[credit for course materials: Prof. Jan von Delft]

Matrix product operators; DMRG

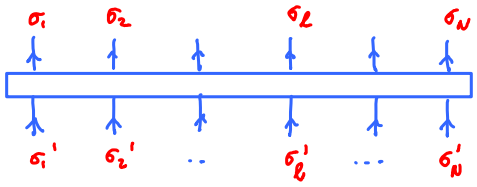
Matrix product operators

$$\hat{O} = |\bar{\sigma}'\rangle\, O^{\bar{\sigma}'}_{\bar{\sigma}} \langle\bar{\sigma}|$$

operator acts on N sites!

[Schollwock2011, Sec 5]

Consider an operator acting on N-site chain:



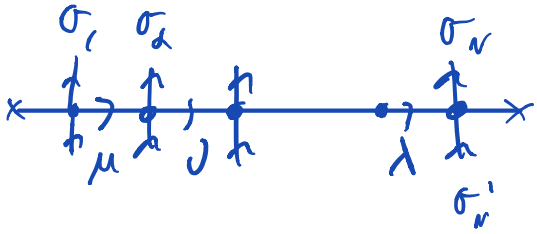
↳ original form but not useful

It can always be written as a

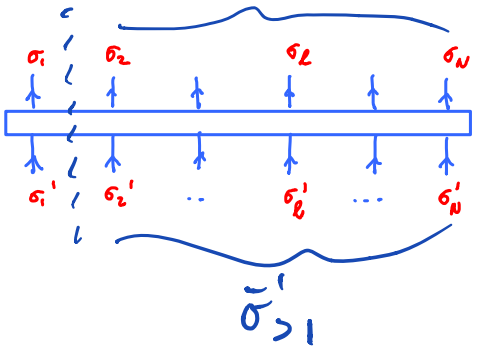
'matrix product operator' (MPO)

$$\hat{O} = |\bar{\sigma}'\rangle\, W^{1\sigma_1'}{}_{\mu\sigma_1} W^{\mu\sigma_2'}{}_{\nu\sigma_2} \cdots W^{\lambda\sigma_N'}{}_{\sigma_N 1} \langle\bar{\sigma}|$$

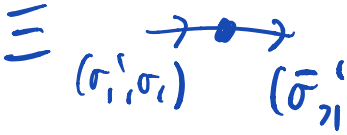
$$\equiv |\bar{\sigma}'\rangle \prod_l W^{\sigma_l'}{}_{\sigma_l} \langle\bar{\sigma}|$$



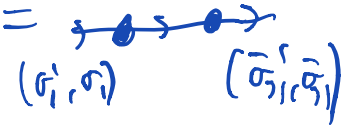
using a sequence of QR decompositions:



reshape as matrix w/ composite indices

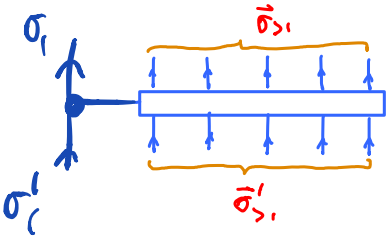


QR Q & R



reshape back

=



⇒ Iterate

tensor at site l

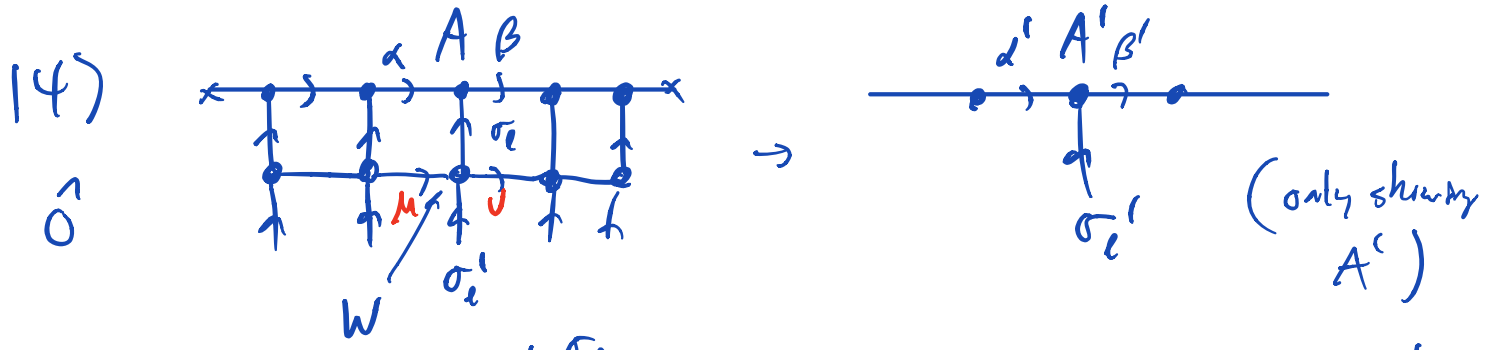
2N-2 less tensors

In general, this produces MPO with growing bond dimensions. $d^2, (d^2)^2, (d^2)^3, \ldots$

But for short-range Hamiltonians, bond dimension is typically small. $\Rightarrow O(1)$

1. Applying MPO to MPS yields MPS

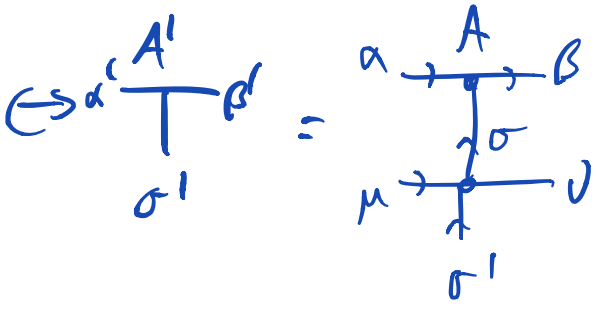
$|\psi'\rangle = \hat{O}|\psi\rangle$



$$|\psi\rangle = |\bar{\sigma}\rangle \prod_\ell A^{[\ell]\,\alpha_\ell \sigma_\ell}_{\alpha_{\ell+1}}$$

$$|\psi'\rangle = \hat{O}|\psi\rangle = |\bar{\sigma}'\rangle \prod_\ell A'^{[\ell]\,\alpha'_\ell \sigma'_\ell}_{\alpha'_{\ell+1}}$$

$$A'^{\alpha'\sigma'}_{\beta'} = W^{\mu\sigma'}_{\nu\sigma} A^{\alpha\sigma}_{\beta}$$

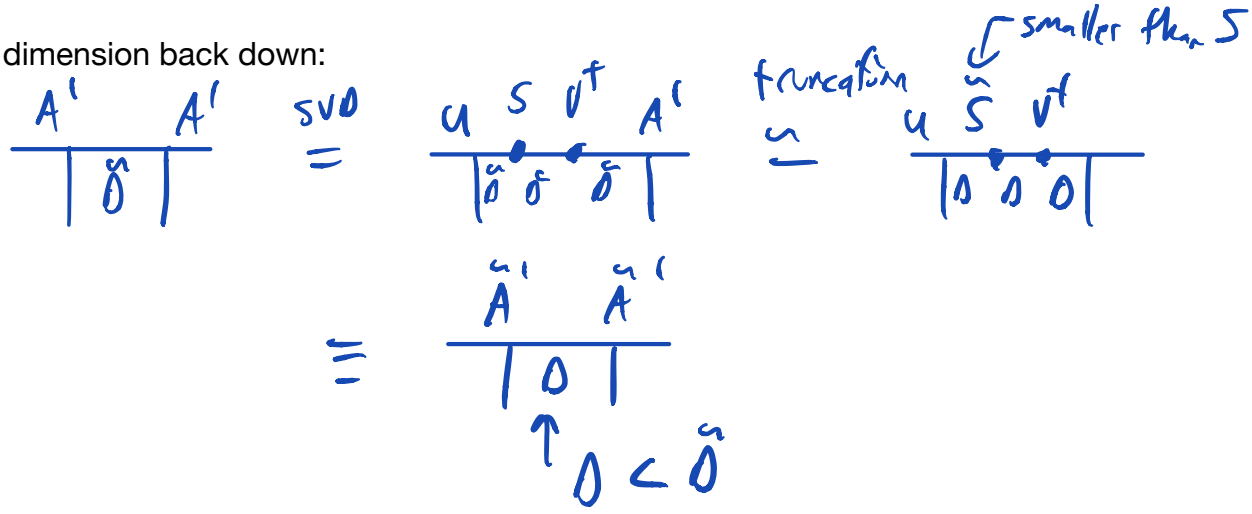


Note: 1. Dropped ℓ for conciseness

2. Convention for W indices CCW

with composite indices, $\alpha' = (\alpha, \mu)$, $\beta' = (\beta, \nu)$ of increased dimension: $D_{A'} = D_W \cdot D_A$

