- The Density Matrix Renormalization Group (DMRG) was invented by Steve White (student of Ken Wilson) to solve general quantum chain models. [White1992], [White1993]
- First realization of connection between MPS and DMRG in limit $N \to \infty$: Ostlund & Rommer [Ostlund1995]
- Realization that finite-size DMRG leads to MPS: Dukelsky, Martin-Delgado, Nishino, Sierra [Dukelski1998]
- Modern formulation: Vidal [Vidal2003], [Vidal2004], Cirac & Verstraete [Verstraete2004]
- Time evolution: Daley, Kollath, Schollwöck, Vidal [Daley2004], White, Feiguin [White2004]
- Connection to NRG: Weichselbaum, Verstraete, Schollwöck, Cirac, von Delft [arXiv:0504305], [Weichselbaum2009]

1. Iterative ground state search

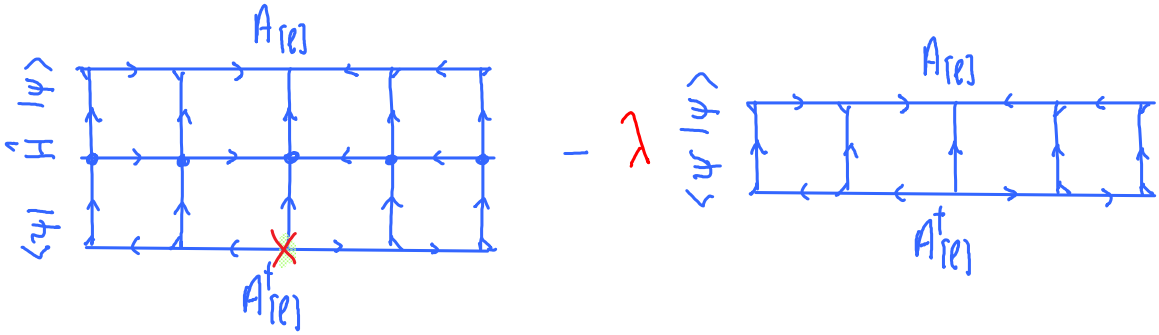
View space of all MPS of given bond dimension, D, as variational space.

Minimize $\langle\psi|\hat{H}|\psi\rangle$ in this space, subject to constraint of unit normalization, $\langle\psi|\psi\rangle = 1$. (1)

Hence extremize $\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle$ (2)

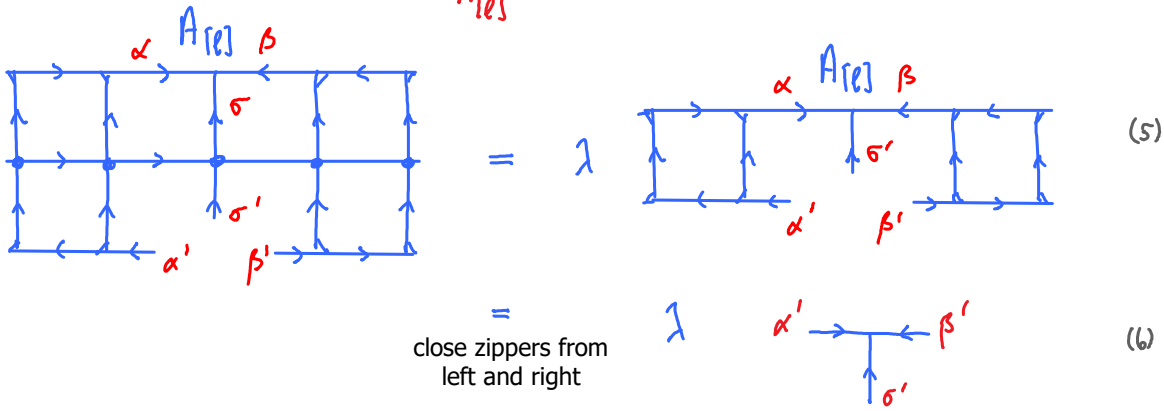
λ: Lagrange multiplier

Graphical representation, assuming mixed-canonical form w.r.t. site ℓ :



