DMRG.1-4: Ground State Search [Schollwöck2011, Sec. 6.3]

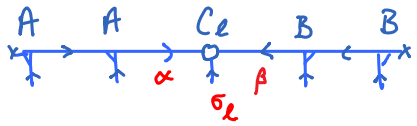
- The Density Matrix Renormalization Group (DMRG) was invented by Steve White (student of Ken Wilson) to solve general quantum chain models. [White1992], [White1993]
- First realization of connection between MPS and DMRG in limit $\mathcal{L} \to \infty$: Ostlund & Rommer [Ostlund1995]
- Realization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

DMRG.1 Iterative ground state search

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

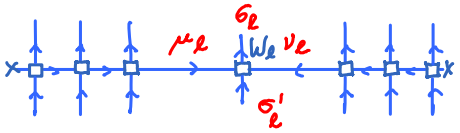
Graphical representation, assuming site-canonical form with orthogonality center at site ℓ :

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



(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, $\top$, $\top$, $\perp$, $\perp$, hence we henceforth drop most (soften all) arrows.

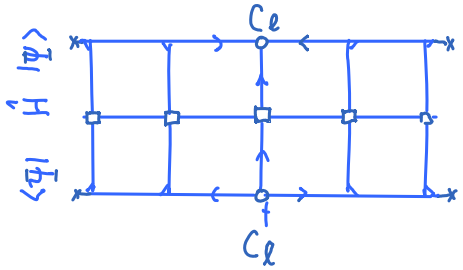
Minimize $\langle\Psi|\hat{H}|\Psi\rangle$ in this space, subject to constraint of unit normalization, $\langle\Psi|\Psi\rangle = 1$.

(2)

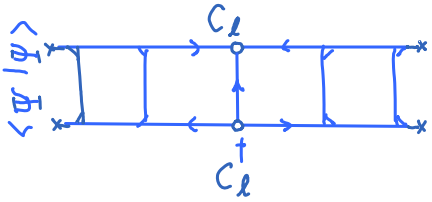
Hence extremize

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

Lagrange multiplier



$-\lambda$

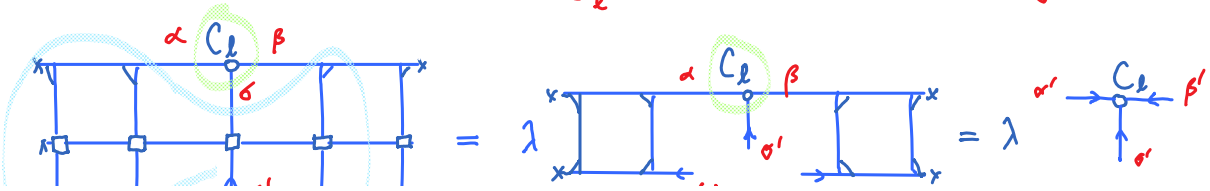


(4)

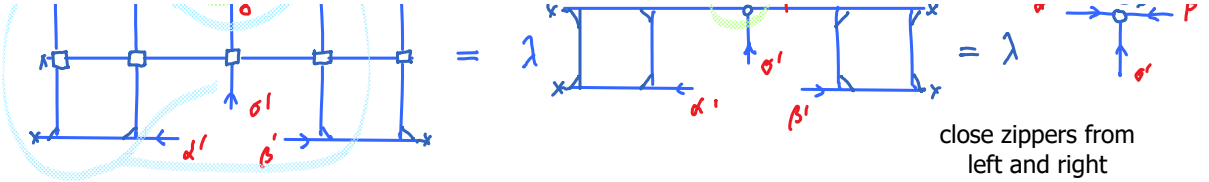
$$\frac{\partial}{\partial x}\left(x^* A x\right) = Ax$$

Do this one tensor at a time:

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



(6)



close zippers from left and right

(6)

Structure of (6): 1-site Schrödinger equation!

$$H_\ell^{(1)} \psi_\ell^{(1)} = \lambda \psi_\ell^{(1)} \qquad \text{with} \qquad \psi_\ell^{(1)} = C_\ell \tag{7}$$

with normalization

$$\psi_\ell^{\dagger(1)} \psi_\ell^{(1)} = 1$$

(8)