In practice, application of MPO is usually followed by SVD+truncation to bring bond dimension back down:



Addition of MPOs:

$$\hat{O} + \hat{\tilde{O}}$$

Let

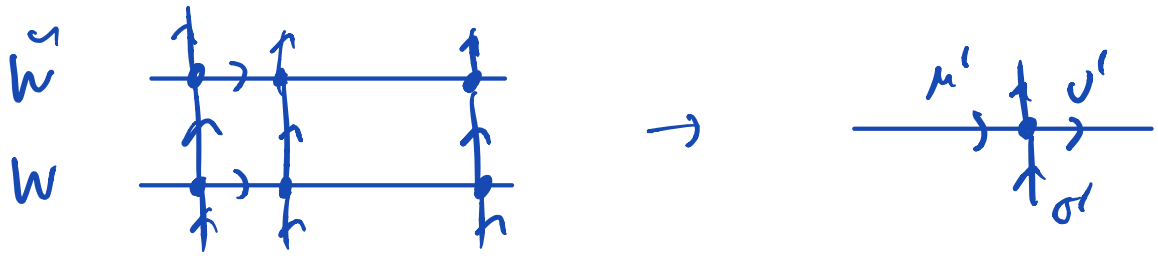
$$\hat{O} = |\bar{\sigma}'\rangle \prod_l W^{\sigma_l' \sigma_l} \langle\bar{\sigma}| \; ; \; \hat{\tilde{O}} = |\bar{\sigma}'\rangle \prod_l \tilde{W}^{\sigma_l' \sigma_l} \langle\bar{\sigma}|$$

$$\hat{O} + \hat{\tilde{O}} = |\bar{\sigma}'\rangle [W W \cdots W + \tilde{W} \tilde{W} \cdots \tilde{W}] \langle\bar{\sigma}|$$

$$= |\bar{\sigma}'\rangle \mathrm{Tr}\left[\begin{pmatrix} W & \tilde{W} \end{pmatrix} \begin{pmatrix} W & \tilde{W} \end{pmatrix} \cdots \begin{pmatrix} W & \tilde{W} \end{pmatrix} \right] \langle\bar{\sigma}|$$

= MPO in enlarged space

Multiplication of MPOs $W\hat{w} = \tilde{w}$



$$\tilde{w}^{\mu'\sigma'}_{\nu'\sigma} = W^{\mu\sigma'}_{\nu\bar{\sigma}}\, \hat{w}^{\mu\bar{\sigma}}_{\nu\sigma}$$

with composite indices, $\mu' = (\mu,\bar{\mu})$, $\nu' = (\nu,\bar{\nu})$ of increased dimension $D_{\tilde{w}} = D_W \cdot D_{\hat{w}}$

2. MPO representation of Heisenberg Hamiltonian

$$\hat{H} = \sum_{l=1}^{N-1}\left[J^z \hat{S}^z_l \hat{S}^z_{l+1} + \frac{1}{2}J\hat{S}^+_l \hat{S}^-_{l+1} + \frac{1}{2}J\hat{S}^-_l \hat{S}^+_{l+1}\right] - h\sum_{l=1}^{N} S^z_l$$

is shorthand for

$$= J^z \hat{S}^z_1 \otimes \hat{S}^z_2 \otimes I \cdots \otimes I$$
$$+ J^z I \otimes \hat{S}^z_1 \otimes \hat{S}^z_2 \otimes \cdots \otimes I + \cdots$$

Contains sum of one and two-site operators. How can we write it as an MPO?

Solution: introduce operator-valued <u>matrices</u> such that product reproduces above form!

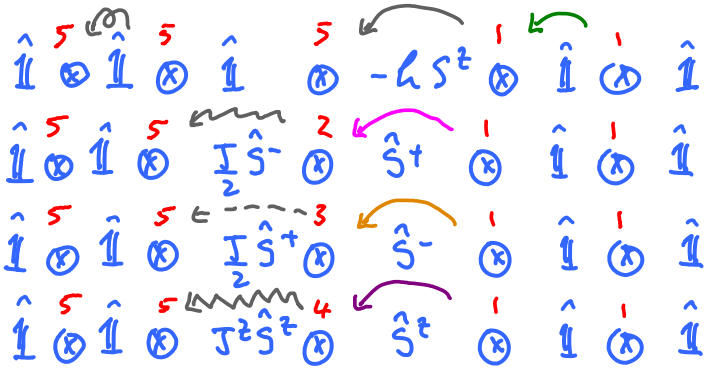
$$\hat{H} = |\bar{\sigma}'\rangle \prod_{\ell} W_{[\ell]}^{\sigma_\ell' \sigma_\ell} \langle\bar{\sigma}|$$

$$= \left(|\sigma_1'\rangle W_{[1]}^{\sigma_1' \sigma_1} \langle\sigma_1|\right) \otimes \left(|\sigma_2'\rangle W_{[2]}^{\sigma_2' \sigma_2} \langle\sigma_2|\right) \otimes \cdots \otimes \left(\quad\right)^{N}$$

$$= \hat{W}^{a}_{[1]} \otimes \hat{W}^{a}_{[2]} \otimes \cdots \otimes \hat{W}^{a}_{[N]} = \text{product of one site operators}$$

Each $\hat{W}^{a}_{[\ell]}$ acts only on site ℓ ; their tensor product gives the full MPO.

Viewed from a bond, the string of operators in each term of can be in one of states.



state 1: only $\hat{I}$ to the right

state 2: only $\hat{S}^+$ just to the right

state 3: one $\hat{S}^-$ just to the right

state 4: one $\hat{S}^z$ just to the right

state 5: one $-h\hat{S}^z$ or completed interaction somewhere to the right

Build matrix with element ij implements transition from 'state' j to i.

$$\hat{w}_{[\ell]} = \begin{pmatrix} \mathbb{1} & 0 & & & \\ \hat{S}^+ & 0 & & & \\ \hat{S}^- & 0 & & & \\ \hat{S}^z & 0 & 0 & 0 & 0 \\ -h\hat{S}^z & \frac{J}{2}\hat{S}^- & \frac{J}{2}\hat{S}^+ & J^z\hat{S}^z & \hat{\mathbb{1}} \end{pmatrix}$$

On site N: $\hat{w}_{[N]} = \begin{pmatrix} \hat{\mathbb{1}} \\ \hat{S}^+ \\ \hat{S}^- \\ \hat{S}^z \\ -hS_z \end{pmatrix}$

and also column 1 of $\hat{w}_{[\ell]}$

One site 1 (= row 1 of $\hat{w}_{[\ell]}$): $\hat{w}^{[1]} = \left[-hS^z, \frac{J}{2}\hat{S}^-, \frac{J}{2}\hat{S}^+, J^zS^z, \mathbb{1}\right]$

$$W_{[\ell]} = \begin{pmatrix} I & 0 & 0 & 0 & 0 \\ S^+ & 0 & 0 & 0 & 0 \\ S^- & 0 & 0 & 0 & 0 \\ S^z & 0 & 0 & 0 & 0 \\ -hS_z & \frac{J}{2}S^- & \frac{J}{2}S^+ & J^zS^z & I \end{pmatrix}$$