(3)

Do this one A -tensor at a time: $\frac{\partial}{\partial A^\dagger_{[\ell]}}\left[\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle\right] = 0$ (4)



(5)

= close zippers from left and right

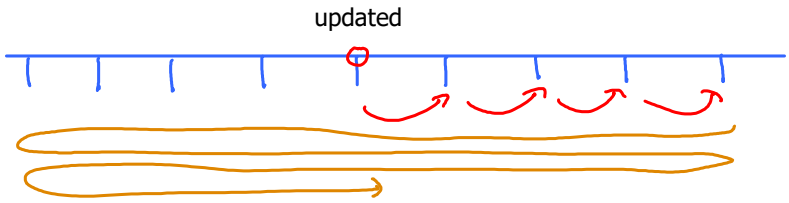
(6)

In the notation of (MPS-V.3.11): $H^{a'}_{\ a} A^{a}_{[\ell]} = \lambda A^{a'}_{[\ell]}$ with $a' = (\alpha', \sigma', \beta')$ (7)

This is an eigenvalue equation for $A_{[\ell]}$ and can be solved with standard linear algebra tools, e.g. Lanczos algorithm (next section).

[More generally: if $|\psi\rangle$ is not represented in mixed-canonical form, one obtains a generalized eigenvalue equation of the form $HA = NA$, with N defined by r.h.s. of (5) . (6)]

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

2. Lanczos method

[Lanczos1950], [Ojalvo1970], [Paige1972], [Koch2011]

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

$\psi_a^* H^a{}_{a'} \psi^{a'}$

We seek the extremal value of $$E[|\psi\rangle] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \quad (1)$$

Denote extremal value by $$E_g = \min E[|\psi\rangle] \equiv E[|\psi_g\rangle] \quad (2)$$

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

'functional gradient': $$\frac{\delta E[|\psi\rangle]}{\delta\langle\psi|} \equiv \frac{H|\psi\rangle}{\langle\psi|\psi\rangle} - \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle^2}|\psi\rangle \quad (3)$$

$$= \frac{H - E[|\psi\rangle]}{\langle\psi|\psi\rangle}|\psi\rangle \equiv |\psi_a\rangle \quad (4)$$

Moving in opposite direction will thus lower the energy:

$$E[|\psi\rangle - \alpha|\psi_a\rangle] < E[|\psi\rangle] \quad \text{for small, positive } \alpha \quad (5)$$

To find optimal value for α , minimize $E[|\psi\rangle - \alpha|\psi_a\rangle]$ w.r.t. the 'variational parameter' α ,

in the space $$K_1 \equiv \text{span}\{|\psi\rangle, |\psi_a\rangle\} = \text{span}\{|\psi\rangle, H|\psi\rangle\} . \quad (6)$$

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

First basis vector: $$|v_0\rangle = \frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}} \quad (7)$$

Second basis vector: $$b_1|v_1\rangle \equiv |\tilde{v}_1\rangle = H|v_0\rangle - |v_0\rangle\langle v_0|H|v_0\rangle \quad (8)$$

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

$|v_0\rangle\langle v_0|H|v_0\rangle$: orthonormalize w.r.t. to $|v_0\rangle$; $\langle v_0|H|v_0\rangle = a_0$

$\langle v_1|(8)$: $$b_1 = \sqrt{\langle\tilde{v}_1|\tilde{v}_1\rangle} = \langle v_1|H|v_0\rangle \quad (9)$$

