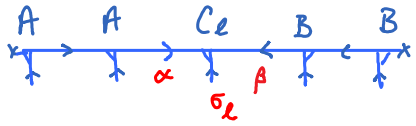
- The Density Matrix Renormalization Group (DMRG) was invented by Steve White (student of Ken Wilson) to solve general quantum chain models. [White1992], [White1993]
- First realization of connection between MPS and DMRG in limit $L \to \infty$: Ostlund & Rommer [Ostlund1995]
- Realization that finite-size 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

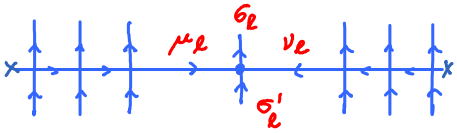
View space of all MPS of given bond dimension, D , as variational space.

Graphical representation, assuming site-canonical form with orthogonality center at site ℓ :

$$|\Psi\rangle = |\beta\rangle |\sigma_\ell\rangle |\alpha\rangle [C_\ell]^{\alpha \sigma_\ell \beta} \qquad (1)$$



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



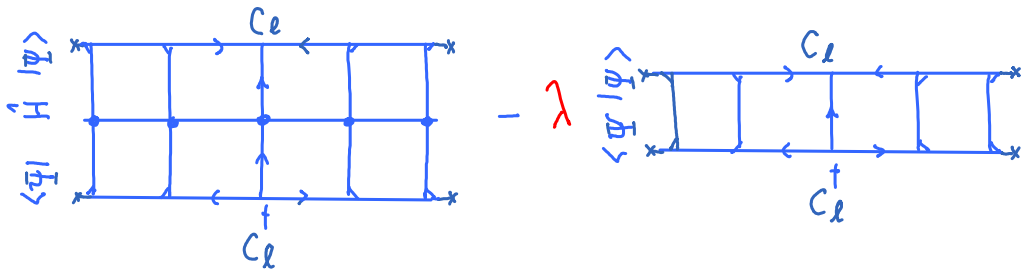
Arrow convention: use same arrow directions on virtual bonds for MPO as in MPS. Then, orientation of MPS triangles, $\uparrow, \downarrow, \nearrow, \searrow$, hence we henceforth drop most (soften all) arrows.

Minimize $\langle\Psi|\hat{H}|\Psi\rangle$ in this space, subject to constraint of unit normalization, $\langle\Psi|\Psi\rangle = 1$. (2)

Hence extremize

$$\langle\Psi|\hat{H}|\Psi\rangle - \lambda \langle\Psi|\Psi\rangle \qquad (3)$$

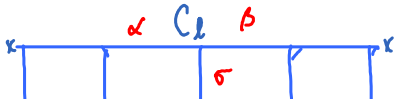
Lagrange multiplier

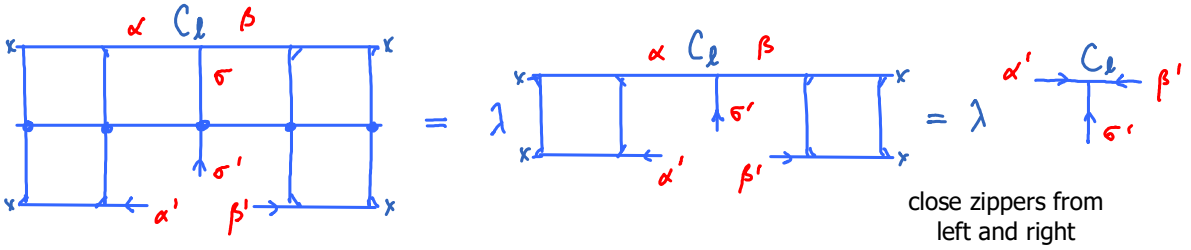


(4)

Do this one tensor at a time:

$$\frac{\partial}{\partial C_\ell^\dagger} \left[\langle\Psi|\hat{H}|\Psi\rangle - \lambda \langle\Psi|\Psi\rangle \right] = 0 \qquad (5)$$