N site: $\hat{w}_{[N]} = \begin{pmatrix} I \\ S^+ \\ S^- \\ S^z \\ -hS^z \end{pmatrix}$ → all unique operators

First site: $\hat{w}_{[1]} = \left[-hS^z, \frac{J}{2}S^-, \frac{J}{2}S^+, J^zS^z, I\right]$

Check: multiplying out a product of such $\hat{W}$'s yields desired result:

$$\hat{W}_{[1]}\hat{W}_{[2]}\hat{W}_{[3]}\hat{W}_{[4]} = \hat{W}_{[1]}\hat{W}_{[2]}\begin{bmatrix} \hat{\mathbb{1}} & 0 \\ \hat{S}^+ & 0 \\ \hat{S}^- & 0 \\ \hat{S}^z & 0 \\ -h\hat{S}^z & \frac{J}{2}\hat{S}^- \quad \frac{J}{2}\hat{S}^+ \quad J^z\hat{S}^z \quad \hat{\mathbb{1}} \end{bmatrix}\begin{bmatrix} \hat{\mathbb{1}} \\ \hat{S}^+ \\ \hat{S}^- \\ \hat{S}^z \\ -hS_z \end{bmatrix}$$

$$= \hat{W}_{[1]}\begin{bmatrix} \hat{\mathbb{1}} & 0 \\ \hat{S}^+ & 0 \\ \hat{S}^- & 0 \\ \hat{S}^z & 0 \\ -h\hat{S}^z & \frac{J}{2}\hat{S}^- \quad \frac{J}{2}\hat{S}^+ \quad J^z\hat{S}^z \quad \hat{\mathbb{1}} \end{bmatrix}\begin{bmatrix} \hat{\mathbb{1}}\otimes\hat{\mathbb{1}} \\ \hat{S}^+\otimes\hat{\mathbb{1}} \\ \hat{S}^-\otimes\hat{\mathbb{1}} \\ \hat{S}^z\otimes\hat{\mathbb{1}} \\ -h\hat{S}^z\otimes\hat{\mathbb{1}} + \frac{J}{2}\hat{S}^-\otimes\hat{S}^+ + \frac{J}{2}\hat{S}^+\otimes\hat{S}^- + J^z\hat{S}^z\otimes\hat{S}^z + \hat{\mathbb{1}}\otimes(-h\hat{S}^z) \end{bmatrix}$$

$$= \begin{bmatrix} -hS^z, & \frac{J}{2}\hat{S}^-, & \frac{J}{2}\hat{S}^+, & J^z\hat{S}^z, & 1 \end{bmatrix}\begin{bmatrix} \mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1} \\ \hat{S}^+\otimes\mathbb{1}\otimes\mathbb{1} \\ \hat{S}^-\otimes\mathbb{1}\otimes\mathbb{1} \\ \hat{S}^z\otimes\mathbb{1}\otimes\mathbb{1} \\ (-h\hat{S}^z\otimes\mathbb{1}\otimes\mathbb{1} + \frac{J}{2}\hat{S}^-\otimes\hat{S}^+\otimes\mathbb{1} + \frac{J}{2}\hat{S}^+\otimes\hat{S}^-\otimes\mathbb{1} + J^z\hat{S}^z\otimes\hat{S}^z\otimes\mathbb{1} \\ + \mathbb{1}\otimes(-h\hat{S}^z)\otimes\mathbb{1} + \mathbb{1}\otimes\frac{J}{2}\hat{S}^-\otimes\hat{S}^+ + \mathbb{1}\otimes\frac{J}{2}\hat{S}^+\otimes\hat{S}^- + \mathbb{1}\otimes J^z\hat{S}^z\otimes\hat{S}^z \\ + \mathbb{1}\otimes\mathbb{1}\otimes(-h\hat{S}^z)) \end{bmatrix}$$

$$= -hS^z\otimes\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1} + \frac{J}{2}\hat{S}^-\otimes\hat{S}^+\otimes\mathbb{1}\otimes\mathbb{1} + \frac{J}{2}\hat{S}^+\otimes\hat{S}^-\otimes\mathbb{1}\otimes\mathbb{1} + J^zS^z\otimes S^z\otimes\mathbb{1}\otimes\mathbb{1}$$

$$+ \mathbb{1}\otimes(-h\hat{S}^z)\otimes\mathbb{1}\otimes\mathbb{1} + \mathbb{1}\otimes\frac{J}{2}\hat{S}^-\otimes\hat{S}^+\otimes\mathbb{1} + \mathbb{1}\otimes\frac{J}{2}\hat{S}^+\otimes\hat{S}^-\otimes\mathbb{1} + \mathbb{1}\otimes J^z\hat{S}^z\otimes\hat{S}^z\otimes\mathbb{1}$$

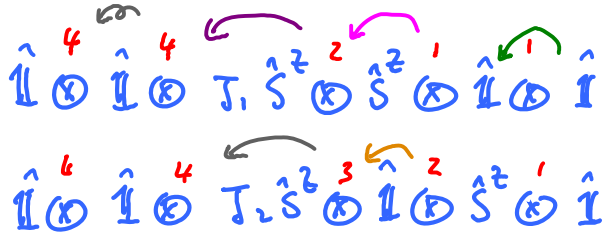
$$+ \mathbb{1}\otimes\mathbb{1}\otimes(-h\hat{S}^z)\otimes\mathbb{1} + \mathbb{1}\otimes\mathbb{1}\otimes\frac{J}{2}\hat{S}^-\otimes\hat{S}^+ + \mathbb{1}\otimes\mathbb{1}\otimes\frac{J}{2}\hat{S}^+\otimes\hat{S}^- + \mathbb{1}\otimes\mathbb{1}\otimes J^z\hat{S}^z\otimes\hat{S}^z$$

$$+ \mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1}\otimes(-h\hat{S}^z)$$

= full Hamiltonian for 4 sites! ✓

Longer-ranged interactions :

$$\hat{H} = J_1 \sum_i \hat{S}_i^z \hat{S}_{i+1}^z + J_2 \sum_i \hat{S}_i^z \hat{S}_{i+2}^z$$



state 1: only $\hat{\mathbb{1}}$ to the right

state 2: only $\hat{S}^z$ just to the right

state 3: one $J_1 \hat{S}^z$ or $J_2 \hat{S}^z$ just to the right

state 4: completed interaction somewhere to the right

$$\hat{W}_{[\ell]} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} \hat{\mathbb{1}} & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 \\ 0 & \hat{\mathbb{1}} & 0 & 0 \\ 0 & J_1 \hat{S}^z & J_2 \hat{S}^z & \hat{\mathbb{1}} \end{pmatrix} \end{array}$$

$$\hat{W}_{[N]} = \begin{pmatrix} \hat{\mathbb{1}} \\ \hat{S}^z \\ 0 \\ 0 \end{pmatrix} = \text{column } 1 \text{ of } \hat{W}_{[\ell]}$$

$$\hat{W}_{[1]} = (0, J_1 \hat{S}^z, J_2 \hat{S}^z, \hat{\mathbb{1}}) = \text{row } 4 \text{ of } \hat{W}_{[\ell]}$$

Check:

$$\hat{W}^{[1]} \hat{W}^{[2]} W^{[3]} = \hat{W}^{(1)} \begin{pmatrix} \hat{\mathbb{1}} & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 \\ 0 & \hat{\mathbb{1}} & 0 & 0 \\ 0 & J_1 \hat{S}^z & J_2 \hat{S}^z & \hat{\mathbb{1}} \end{pmatrix} \begin{pmatrix} \hat{\mathbb{1}} \\ \hat{S}^z \\ 0 \\ 0 \end{pmatrix}$$

$$= (0, J_1 \hat{S}^z, J_2 \hat{S}^z, \hat{\mathbb{1}}) \begin{pmatrix} \hat{\mathbb{1}} \otimes \hat{\mathbb{1}} \\ \hat{S}_2 \otimes \hat{\mathbb{1}} \\ \hat{\mathbb{1}} \otimes \hat{S}^z \\ 0 + J_1 \hat{S}^z \otimes \hat{S}^z + 0 + 0 \end{pmatrix}$$