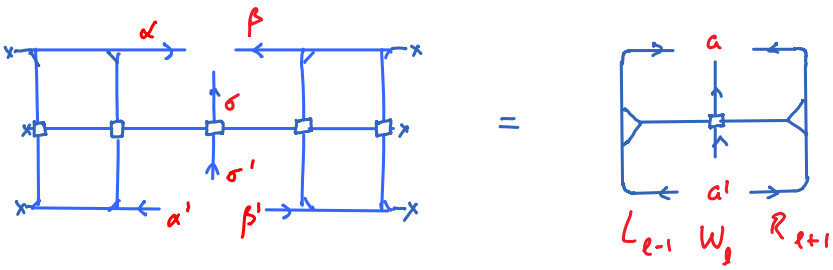
Here, C_ℓ is viewed as vector, labeled by composite index $a' = (\alpha', \sigma_\ell', \beta')$, and $H_\ell^{(1)}$ as a matrix:

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

compare (MPS.15.11)

$(D^2 d) \times (D^2 d)$

$\left[H_\ell^{(1)}\right]^{a'}{}_{a} =$

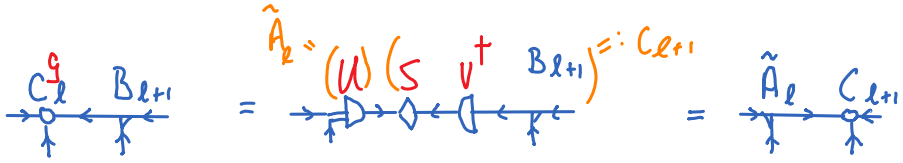


(10)

(7) is an eigenvalue equation for C_ℓ. The lowest eigenvalue and eigenvector can be found with standard linear algebra tools (e.g. Lanczos algorithm, next section), <u>without</u> having to construct $H_\ell^{(1)}$ fully.
It suffices to know how to compute $H_\ell^{(1)} C_\ell$.

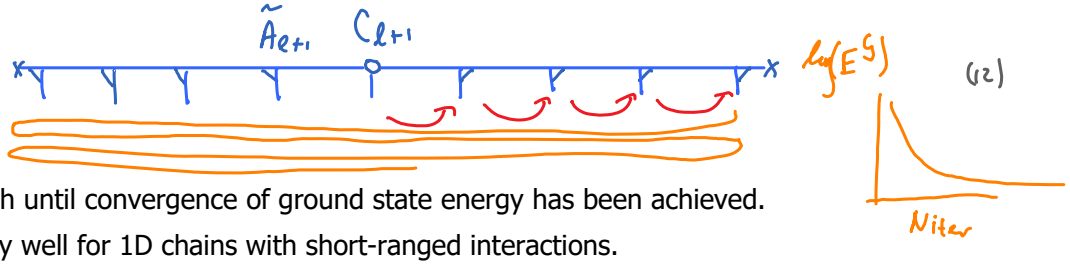
[More generally: if $|\psi\rangle$ is not represented in site-canonical form, one obtains a generalized eigenvalue equation of the form $H_\ell^{(1)} C_\ell = N_\ell^{(1)} C_\ell$, with $N_\ell^{(1)}$ defined by r.h.s. of (6) .]

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



(11)

Compute new environments L_ℓ and $R_{\ell+2}$ for site ℓ , then 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.

Cost of 1-site DMRG = cost of computing $H_\ell^{(1)} \psi_\ell^{(1)}$: $O(D^3 d w + D^2 d^2 w^2)$ (13)

Note: the full $H_\ell^{(1)}$ of dimension $D^2 d \times D^2 d$ (expensive!) need not be constructed explicitly!

DMRG.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 $$E[|\psi\rangle] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \quad (1)$$

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

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

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

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

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 'Krylov space' $$K_1 := \text{span}\{|\psi\rangle, |\psi_a\rangle\} = \text{span}\{|\psi\rangle, H|\psi\rangle\} . \quad (6)$$

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

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

First Krylov step: explore the second direction in Krylov space by applying H to $|v_0\rangle$:

Define $$|\tilde{v}_1\rangle := H|v_0\rangle \quad (8)$$

Orthogonalize w.r.t. $|v_0\rangle$: $$|v_1^\perp\rangle := |\tilde{v}_1\rangle - |v_0\rangle\langle v_0|\tilde{v}_1\rangle \quad (9)$$

ensuring $$\langle v_0|v_1^\perp\rangle = 0 \quad (10)$$

Compute norm and normalize: $$b_1 := \sqrt{\langle v_1^\perp|v_1^\perp\rangle} \in \mathbb{R} \quad (11)$$