(6)

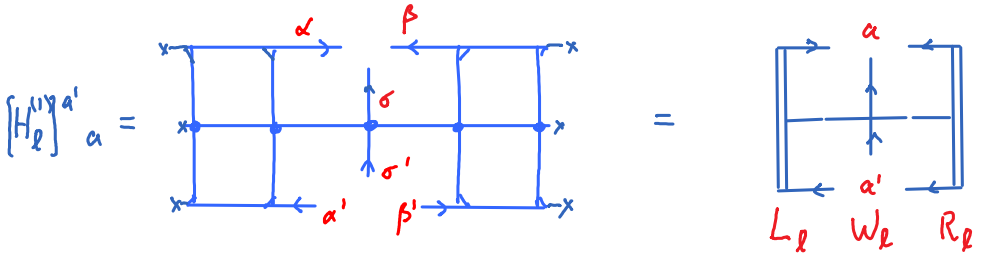
Structure of this equation: $H_\ell^{(1)} C_\ell = \lambda C_\ell$ (7)

with normalization $C_\ell^\dagger C_\ell = 1$ (8)

Here, C_ℓ is viewed as vector, labeled by composite index $a' = (\alpha', \sigma', \beta')$, and $H_\ell^{(1)}$ as a matrix:

$$\left[H_\ell^{(1)}\right]^{a}_{\ a'} \left[C_\ell\right]^{a'} = \lambda \left[C_\ell\right]^{a} \qquad \text{with normalization} \qquad \left[C_\ell^\dagger\right]_a \left[C_\ell\right]^a = 1 \qquad (9)$$

compare (MPS-IV.3.11)

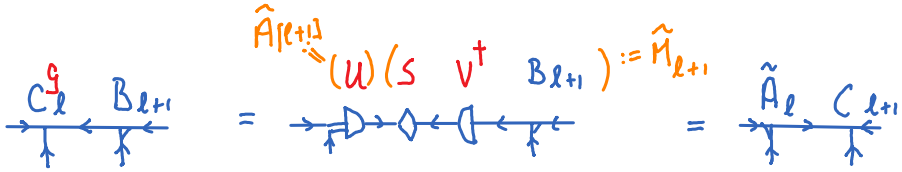


(10)

(7) is an eigenvalue equation for C_ℓ and can be solved with standard linear algebra tools, e.g. Lanczos algorithm (next section).

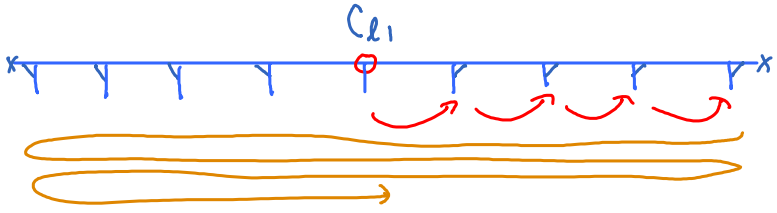
[More generally: if $|\psi\rangle$ is not represented in site-canonical form, one obtains a generalized eigenvalue equation of the form $H_\ell^{(1)} C_\ell = G_\ell^{(1)} C_\ell$, with $G_\ell^{(1)}$ defined by r.h.s. of (6) .]

Use the 'eigenvector' with the lowest eigenvalue (= current estimate of ground state energy), say C_ℓ^G, to 'update' MPS, then move to next site, use SVD on $\tilde{C}_{[\ell]}$ to shift orthogonality center to site $\ell+1$:



(11)

optimize $C_{\ell+1}$, etc..