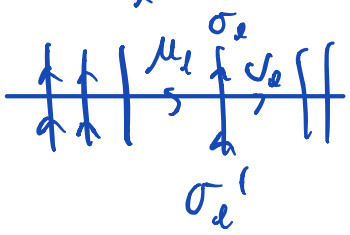
$$= J_1 \hat{S}^z \otimes \hat{S}^z \otimes \hat{\mathbb{1}} + J_2 \hat{S}^z \otimes \hat{\mathbb{1}} \otimes \hat{S}^z + \hat{\mathbb{1}} \otimes J_1 \hat{S}_2 \otimes \hat{S}_2 \quad \checkmark$$

3. Applying MPO to mixed-canonical state

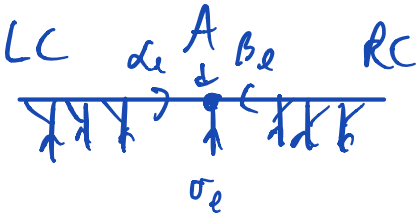
[Schollwock2011, Sec 6.2]

How does an MPO act on an MPS in mixed-canonical representation wrt site ℓ ?

Consider $\hat{O} = |\tilde{\sigma}'\rangle \prod_\ell W_{[\ell]}^{\sigma_\ell' \sigma_\ell} \langle\tilde{\sigma}|$



$$|\psi\rangle = |\alpha_\ell\rangle|\sigma_\ell\rangle|\beta_\ell\rangle A^{\alpha_\ell \sigma_\ell \beta_\ell} \equiv |a\rangle A^a$$

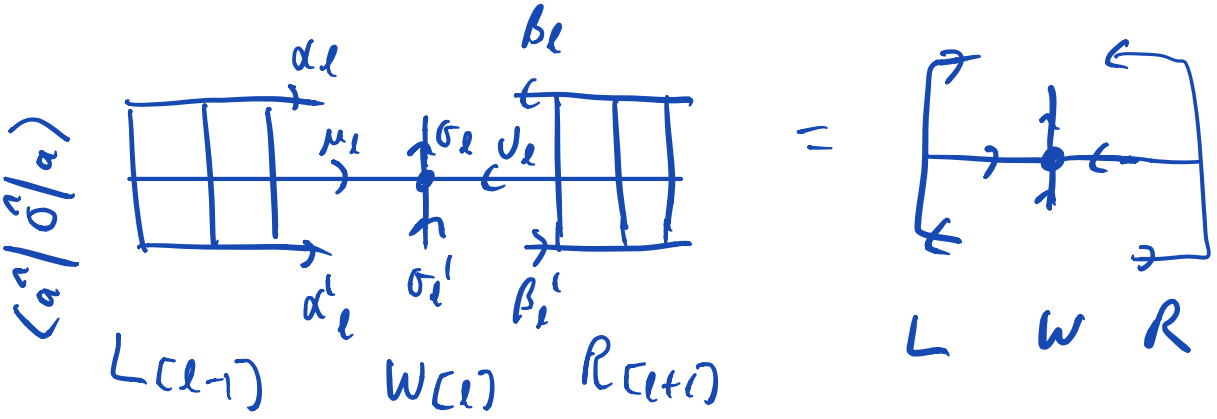


Here $\{|a\rangle\}$ form a basis for the mixed-canonical representation. Express operator in this basis: $\hat{O} = |a'\rangle O^{a'}_{\ a} \langle a|$, matrix elements $O^{a'}_{\ a} = \langle a'|\hat{O}|a\rangle$

$$|\psi'\rangle = \hat{O}|\psi\rangle = |a'\rangle A'^{a} = |a'\rangle O^{a'}_{\ a} A^a$$

then

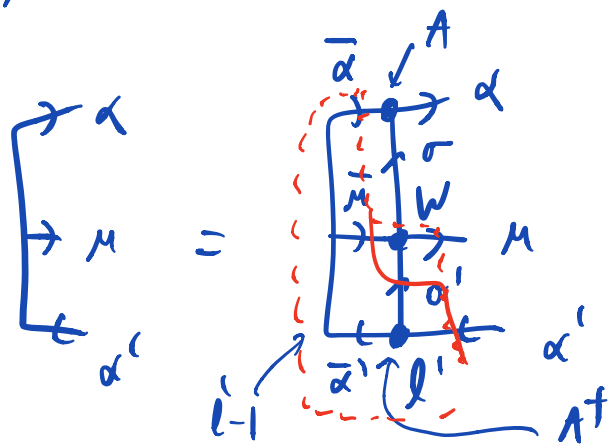
$O^{a'}_{\ a} = \langle a'|\hat{O}|a\rangle$



L can be computed iteratively, for $\ell' \le \ell - 1$

(Similarly for R, for $\ell' \ge \ell + 1$)

$$L^{\alpha'}_{[\ell'],\mu\alpha} = A^{\dagger}_{[\ell'],\sigma'\bar{\alpha}'} L^{\bar{\alpha}'}_{[\ell'-1],\bar{\mu}\bar{\alpha}} A^{\bar{\alpha}\sigma}_{[\ell']} W^{\bar{\mu}\sigma'}_{[\ell'],\mu\sigma}$$

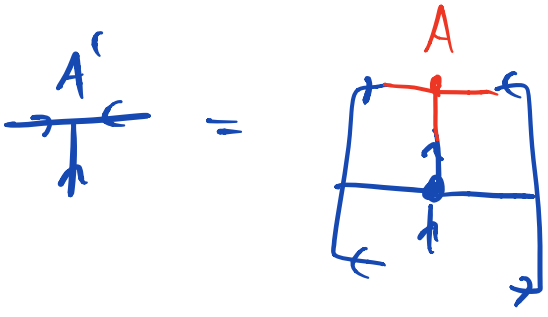


For efficient computation, perform sums in this order:

1. Sum over $\bar{\alpha}', \sigma'$ for fixed $\alpha', \bar{\alpha}, \bar{\mu}$ at cost $(D_d) \cdot (D' \cdot D_w)$
2. Sum over $\bar{\mu}, \sigma$ for fixed $\alpha', \bar{\alpha}, \mu$ at cost $(D_w \cdot d) \cdot (D' \cdot D_w)$
3. Sum over $\bar{\alpha}$ for fixed α', α, μ at cost $D \cdot (D' D_w)$

The application of MPO to MPS is then represented as:

$$A'^{a'} = O^{a'}_{\ a} A^{a}$$



DMRG I: Ground state search

- The density matrix renormalization group (DMRG) was invented by Steve White (student of Ken Wilson) to solve general quantum chain models. [White1992, 1993]
- First realization of connection between MPS and DMRG in limit : Ostlund & Rommer [Ostlund 1995]
- Realization that finite-size DMRG leads to MPS: Dukelski, Martin-Delgado, Nishino, Sierra [Dukelski1998]
- Modern formulation: Vidal [Vidal2003, 2004], Cirac and Verstraete [Verstraete2004]
- Time evolution: Daley, Kollath, Schollwock, Vidal [Daley2004], White, Feiguin [White2004]

1. Iterative ground state search

View space of all MPS of given bond dimension, D , as variational space.