2nd basis vector: $$|v_1\rangle := |v_1^\perp\rangle / b_1 \quad (12)$$

Rewrite (9): $$|v_1\rangle b_1 \overset{(11)}{=} |v_1^\perp\rangle = H|v_0\rangle - |v_0\rangle\underbrace{\langle v_0|H|v_0\rangle}_{\text{define } := a_0 = \langle v_0|\tilde{v}_1\rangle} \quad (13)$$

(13)

Rewrite (9): $|v_1\rangle b_1 = \ldots$ define $:= a_0 = \langle v_0|\tilde{v}_1\rangle$

Rearrange (13): $H|v_0\rangle \overset{(13)}{=} |v_0\rangle a_0 + |v_1\rangle b_1$ (14)

$\langle v_1|$ (14) and (10) yield: $\langle v_1|H|v_0\rangle \overset{(10)}{=} 0 + b_1 = \langle v_0|H|v_1\rangle$ (15)

since b_1 is real, (11)

Finally, define $a_1 := \langle v_1|H|v_1\rangle \overset{(27)}{=}$ (16)

Now we have orthonormal basis for 2-dimensional Krylov space: $K_1 := \text{span}\{|v_0\rangle, |v_1\rangle\} = \text{span}\{|v_0\rangle, H|v_0\rangle\}$ (17)

In the space K_1, the Hamiltonian has the matrix representation

$$H_{K_1} = \begin{pmatrix} \langle v_0|H|v_0\rangle & \langle v_0|H|v_1\rangle \\ \langle v_1|H|v_0\rangle & \langle v_1|H|v_1\rangle \end{pmatrix} = \begin{pmatrix} a_0 & b_1 \\ b_1 & a_1 \end{pmatrix} \quad (18)$$

The ground state of H_{K_1}, say $|g\rangle_{K_1}$ with energy $E^g_{K_1}$, 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,

$$\tau[|\psi\rangle] \equiv \|(H-E)|\psi\rangle\|^2 = \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2 \quad (19)$$

for $|\psi\rangle = |g\rangle_{K_1}$, $E = E^g_{K_1}$ and stop when it drops below some threshold.

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

$$K_N(|v_0\rangle) = \text{span}\{|v_0\rangle, H|v_0\rangle, H^2|v_0\rangle, \ldots, H^N|v_0\rangle\} \quad (20)$$

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

Instead of repeatedly minimizing in 2x2 subspaces, we could <u>first</u> construct K_N, <u>then</u> compute its ground state. (This is faster, since it amounts to using N <u>simultaneous</u> variational parameters instead of N separate ones.) To do this, iteratively construct a 'Krylov basis' for K_N, such that

$$K_N(|v_0\rangle) = \text{span}\{|v_0\rangle, |v_1\rangle, \ldots, |v_N\rangle\}, \quad \text{with} \quad \langle v_n|v_{n'}\rangle = \delta_{nn'} \quad (21)$$

We now elaborate this iteration strategy, first for the 2nd Krylov step, then for the (n+1)-th step.

<u>Second Krylov step:</u> explore a new direction in Krylov space by applying H to $|v_1\rangle$:

Define $|\tilde{v}_2\rangle := H|v_1\rangle$ Proj. on $K_1(|v_0\rangle)$ (22)

Orthogonalize: $|v_2^\perp\rangle := |\tilde{v}_2\rangle - \sum_{j=0}^{1} |v_j\rangle\langle v_j|\tilde{v}_2\rangle$ (23)

ensuring $\langle v_j | v_2^\perp \rangle = 0 \qquad j = 0, 1$ (24)

Normalize: $b_2 := \sqrt{\langle v_2^\perp | v_2^\perp \rangle}$ (25)

3rd basis vector: $|v_2\rangle = |v_2^\perp\rangle / b_2$ (26)

Rewrite (23): $|v_2\rangle b_2 \overset{(26)}{=} |v_2^\perp\rangle \overset{(23,27)}{=} H|v_1\rangle - |v_1\rangle\underbrace{\langle v_1|H|v_1\rangle}_{\text{define } := a_1 = \langle v_1|\hat{v}_2\rangle \overset{(15)}{=} b_1} - |v_0\rangle\langle v_0|H|v_1\rangle$ (27)

Rearrange (27): $H|v_1\rangle \overset{(27)}{=} |v_0\rangle b_1 + |v_1\rangle a_1 + |v_2\rangle b_2$ (28)