(12)

'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]
original idea — stable version — nice discussion

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

We seek the extremal value of

$$E[|\psi\rangle] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{1}$$

Denote extremal value by

$$E_g = \min E[|\psi\rangle] \equiv E[|\psi_g\rangle] \tag{2}$$

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

'functional gradient':

$$\frac{\delta E[|\psi\rangle]}{\delta\langle\psi|} \equiv \frac{H|\psi\rangle}{\langle\psi|\psi\rangle} - \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle^2}|\psi\rangle \tag{3}$$

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

Moving in opposite direction will thus lower the energy:

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

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

in the space

$$K_1 := \text{span}\{|\psi\rangle, |\psi_a\rangle\} = \text{span}\{|\psi\rangle, H|\psi\rangle\} . \tag{6}$$

Starting from the random initial state $|\psi\rangle$, construct a normalized basis $\{|v_0\rangle, |v_1\rangle\}$ for this space:

First basis vector:

$$|v_0\rangle := \frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}} \tag{7}$$

Second basis vector:

$$b_1|v_1\rangle := |\tilde{v}_1\rangle := H|v_0\rangle - |v_0\rangle\underbrace{\langle v_0|H|v_0\rangle}_{:= a_0} \tag{8}$$

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

$|v_0\rangle$: orthonormalize w.r.t. to $|v_0\rangle$

$$b_1 := \sqrt{\langle\tilde{v}_1|\tilde{v}_1\rangle} \quad \text{(real)} \qquad \overset{\langle v_1|(8)}{=} \langle v_1|H|v_0\rangle + \underbrace{0}_{\text{since } \langle v_1|v_0\rangle \overset{(8)}{=} 0} \tag{9}$$

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

$$a_0 := \langle v_0|H|v_0\rangle , \quad a_1 := \langle v_1|H|v_1\rangle , \quad b_1^2 = \langle\tilde{v}_1|\tilde{v}_1\rangle \tag{10}$$

then

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

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

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

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

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 $\{|v_0\rangle, |v_1\rangle, \ldots, |v_L\rangle\}$

As before: $b_1|v_1\rangle := |\tilde{v}_1\rangle := H|v_0\rangle - a_0|v_0\rangle \quad (16)$

normalize

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

$$= H|v_1\rangle - |v_1\rangle a_1 - |v_0\rangle b_1^* \quad (18)$$

($\langle v_1|H|v_1\rangle$, $\langle v_0|H|v_1\rangle$)

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

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

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

$$= H|v_2\rangle - |v_2\rangle a_2 - |v_1\rangle b_2^* - |v_0\rangle 0 \quad (22)$$

($\langle v_2|H|v_2\rangle$, $\langle v_1|H|v_2\rangle$, $\overset{(20)}{=} \langle v_0|H|v_2\rangle$)

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

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

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

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

[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: $$\langle v_n|H|v_j\rangle = 0 \quad \text{for} \quad j = 0, \ldots, n-2 \quad (26)$$

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

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

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

are the best approximations, within the Krylov space 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) $b_n = \sqrt{\langle \tilde{v}_n | \tilde{v}_n \rangle}$

   (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

DMRG-I.3

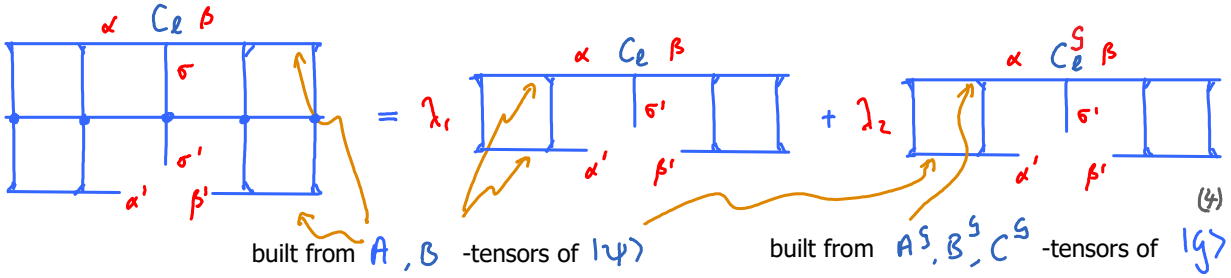
Suppose we have an MPS representation for ground state, $|g\rangle =$  (1)

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. $C_\ell^\dagger$ yields



(4)