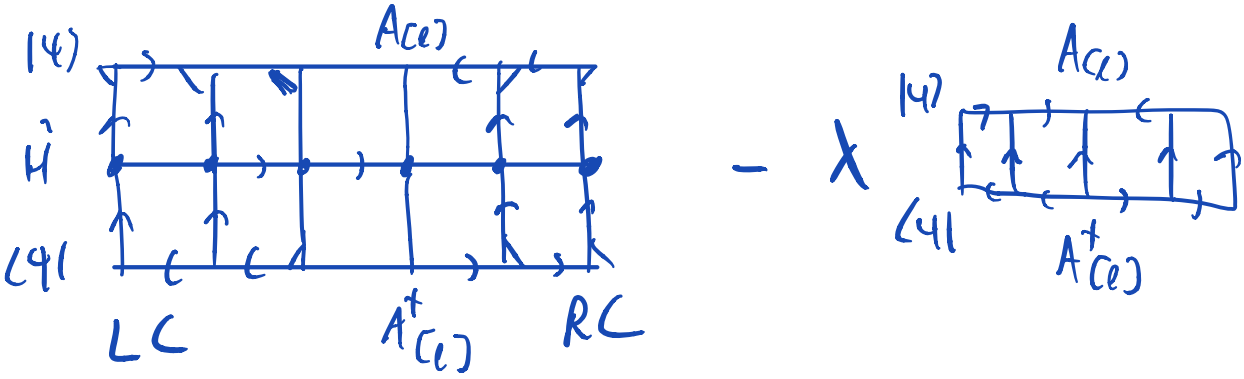
Minimize $\langle\psi|\hat{H}|\psi\rangle$ in this space, subject to constraint of unit normalization,

$$\Rightarrow \quad \langle\psi|\psi\rangle = 1$$

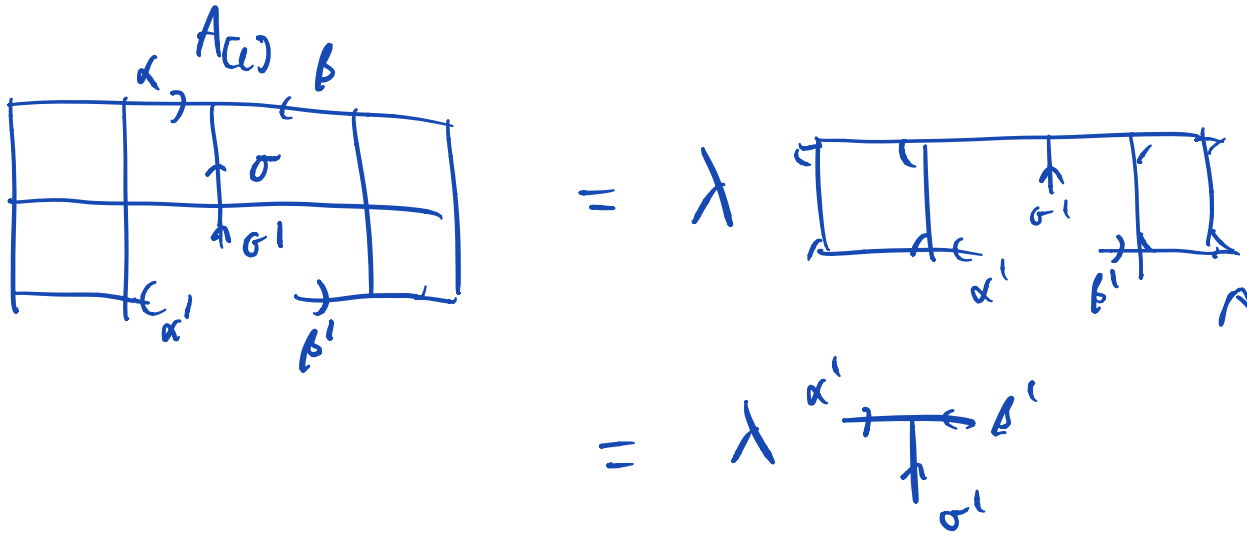
Hence extremize: $\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle$

λ Lagrange multiplier

Graphical representation, assuming mixed-canonical form wrt to site :



Do this one A tensor at a time: $\frac{\partial}{\partial A^{\dagger}_{[l]}}\left[\langle\psi|H|\psi\rangle - \lambda\langle\psi|\psi\rangle\right] = 0$



In index notation:

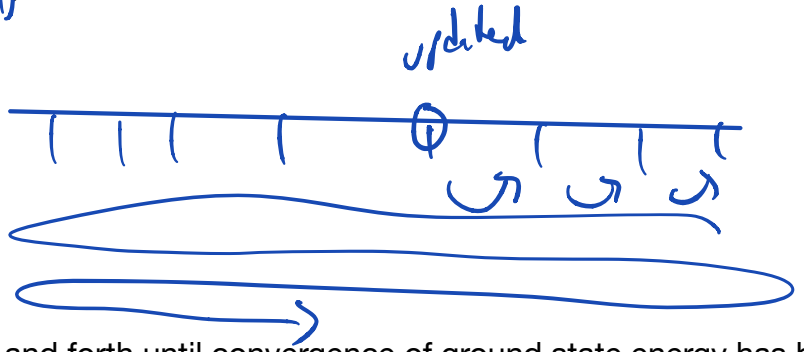
$$H^{a'}_{\ a}\, A^{a}_{[l]} = \lambda A^{a'}_{[l]} \quad \text{with} \quad a' = (\alpha', \sigma', \beta')$$

This is an eigenvalue equation for $A_{[l]}$ can can be solved with standard linear algebra tools such as a Lanczos algorithm.

Note: if $|\psi\rangle$ is not represented in mixed-canonical form, one obtains a generalized eigenvalue equation of the form $HA = NA$ with N defined above.

Use that 'eigenvector' $A_{[s]}$ yielding lowest eigenvalue (=current estimate of ground state energy) to 'update' MPS, then move to next site, switch to mixed-canonical form on site $l+1$,

optimize $A_{[s+1]}$, etc.



'Sweep' back and forth until convergence of ground state energy has been achieved.

This works remarkably well for 1D chains with short-ranged interactions.

ground states of

Due to area law, entanglement entropy grows at most as $\ln L$. ⇒ Bond dimension required grows at most polynomially in L.

2. Lanczos method

[Lanczos1950, Ojalvo1970, Paige1972, Koch2011]

- Fast way of finding extremal eigenvalues of a Hermitian NxN matrix, H.
- Prerequisite: an algorithm for computing $H|\psi\rangle$, for any vector $|\psi\rangle$.

We seek the extremal value of $$E[|\psi\rangle] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

Denote extremal value by $$E_g = \min E[|\psi\rangle] \equiv E[|\psi_g\rangle]$$

The direction of steepest ascent of the functional $E[|\psi\rangle]$ evaluated at $|\psi\rangle$ is given by

'functional gradient': $$\frac{\delta E[|\psi\rangle]}{\delta\langle\psi|} \equiv \frac{H|\psi\rangle}{\langle\psi|\psi\rangle} - \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle^2}|\psi\rangle$$

$$= \frac{H - E[|\psi\rangle]}{\langle\psi|\psi\rangle}|\psi\rangle$$

$$\equiv |\psi_a\rangle$$

Moving in opposite direction will thus lower the energy:

$$E[|\psi\rangle - \alpha|\psi_a\rangle] < E[|\psi\rangle] \text{ for "small" } \alpha > 0.$$

To find optimal value for α, minimize $E[|\psi\rangle - \alpha|\psi_a\rangle]$ wrt to 'variational parameter' α,

in the space $K_1 \equiv \text{span}\{|\psi\rangle, |\psi_a\rangle\} = \text{span}\{|\psi\rangle, H|\psi\rangle\}$

Construct a normalized basis for this space (for a random initial state $|\psi\rangle$):

First basis vector: $$|v_0\rangle = \frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}}$$

Second basis vector: $$b_1|v_1\rangle \equiv |\tilde{v}_1\rangle = H|v_0\rangle - |v_0\rangle\underbrace{\langle v_0|H|v_0\rangle}_{a_0}$$

b_1: normalization factor so that $\langle v_1|v_1\rangle = 1$

orthogonalize wrt $|v_0\rangle$

Now find a matrix representation of H in this space. Define:

