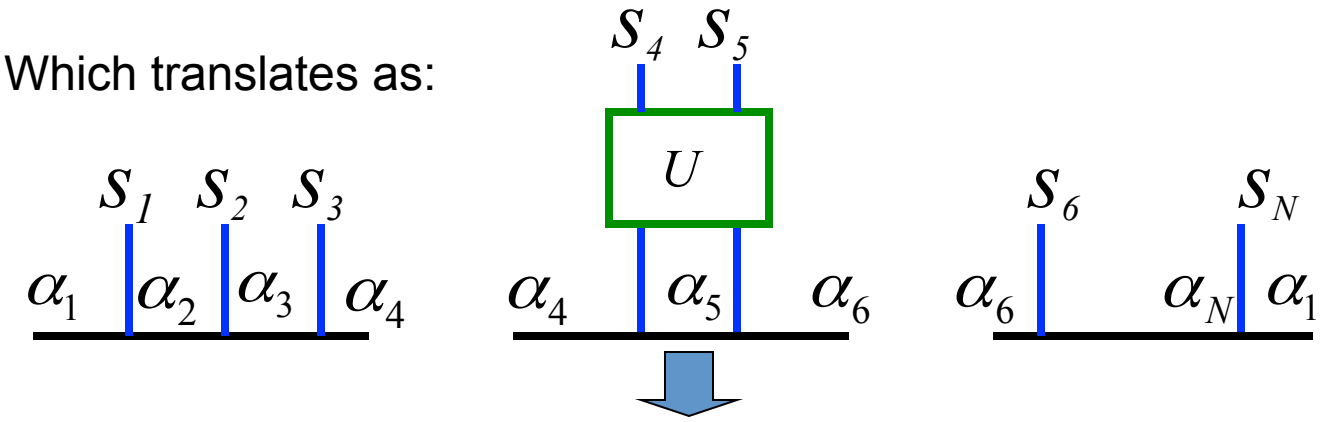
The operator acts on the spin index only

Pairwise unitary tranformations

The two-site time-evolution operator will act as:



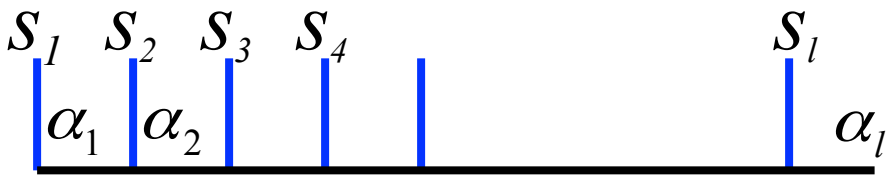
Which translates as:



$$\sum_{s'_4,s'_5} A_4[s'_4]_{\alpha_4\alpha_5} U^{s_4,s_5}_{s'_4,s'_5} A_5[s'_5]_{\alpha_5\alpha_6}$$

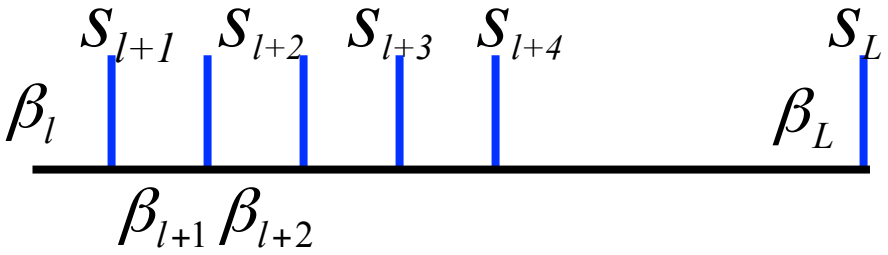
Matrix product basis

$$|\alpha_l\rangle = \sum_{\{s\}} A[s_1]_{\alpha_1} A[s_2]_{\alpha_1,\alpha_2} \ldots A[s_l]_{\alpha_{l-1}\alpha_l} |s_1 \ldots s_l\rangle$$