Now find a matrix representation of H in this space: define

$$a_0 \equiv \langle v_0|H|v_0\rangle , \quad a_1 \equiv \langle v_1|H|v_1\rangle , \quad b_1^2 \equiv \langle\tilde{v}_1|\tilde{v}_1\rangle \quad (10)$$

then $$H|v_0\rangle \overset{(8)}{=} |v_1\rangle b_1 + |v_0\rangle a_0 \quad (11)$$

hence in the space K_1 , the Hamiltonian has the matrix representation

$$\begin{pmatrix} \langle v_0|H|v_0\rangle & \langle v_0|H|v_1\rangle \\ b_1^* & \end{pmatrix}$$

hence in the space K_1, the Hamiltonian has the matrix representation

$$H_{K_1} = \begin{pmatrix} \langle v_0|H|v_0\rangle & \langle v_0|H|v_1\rangle \\ \langle v_1|H|v_0\rangle & \langle v_1|H|v_1\rangle \end{pmatrix} = \begin{pmatrix} a_0 & b_1^* \\ b_1 & a_1 \end{pmatrix} \quad (12)$$

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,

$$\tau[|\psi\rangle] \equiv \| (H - E)|\psi\rangle \|^2 = \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2 \quad (13)$$

and stop when it drops below some threshold.

Krylov space

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

$$K(|\ \rangle) = \text{span}\{|v_0\rangle, H|v_0\rangle, H^2|v_0\rangle, \ldots, H^L|v_0\rangle\} \quad (14)$$

$$= \text{'Krylov space of } H \text{ over } |v_0\rangle\text{'} \quad \text{(dimension } L+1\text{)}. \quad (15)$$

Instead of repeatedly minimizing in 2x2 subspaces, we could first construct K_L, then compute its ground state. (This 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: $$b_1|v_1\rangle \equiv |\tilde{v}_1\rangle = H|v_0\rangle - a_0|v_0\rangle \quad (16)$$

normalize

Third vector: $$b_2|v_2\rangle \equiv |\tilde{v}_2\rangle \equiv H|v_1\rangle - \sum_{j=0}^{1} |v_j\rangle\langle v_j|H|v_1\rangle \quad (17)$$

$$= H|v_1\rangle - |v_1\rangle \underbrace{a_1}_{\langle v_1|H|v_1\rangle} - |v_0\rangle \underbrace{b_1^*}_{\langle v_0|H|v_1\rangle} \quad (18)$$

where $$b_2 \overset{(17)}{=} \sqrt{\langle \tilde{v}_2|\tilde{v}_2\rangle} \overset{(18)}{=} \langle v_2|H|v_1\rangle \quad (19)$$

Note: $\langle v_2|H|v_0\rangle = 0$, since $H|v_0\rangle \in \text{span}\{|v_0\rangle, |v_1\rangle\}$ (20)

Fourth vector: $$b_3|v_3\rangle \equiv |\tilde{v}_3\rangle \equiv H|v_2\rangle - \sum_{j=0}^{2} |v_j\rangle\langle v_j|H|v_2\rangle \quad (21)$$

$$= H|v_2\rangle - |v_2\rangle \underbrace{a_2}_{\langle v_2|H|v_2\rangle} - |v_1\rangle \underbrace{b_2^*}_{\langle v_1|H|v_2\rangle} - |v_0\rangle \underbrace{0}_{(20)\ \langle v_0|H|v_2\rangle} \quad (22)$$

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

nth step: $b_{n+1}|v_{n+1}\rangle \equiv |\tilde{v}_{n+1}\rangle = H|v_n\rangle - \sum_{j=0}^{n} |v_j\rangle\langle v_j|H|v_n\rangle$ (23)

$= H|v_n\rangle - |v_n\rangle a_n - |v_{n-1}\rangle b_n^*$ (24)

with $a_n = \langle v_n|H|v_n\rangle$, $b_n = \langle v_n|H|v_{n-1}\rangle$ (25)

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

Throughout we have: $\langle v_{n+1}|H|v_j\rangle = 0$ for $j = 0, \ldots, n-1$ (26)

since

$H|v_j\rangle \overset{(24)}{\in} \text{span}\{|v_{j+1}\rangle, |v_j\rangle, |v_{j-1}\rangle\}$ (27)

Hence, rearranging (24): $H|v_n\rangle = |v_{n-1}\rangle b_n^* + |v_n\rangle a_n + |v_{n+1}\rangle b_{n+1}$ (28)