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

$$H_\ell C_\ell = \lambda_1 C_\ell + \lambda_2 g_\ell \quad (5)$$

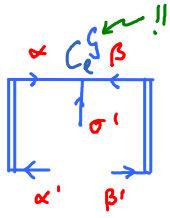
cf. (DMRG-I.1.7)

with $C_\ell^\dagger \cdot C_\ell \overset{(3)}{=} 1$, $C_\ell^\dagger g_\ell \overset{(3)}{=} 0$ (6)

Displaying indices: $a' = (\alpha', \sigma', \beta')$

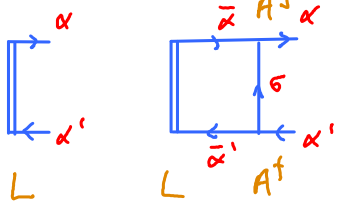
$$[H_\ell]^{a'}_{\ a}[C^\ell]^a = \lambda_1[C_\ell]^{a'} + \lambda_2[g_\ell]^{a'} \qquad [C_\ell^\dagger]_a[C_\ell]^a = 1\,, \quad [C_\ell^{\dagger g}]_a[g_\ell]^a = 1 \quad (7)$$

$$[g_\ell]^{a'} = [g_\ell]^{\alpha'\sigma'\beta'} = [L_{\ell-1}]^{\alpha'}{}_{\alpha}[A_\ell^g]^{\alpha\sigma'\beta}[R_{\ell+1}]_{\beta}{}^{\beta'} \quad (8)$$



with L and R computed iteratively,

$$[L_\ell]^{\alpha'}{}_{\alpha} = [A_\ell^\dagger]^{\alpha'}{}_{\sigma\bar\alpha'}[L_{\ell-1}]^{\bar\alpha'}{}_{\bar\alpha}[A_\ell^g]^{\bar\alpha\sigma}{}_{\alpha} \quad (9)$$



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: $P_g \, H \overbrace{(P_g + |g\rangle\langle g|)}^{(9)\,\mathbb{1}} |A\rangle = \lambda_1 P_g |A\rangle + \underbrace{0}_{(8)=0}$ (11)

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

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,

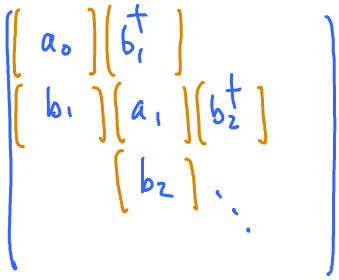
$|v_{0,i}\rangle$, $i = 1, \ldots, M$, and represent action of H as

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

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

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

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



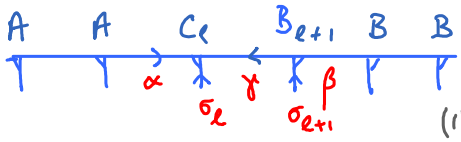
4. Two-site update

[Schollwöck2011, Sec. 6.4]

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:

$$|\Psi\rangle = |\beta\rangle\,|\sigma_{\ell+1}\rangle\,|\sigma_\ell\rangle\,|\alpha\rangle\,[C_\ell]^{\alpha\sigma_\ell}{}_{\gamma}\,[B_{\ell+1}]^{\gamma\sigma_{\ell+1}\beta}$$



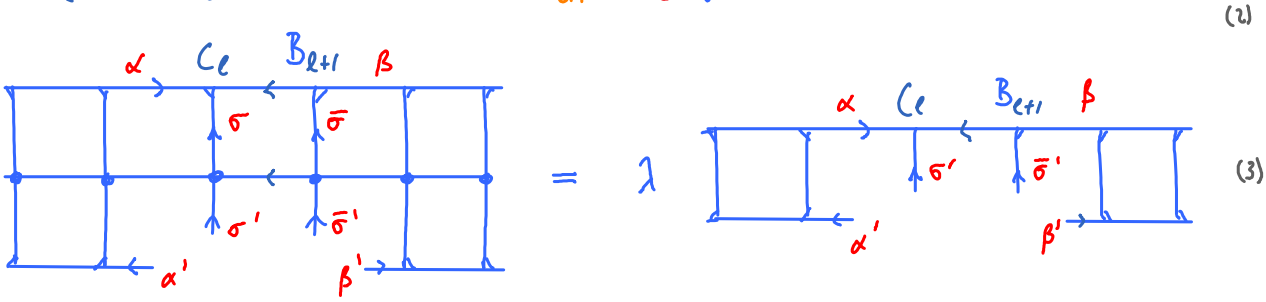
(1)