$a_0 \equiv \langle v_0|H|v_0\rangle \quad a_1 \equiv \langle v_1|H|v_1\rangle$

$b_1^* \equiv \langle\tilde{v}_1|\tilde{v}_1\rangle$

$b_1 = \sqrt{\langle\tilde{v}_1|\tilde{v}_1\rangle}$

$= \langle v_1|H|v_0\rangle$

Apply $\langle v_1|$ to

then $$H|v_0\rangle = |v_1\rangle b_1 + |v_0\rangle a_0$$

rearrange

Hence in the space K_1, the Hamiltonian has the matrix representation:

$$H_{K_1} = \begin{bmatrix} \langle v_0|H|v_0\rangle & \langle v_0|H|v_1\rangle \\ \langle v_1|H|v_0\rangle & \langle v_1|H|v_1\rangle \end{bmatrix} = \begin{pmatrix} a_0 & b_1^* \\ b_1 & a_1 \end{pmatrix}$$

The ground state of H_{K_1}, say $|g\rangle_{K_1}$, yields the optimal choice for α.

Now we could iterate: use $|g\rangle_{K_1}$ as starting point for another optimization step. Convergence is rapid. Monitor quality of result by computing the residual energy variance,

$$r(|\psi\rangle) \equiv \| (H-\epsilon)|\psi\rangle \|^2$$
$$= \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2$$

and stop when it drops below some threshold.

Krylov space

After L steps, starting from $|v_0\rangle$, the resulting vector will live in

$$K_L(|v_0\rangle) = \text{span}\{|v_0\rangle, H|v_0\rangle, H^2|v_0\rangle, \ldots, H^L|v_0\rangle\}$$

='Krylov space of H over $|v_0\rangle$' (dimension $L+1$).

Instead of repeatedly minimizing in 2x2 subspaces, we could first construct K_L, then compute its ground state. (This way is faster, since it amounts to using L simultaneous variational parameters instead of L separate ones). To do this, iteratively construct a 'Krylov basis' for K_L:

Krylov basis

As before: $b_1|v_1\rangle \equiv |\tilde{v}_1\rangle = H|v_0\rangle - a_0|v_0\rangle$

Third vector: $b_2|v_2\rangle \equiv |\tilde{v}_2\rangle \equiv H|v_1\rangle - \sum_{j=0}^{1} |v_j\rangle\langle v_j|H|v_1\rangle$

$= H|v_1\rangle - |v_1\rangle a_1 - |v_0\rangle b_1^*$

where $b_2 = \sqrt{\langle\tilde{v}_2|\tilde{v}_2\rangle} = \langle v_2|H|v_1\rangle$

Note: $\langle v_2|H|v_0\rangle = 0$, since $H|v_1\rangle \in \text{span}\{|v_2\rangle, |v_1\rangle\}$

Fourth vector: $b_3|v_3\rangle \equiv |\tilde{v}_3\rangle \equiv H|v_2\rangle - \sum_{j=0}^{2} |v_j\rangle\langle v_j|H|v_2\rangle$

$= H|v_2\rangle - |v_2\rangle a_2 - |v_1\rangle b_2^* - |v_0\rangle \cdot 0$

Thus we obtain a two-term iteration scheme: we only need to store 3 vectors at a time!

nth step: $b_{n+1}|v_{n+1}\rangle \equiv |\tilde{v}_{n+1}\rangle = H|v_n\rangle - \sum_{j=0}^{n} |v_j\rangle\langle v_j|H|v_n\rangle$

$= H|v_n\rangle - |v_n\rangle a_n - |v_{n-1}\rangle b_n^*$

with $a_n = \langle v_n|H|v_n\rangle$, $b_n = \langle v_n|H|v_{n-1}\rangle$

[If it happens that $b_{n+1}=0$, pick an arbitrary $|v_{n+1}\rangle$ orthonormal to all $|v_j\rangle$]. $(j=0,\dots,n)$

Throughout we have $\langle v_{n+1}|H|v_j\rangle = 0$ for $j=0,\dots,n-1$

since $H|v_j\rangle \in \text{span}\{|v_{j+1}\rangle, |v_j\rangle, |v_{j-1}\rangle\}$

Hence, rearranging: $H|v_n\rangle = |v_{n-1}\rangle b_n^* + |v_n\rangle a_n + |v_{n+1}\rangle b_{n+1}$

So in $\mathcal{K}_L$, H has tridiagonal form:

$$H_{\mathcal{K}_L} = \begin{pmatrix} a_0 & b_1^* & & & \\ b_1 & a_1 & b_2^* & & \\ & b_1 & \ddots & \ddots & \\ & & \ddots & \ddots & b_L^* \\ & & & b_L & a_n \end{pmatrix}$$

Ground state of $H_{\mathcal{K}_L}$ satisfies the eigenvalue equation

$$(H_{\mathcal{K}_L})^i_j \, (\psi_g^L)^j = E_g^L \, (\psi_g^L)^i$$

Thus

$$E_g^L \quad \text{and} \quad |\psi_g^L\rangle = \sum_{j=0}^{L} |v_j\rangle \, (\psi_g^L)^j$$

are the best approximations, within the Krylov space $\mathcal{K}_L$, of the true ground state energy and ground state.

Note: $|\psi_g^{(c)}\rangle$ can be constructed 'on the fly', one term at a time, by restarting Lanczos iteration from $|v_0\rangle$.

The Lanczos scheme converges exponentially fast, with a rate constant ~ [gap to first excited state]$^{1/2}$.

Summary

1. Start with arbitrary $|v_0\rangle$
2. First iteration step
   i. $|\tilde{v}_1\rangle = H|v_0\rangle$
   ii. $a_0 = \langle \tilde{v}_1 | v_0 \rangle$
   iii. $|v_1\rangle = |\tilde{v}_1\rangle - a_0|v_0\rangle$ ← orthogonal
3. General iteration step for $n \geq 1$:
   i. $b_n = \langle \tilde{v}_n | \tilde{v}_n \rangle$
   ii. If $b_n \neq 0$, $|v_n\rangle = |\tilde{v}_n\rangle / b_n$ ← normalization
   else, pick $|v_n\rangle$ as orthogonal to $|v_0\rangle \ldots |v_n\rangle$
   iii. $|\tilde{v}_{n+1}\rangle = H|v_n\rangle$
   iv. $a_n = \langle \tilde{v}_{n+1} | v_n \rangle$
   v. $|\tilde{v}_{n+1}\rangle = |\tilde{v}_{n+1}\rangle - |v_n\rangle a_n - |v_{n-1}\rangle b_n^*$

and repeat 3 until convergence.