Hence, in K_L ,

H has tridiagonal form:

$$H_{K_L} = \begin{pmatrix} a_0 & b_1^* & & & & \\ b_1 & a_1 & b_2^* & & & \\ & b_2 & a_2 & b_3^* & & \\ & & b_3 & a_3 & \ddots & \\ & & & & a_{L-1} & b_L^* \\ & & & & b_L & a_L \end{pmatrix}$$

Ground state of H_{K_L} satisfies the eigenvalue equation $(H_{K_L})^i{}_j (\psi_g^L)^j = E_g^L (\psi_g^L)^i$

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

are the best approximations, within the Krylov space K_L, of true ground state energy and ground state.

Note: $|\psi_g^L\rangle$ 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 $\sim$ [gap to first excited state]$^{1/2}$.

Summary

1. Start with arbitrary $|v_0\rangle$
2. First iteration step: (i) $|\tilde{\tilde{v}}_1\rangle = H|v_0\rangle$

   (ii) $a_0 = \langle \tilde{\tilde{v}}_1 | v_0 \rangle$

   (iii) $|\tilde{v}_1\rangle = |\tilde{\tilde{v}}_1\rangle - a_0 |v_0\rangle$

3. General iteration step, for $n \geq 1$:

   (i) $b_n = \langle \tilde{v}_n | \tilde{v}_n \rangle$

   (ii) If $b_n \neq 0$, then $|v_n\rangle = |\tilde{v}_n\rangle / b_n$

   else, pick $|v_n\rangle$ as arbitrary normalized vector orthogonal to all $|v_0\rangle, \ldots, |v_{n-1}\rangle$

   (iii) $|\tilde{\tilde{v}}_{n+1}\rangle = H|v_n\rangle$

   (iv) $a_n = \langle \tilde{\tilde{v}}_{n+1} | v_n \rangle$

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

   and back to 3(i).

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

3. DMRG for excited states

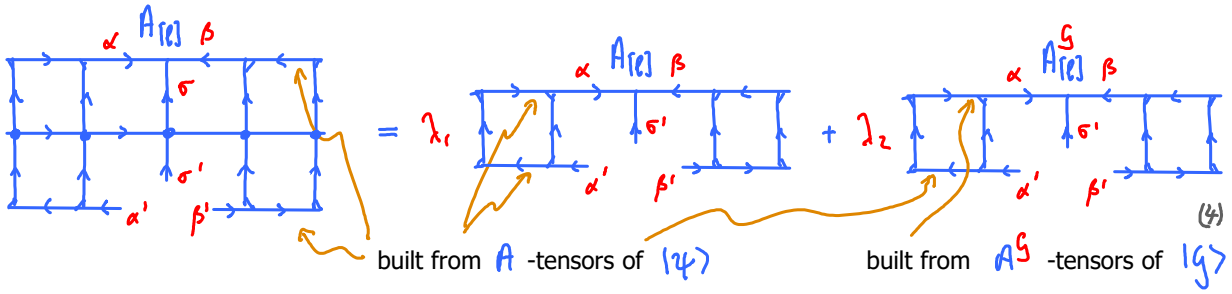
Suppose we have an MPS representation for ground state, $|g\rangle = |\vec{\sigma}\rangle \prod_\ell A^{g\sigma_\ell}_{[\ell]}$ (1)

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

Extremize: $\langle\psi|H|\psi\rangle - \lambda_1\langle\psi|\psi\rangle - \lambda_2\langle\psi|g\rangle$ (2)

Lagrange multipliers enforce $\langle\psi|\psi\rangle = 1$ and $\langle\psi|g\rangle = 0$. (3)

Extremization w.r.t. $A^\dagger_{[\ell]}$ yields



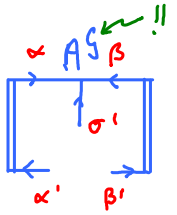
(4)