Then extremize simultaneously w.r.t.

$C_\ell^\dagger$ and $B_{\ell+1}^\dagger$

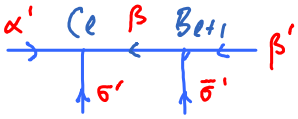
$$\frac{\partial}{\partial B_{\ell+1}^\dagger}\,\frac{\partial}{\partial C_\ell^\dagger}\left[\langle\Psi|\hat{H}|\Psi\rangle - \lambda\langle\Psi|\Psi\rangle\right] = 0$$

(2)



(3)

close zippers from left and right = λ



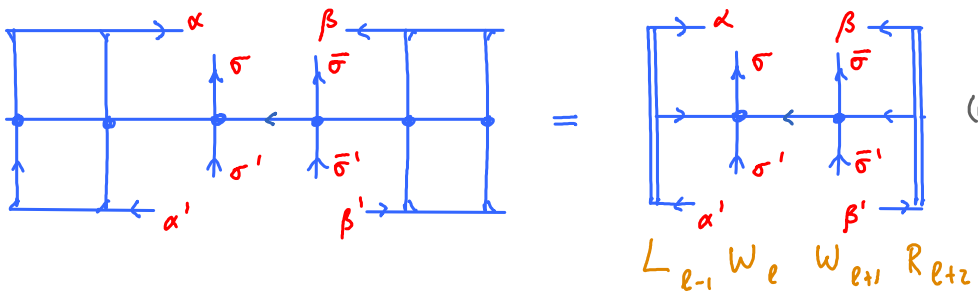
(4)

Compact notation: $\left[H_\ell^{(2)}\right]^{a'}_{a}\left[\psi_\ell^{(2)}\right]^{a} = \lambda\left[\psi_\ell^{(2)}\right]^{a'}$ with composite index $a = (\alpha, \sigma, \bar{\sigma}, \beta)$

(5)

and

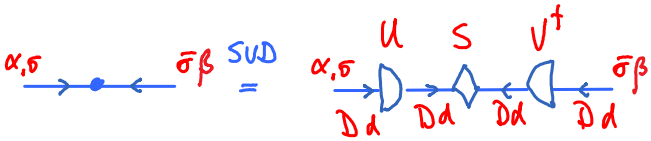
$\left[H_\ell^{(2)}\right]^{a'}_{a} =$



(6)

Use Lanczos to find lowest eigenvalue of eigenvalue equation (5), and reshape updated $\tilde{\psi}_\ell^{(2)}$:

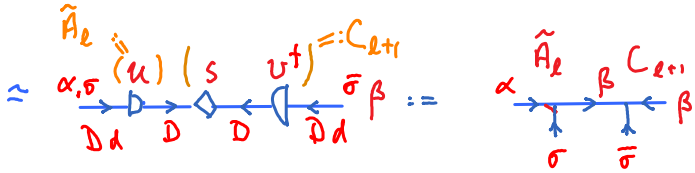
updated $\left[\tilde{\psi}_\ell^{(2)}\right]^{a}$ reshape =



(7)

Key point: S has Dd singular values, larger than the virtual bond dimension D of M and B. Hence, it explores a larger state space, in general also including more symmetry sectors!

Truncate down to D and reshape:



(8)

This concludes optimization of site ℓ. Now move one site to the right and repeat. Sweep back and forth until convergence of full chain.