There are other ways of organizing this iteration loop, but this one is most numerically stable [Paige1972]

3. DMRG for excited states

Suppose we have an MPS representation for ground state,

$$|g\rangle = (\bar{\sigma}) \prod_\ell A^{g\sigma_\ell}_{[\ell]}$$

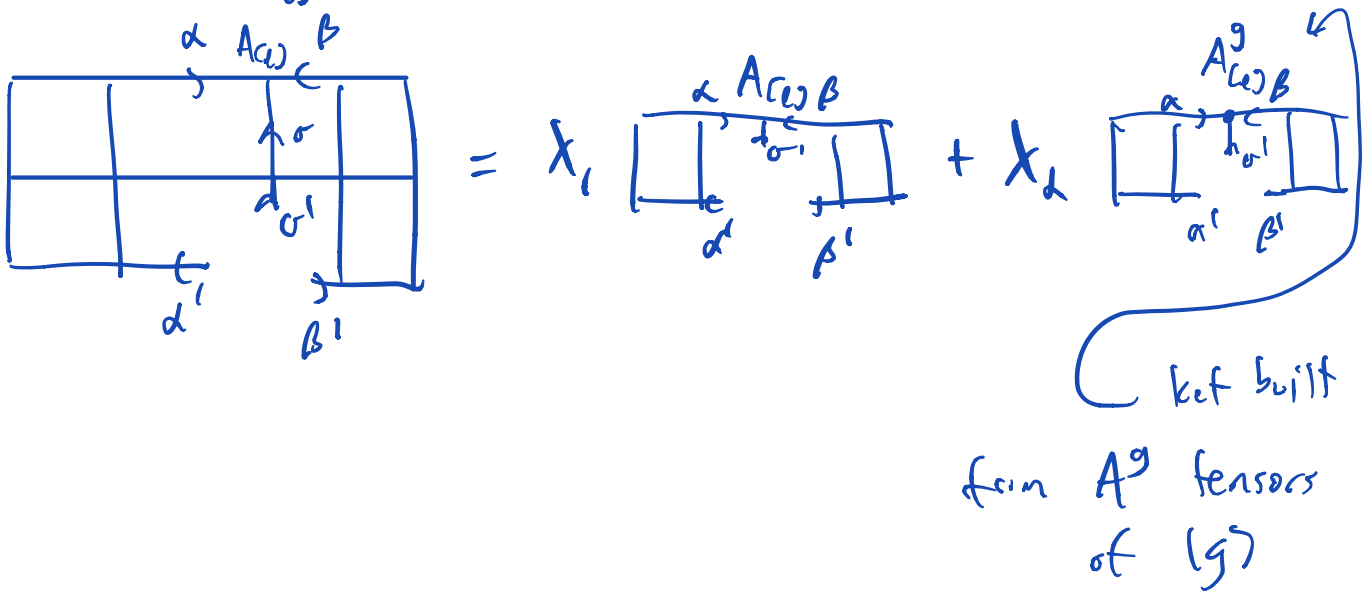
ground state

found by DMRG. Excited states can be constructed by repeating a DMRG sweep in space orthogonal to $|g\rangle$.

Extremize: $\langle\psi|H|\psi\rangle - \lambda_1\langle\psi|\psi\rangle - \lambda_2\langle\psi|g\rangle$

Lagrange multipliers enforce $\langle\psi|\psi\rangle = 1$, $\langle\psi|g\rangle = 0$.

Extremization wrt $A^\dagger_{[\ell]}$ yields:



All other tensors are A tensors for desired excited state.

Generic structure of this equation, in mixed-canonical representation of site ℓ

$$H^{a'}_{\ a}\, A^{a}_{[\ell]} = \lambda_1 A^{a'} + \lambda_2 g^{a'}$$

with $a' = (\alpha', \sigma', \beta')$, $A^{\dagger}_{a} A^{a} = I$, $A^{\dagger}_{a} g^{a} = 0$

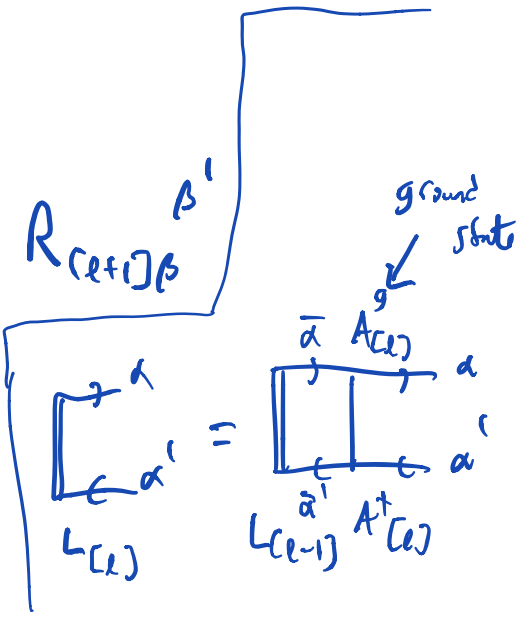
$$A^{g\dagger}_{a} A^{ga} = I$$

[left-norm.]

$$g^{a'} \equiv g^{\alpha'\sigma'\beta'} = L^{\alpha'}_{[\ell-1]\alpha}\, A^{g\,\sigma'}_{[\ell]}\, R_{[\ell+1]\beta'}$$

w/ L+R computed iteratively:

$$L^{\alpha'}_{[\ell]\alpha} = A^{\dagger\,\alpha'}_{[\ell]\,\sigma\bar{\alpha}'}\, L^{\bar{\alpha}'}_{[\ell-1]\bar{\alpha}}\, A^{g\,\bar{\sigma}}_{[\ell]\,\alpha}$$



Index-free notation:

$$H|A\rangle = \lambda_1 |A\rangle + \lambda_2 |g\rangle \quad , \quad \langle A|g\rangle = 0$$

Define projector onto subspace orthogonal to $|g\rangle$: $P_g = I - |g\rangle\langle g|$

[with indices: $P_{g\ a}^{\ a'} = I^{a'}_{\ a} - g^{a'} g^{\dagger}_{a}$ $\quad \left[P_{g\ a}^{\ a'} g^{a} = 0 \right]$

Project eigenvalue equation into this subspace:

$$P_g H \left(\underbrace{P_g}_{I} + \underbrace{|g\rangle\langle g|}_{=0} \right) |A\rangle = \lambda_1 P_g |A\rangle + 0$$

$$P_g H P_g |A\rangle = \lambda_1 P_g |A\rangle$$

This is simply an eigenvalue problem, for $P_g H$, in subspace orthogonal to $|g\rangle$. It can be solved using straightforward generalization of Lanczos scheme, using Krylov subspace orthogonal to $|g\rangle$.

Given an arbitrary initial state $|v_0\rangle$, project it onto orthogonal subspace, $|v_0'\rangle = P_g |v_0\rangle$ and construct new Krylov vectors using

$$|\tilde{v}_{n+1}\rangle = P_g H |v_{n+1}\rangle - |v_n\rangle a_n - |v_{n-1}\rangle b_n^*$$

Why not simply use excited states in K_L ? Because numerical noise can cause the $|v_n\rangle$ to be not exactly orthogonal, hence for $j < n-2$, $\langle v_n | v_j \rangle \sim 10^{-16}$ rather than 0.

This leads to spurious multiple copies of eigenstates ('ghost states'). For the ground state, the variational principle ensures that the loss of orthogonality does not become a severe problem. But for excited states, it does. To prevent this, explicit reorthogonalization is needed at every step, using P_g , as above.

Block-Lanczos for excited states

Standard Lanczos: represent action of H as

$$H|v_1\rangle = |v_1\rangle a_1 + |v_2\rangle b_1 \Rightarrow$$

$$\begin{pmatrix} a_1 & b_1^\dagger & & \\ b_1 & a_1 & b_2^\dagger & \\ & b_2 & \ddots & \ddots \\ & & \ddots & \end{pmatrix}$$

Block-Lanczos: start with set of M orthogonal vectors,

$|v_{0,i}\rangle$, $i = 1 \ldots M$, and represent action of H as

$$H|v_{0,i}\rangle = |v_{0,j}\rangle \underbrace{\delta^j{}_i}_{\text{orthogonal}} (a_1)^i{}_j + |v_{1,j}\rangle (b_1)^j{}_i$$

with $\langle v_{0,j}|v_{1,i}\rangle = 0$, $\langle v_{1,j}|v_{1,i}\rangle = \delta^j{}_i$

$(a_1)^i{}_j = \langle v_{0,i}|H|v_{0,j}\rangle$, $(b_1)^j{}_i = \langle v_{1,j}|H|v_{0,i}\rangle$

etc. Then the lowest M eigenstates of block-tridiagonal matrix

gives the Lanczos approximation for lowest M eigenstates of H

$M \times M$ matrix

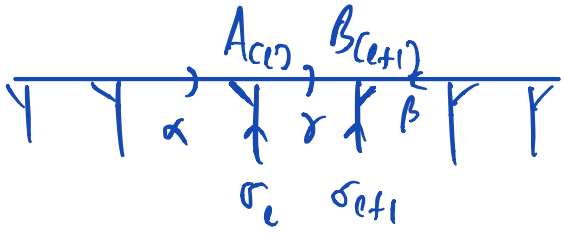
$$\begin{bmatrix} [a_0] & [b_1^\dagger] & & \\ [b_1] & [a_1] & [b_2^\dagger] & \\ & [b_2] & \ddots & \ddots \\ & & \ddots & \end{bmatrix}$$

4. Two-site update

If one encodes symmetries, then 'one-site update' as discussed above can get stuck: if one starts in the wrong symmetry sector, one stays there, because one-site update offers no way of enlarging the Hilbert space during the variational search to explore other symmetry sectors. Cure: 'two-site' update, which variational optimizes two A-tensors at a time.