Generic structure of this equation, in mixed-canonical representation of site ℓ [compare (DMRG-I.1.7)]:

$$H^{a'}{}_a\, A^a_{[\ell]} = \lambda_1 A^{a'} + \lambda_2 g^{a'}, \quad \text{with} \quad A^\dagger_a A^a \overset{(3)}{=} 1, \quad A^\dagger_a g^a \overset{(3)}{=} 0, \tag{5}$$

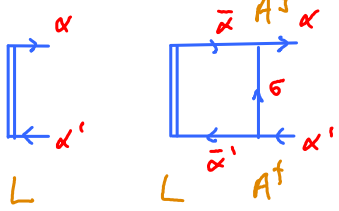
with $a' = (\alpha', \sigma', \beta')$

$$g^{a'} \equiv g^{\alpha'\sigma'\beta'} = L_{[\ell-1]\alpha}{}^{\alpha'} A^{g\,\alpha\sigma'\beta}_{[\ell]} R_{[\ell+1]\beta}{}^{\beta'} \tag{6}$$



with L and R computed iteratively,

$$L_{[\ell]}{}^{\alpha'}{}_{\alpha} = A^{\dagger\,\alpha'}_{[\ell]\,\sigma\bar{\alpha}'} L_{[\ell-1]}{}^{\bar{\alpha}'}{}_{\bar{\alpha}} A^{g\,\bar{\alpha}\sigma}_{[\ell]\,\alpha} \tag{7}$$



Index-free notation for (5): $H|A\rangle = \lambda_1|A\rangle + \lambda_2|g\rangle, \quad \langle A|g\rangle = 0$ (8)

Define projector onto subspace orthogonal to $|g\rangle$: $P_g = \mathbb{1} - |g\rangle\langle g|$ (9)

with indices: $P_g{}^{a'}{}_a = \mathbb{1}^{a'}{}_a - g^{a'} g^\dagger_a$, so that $P_g{}^{a'}{}_a\, g^a = 0$ (10)

Project (8) onto this subspace: $P_g H \underbrace{(P_g + |g\rangle\langle g|)}_{(9)\ \mathbb{1}}|A\rangle = \lambda_1 P_g|A\rangle + \underbrace{0}_{(8)=0}$ (11)

$(g) = 0$

$$P_g H P_g |A\rangle = \lambda_1 P_g |A\rangle \qquad (12)$$

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, $|v_0'\rangle = P_g |v_0\rangle$, (13)

and construct new Krylov vectors using

$$|\tilde{v}_{n+1}\rangle = P_g H |v_{n+1}\rangle - |v_n\rangle a_n - |v_{n-1}\rangle b_n^* \qquad (14)$$

Why not simply use excited states in K_L? Because numerical noise can cause the $|v_n\rangle$ to be not <u>exactly</u> orthogonal, hence for $j < n-2$, $\langle v_n | v_j \rangle \simeq 10^{-16}$ 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 <u>does</u>. To prevent this, explicit reorthogonalization is needed at every step, using P_g, as indicated above.

<u>Block-Lanczos for excited states</u>

Standard Lanczos: represent action of H as

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

$$\begin{pmatrix} a_0 & b_1^* & & \\ b_1 & a_1 & b_2^* & \\ & b_2 & \ddots & \\ & & & \end{pmatrix}$$

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

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

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

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

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

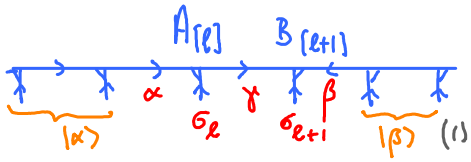
etc. Then the lowest M eigenstates of block-tridiagonal matrix give the Lanczos approximation for lowest M eigenstates of H

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

If one encodes symmetries (see Sym-I to Sym-III), then 'one-site update' (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 variationally optimizes two A-tensors at a time.