"left canonical"

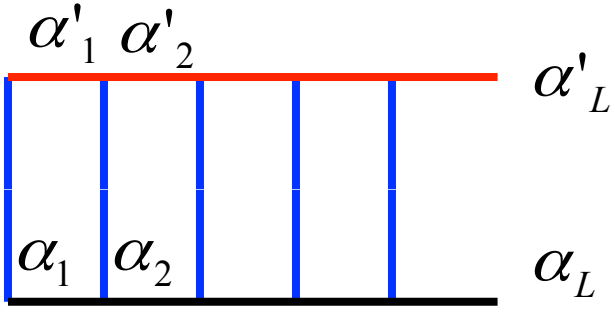
$$|\beta_l\rangle = \sum_{\{s\}} B[s_l]_{\beta_l,\beta_{l+1}} B[s_{l+2}]_{\beta_{l+2},\beta_{l+3}} \ldots B[s_L]_{\beta_L} |s_l \ldots s_L\rangle$$



"right canonical"

As we saw before, in the dmrg basis we get:

$$\langle \alpha_l | \alpha'_l \rangle =$$



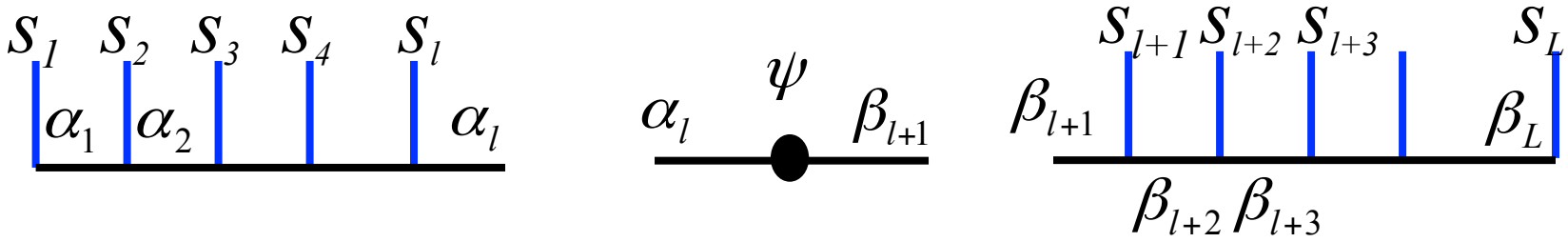
$$= \delta_{\alpha_l,\alpha'_l}$$

The DMRG w.f. in diagrams

$$|\psi\rangle =$$

$$\sum_{\{s\}} A[s_1]_{\alpha_1} A[s_2]_{\alpha_1,\alpha_2} \ldots A[s_l]_{\alpha_{l-1}\alpha_l} \langle \alpha_l \beta_{l+1} | \psi \rangle B[s_{l+1}]_{\beta_{l+1},\beta_{l+2}} B[s_{l+2}]_{\beta_{l+2},\beta_{l+3}} \ldots B[s_L]_{\beta_L} \, | \, s_1 \ldots s_L \rangle =$$

$$\sum_{\{s\}} A[s_1]_{\alpha_1} A[s_2]_{\alpha_1,\alpha_2} \ldots A[s_l]_{\alpha_{l-1}\alpha_l} \psi_{\alpha_l \beta_{l+1}} B[s_{l+1}]_{\beta_{l+1},\beta_{l+2}} B[s_{l+2}]_{\beta_{l+2},\beta_{l+3}} \ldots B[s_L]_{\beta_L} \, | \, s_1 \ldots s_L \rangle$$



(It's a just little more complicated if we add the two sites in the center)

The AKLT State

$$H_{AKLT} = \sum_i S_i \cdot S_{i+1} + \frac{1}{3}\left(S_i \cdot S_{i+1}\right)^2 \quad \text{with} \quad S = 1$$