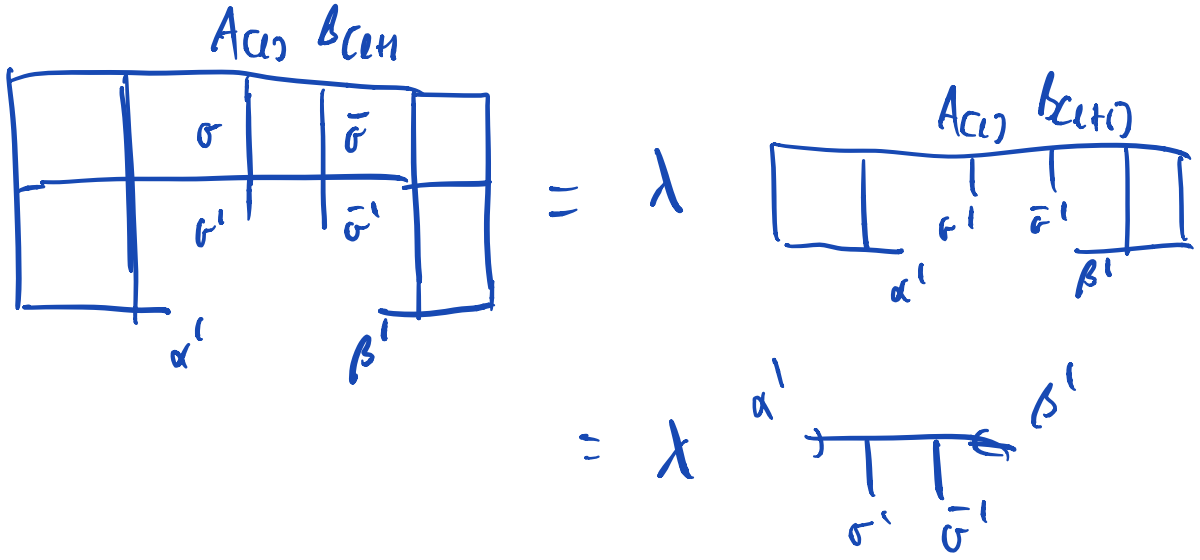
Represent MPS in mixed-canonical two-site basis:

$$|\psi\rangle = |\beta\rangle|\sigma_{\ell+1}\rangle|\sigma_\ell\rangle|\alpha\rangle \times A^{\alpha\sigma_\ell}_{[\ell]\gamma} B^{\gamma\sigma_{\ell+1}\beta}_{[\ell+1]}$$



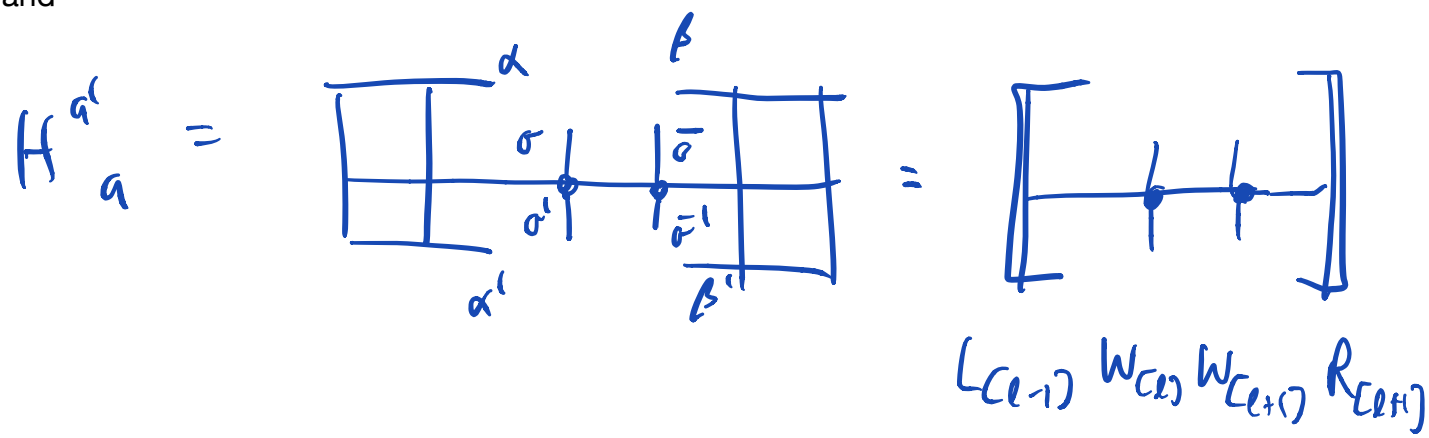
Then extremize simultaneously wrt $A^\dagger_{[\ell]}$, $B^\dagger_{[\ell+1]}$

$$\frac{\partial}{\partial B^\dagger_{[\ell+1]}} \frac{\partial}{\partial A^\dagger_{[\ell]}} \left[\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle \right] = 0$$



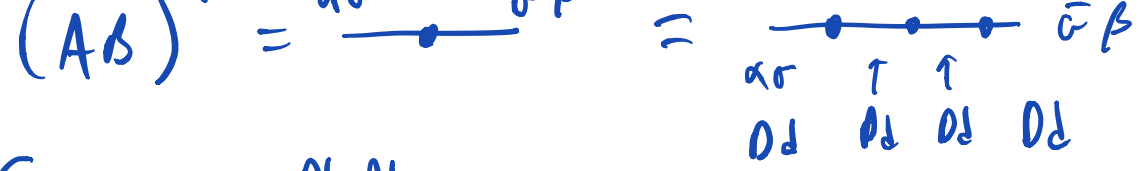
Compact notation: $H^{a'}_{\ a}(AB)^a = \tilde{A}(AB)^{a'}$ with composite index $a = (\alpha, \sigma, \bar{\sigma}, \beta)$

and



Use Lanczos to find lowest eigenvalue of variational equation, reshape updated $(\tilde{AB})$:

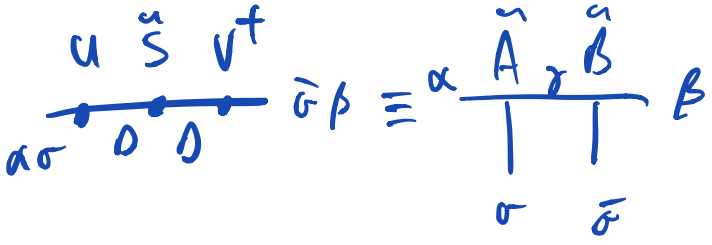
updated $(\tilde{AB})^a =$



Key point: S has dimensions $D \times D$, hence explores a larger state space than previously, in general also including different symmetry sectors!

1 site →

Truncate down to D and reshape;



two sites

This concludes optimization of $\tilde{A}$. Now move one site to right and repeat. Sweep back and forth until convergence of full chain.

$$\tilde{A} = U\sqrt{\tilde{S}}$$

$$\tilde{A}^\dagger \tilde{A} = \sqrt{S}\, U^\dagger U \sqrt{S}$$