Represent MPS in mixed-canonical two-site basis:

$$|\psi\rangle = \sum_{\alpha\sigma_\ell\sigma_{\ell+1}\beta} |\beta\rangle |\sigma_{\ell+1}\rangle |\sigma_\ell\rangle |\alpha\rangle A_{[\ell]}^{\alpha\sigma_\ell\gamma} B_{[\ell+1]}^{\gamma\sigma_{\ell+1}\beta}$$



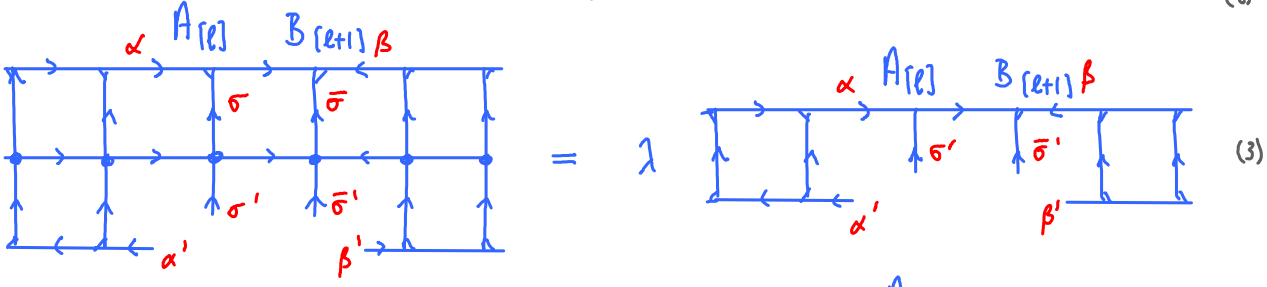
(1)

Then extremize simultaneously w.r.t.

$A^\dagger_{[\ell]}$ and $B^\dagger_{[\ell+1]}$

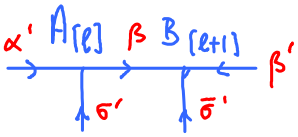
$$\frac{\partial}{\partial B^\dagger_{[\ell+1]}} \frac{\partial}{\partial A^\dagger_{[\ell]}} \left[\langle\psi|\hat{H}|\psi\rangle - \lambda \langle\psi|\psi\rangle \right] = 0$$

(2)



(3)

close zippers from left and right = λ

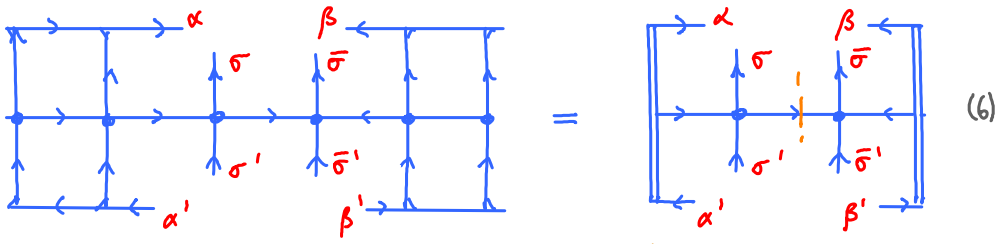


(4)

Compact notation: $H^{a'}{}_{a} (AB)^a = \lambda (AB)^{a'}$ with composite index $a = (\alpha, \sigma, \bar{\sigma}, \beta)$ (5)

and

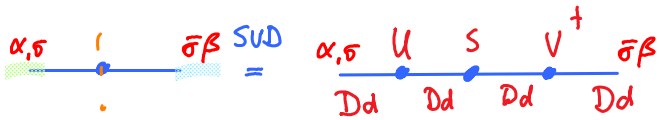
$H^{a'}{}_{a}$ =



(6)

Use Lanczos to find lowest eigenvalue of eigenvalue equation (5), and reshape updated $(\widetilde{AB})$:

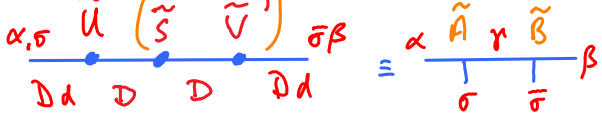
updated $(\widetilde{AB})^a$ reshape =



(7)

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

Truncate down to D and reshape:



(8)

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