We replace the spins S=1 by a pair of spins S=1/2 that are completely symmetrized

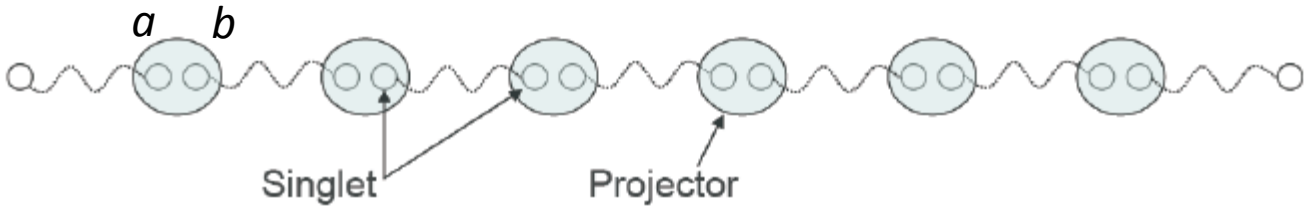
$$|+\rangle_i = |\uparrow\rangle_{ia}|\uparrow\rangle_{ib}$$

$$|0\rangle_i = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{ia}|\downarrow\rangle_{ib} + |\downarrow\rangle_{ia}|\uparrow\rangle_{ib}\right)$$

$$|-\rangle_i = |\downarrow\rangle_{ia}|\downarrow\rangle_{ib}$$

… and the spins on different sites are forming a singlet

$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{i,a}|\downarrow\rangle_{i+1,b} - |\downarrow\rangle_{i,a}|\uparrow\rangle_{i+1,b}\right)$$



The AKLT as a MPS

The singlet wave function with singlet on all bonds is

$$\left|\psi_{\Sigma}\right\rangle = \sum_{\{s\}}\sum_{a,b}\Sigma_{b_1,a_2}\Sigma_{b_2,a_3}...\Sigma_{b_L,a_1}\left|\{a,b\}\right\rangle \text{ with } \quad \Sigma_{ab} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

The local projection operators onto the physical S=1 states are

$$M^{+}_{ab} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}; M^{0}_{ab} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix}; M^{-}_{ab} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

The mapping on the spin S=1 chain then reads

$$\sum_{\{s\}}\sum_{a,b} M^{s_1}_{a_1,b_1} M^{s_2}_{a_2,b_2}...M^{s_L}_{a_L,b_L}\left|\{s\}\right\rangle\left\langle\{a,b\}\right|$$

Projecting the singlet wave-function we obtain

$$\left|\psi_{AKLT}\right\rangle = P\left|\psi_{\Sigma}\right\rangle = \sum_{\{s\}} M^{s_1}_{a_1,b_1}\Sigma_{b_1,a_2} M^{s_2}_{a_2,b_2}\Sigma_{b_2,a_3}...M^{s_L}_{a_L,b_L}\Sigma_{b_L,a_1}\left|\{s\}\right\rangle$$

$$\left|\psi_{AKLT}\right\rangle = \sum_{\{s\}} A^{s_1}_{a_1,a_2} A^{s_2}_{a_2,a_3}...A^{s_L}_{a_L,a_1}\left|\{s\}\right\rangle \text{ with } A^{s_l}_{a_l,a_{l+1}} = M^{s_l}_{a_l,b_l}\Sigma_{b_l,a_{l+1}}$$

Variational MPS

We can postulate a variational principle, starting from the assumption that the MPS is a good way to represent a state. Each matrix A has DxD elements and we can consider each of them as a variational parameter. Thus, we have to minimize the energy with respect to these coefficients, leading to the following optimization problem:

$$\min_{A_\alpha}\left[\langle\psi|H|\psi\rangle - \lambda\langle\psi|\psi\rangle\right]$$

DMRG does something very close to this…