$\langle v_2|$ (28) and (24) yield: $\langle v_2|H|v_1\rangle = \overset{\overset{(24)}{\uparrow}}{0} + 0 + b_2 = \langle v_1|H|v_2\rangle$ (29)

since b_2 is real, (25)

next-to-diagonal elements

Note: $\langle v_2|H|v_0\rangle = 0$, since $H|v_0\rangle \overset{(13)}{\in} \text{span}\{|v_0\rangle, |v_1\rangle\}$ (30)

i.e. K_2: $H_{k_2} = \begin{pmatrix} a_0 & b_1 & 0 \\ b_1 & a_1 & b_2 \\ 0 & b_2 & a_2 \end{pmatrix}$ and we orthogonalized $|v_2\rangle$ w.r.t. $|v_0\rangle, |v_1\rangle$ [see (23,24)]

$a_2 = \langle v_2|H|v_2\rangle$

<u>(n+1)-th Krylov step:</u> explore a new direction in Krylov space by applying H to $|v_n\rangle$:

Define $|\tilde{v}_{n+1}\rangle := H|v_n\rangle$ (31)

Define: $a_n := \langle v_n|\tilde{v}_{n+1}\rangle = \langle v_n|H|v_n\rangle$ diagonal elements (32)

Orthogonalize: $|v_{n+1}^\perp\rangle := |\tilde{v}_{n+1}\rangle - \sum_{j=0}^{n} |v_j\rangle\langle v_j|\tilde{v}_{n+1}\rangle$ (33)

ensuring $\langle v_j|v_{n+1}^\perp\rangle = 0$ for $0 \le j \le n$ (34)

Normalize: $b_{n+1} := \sqrt{\langle v_{n+1}^\perp | v_{n+1}^\perp\rangle}$ (35)

(n+1)-th basis vector: $|v_{n+1}\rangle := |v_{n+1}^\perp\rangle / b_{n+1}$ (36)

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

Rewrite (33):

$|v_{n+1}\rangle b_{n+1} \overset{(34)}{=} |v_{n+1}^\perp\rangle \overset{(31,30)}{=} H|v_n\rangle - |v_n\rangle\underbrace{\langle v_n|H|v_n\rangle}_{(32)\ a_n} - |v_{n-1}\rangle\underbrace{\langle v_{n-1}|H|v_n\rangle}_{(36)\ b_{n-1}} - \underbrace{0}_{(38)}$ (37)

All other terms vanish: $\langle v_j|H|v_n\rangle = \langle v_n|H|v_j\rangle = 0$ for $j < n-1$ (38)

farther-than-next-to-diagonal

since by construction, $H|v_j\rangle \in \text{span}\{|v_i\rangle, 0 \le i \le j+1\}$ and for $j < n-1$,

i.e. $i \le j+1 < n$, $|v_n\rangle$ is orthogonal to them all: $\langle v_n|v_i\rangle \overset{(34)}{=} 0$ for $i < n$ (39)

orthonormal Krylov basis: $|v_0\rangle, \ldots, |v_j\rangle, |v_{j+1}\rangle, \ldots, |v_{n-2}\rangle, |v_{n-1}\rangle, |v_n\rangle$

$|v_{j<n-1}\rangle$ is one of these states

$H|v_{j<n-1}\rangle$ lies in span of these states, hence has no overlap with $|v_n\rangle$

Rearrange (37): $$H|v_n\rangle = |v_{n-1}\rangle b_n + |v_n\rangle a_n + |v_{n+1}\rangle b_{n+1} \qquad (40)$$

$\langle v_n|$(40) and (34) yield $$b_{n+1} = \langle v_{n+1}|H|v_n\rangle = \langle v_n|H|v_{n+1}\rangle \qquad (41)$$ next-to-diagonal elements

(38) holds if computations are done using <u>exact</u> arithmetic. In numerical practice, it does not hold strictly (typical violations are $O(10^{-12})$), and errors accumulate. Hence it is advisable to orthogonalize a second time, directly after (32), before proceeding. This will be made explicit see below.

Hence, in K_N,

H has tridiagonal form:

$$H_{K_N} \overset{(36)}{=} \begin{array}{c|cccccc} & |v_0\rangle & |v_1\rangle & & & & |v_N\rangle \\ \hline \langle v_0| & a_0 & b_1 & & & & \\ \langle v_1| & b_1 & a_1 & b_2 & & & \\ & & b_2 & a_2 & b_3 & & \\ & & & b_3 & a_3 & \ddots & \\ & & & & & a_{N-1} & b_N \\ \langle v_N| & & & & & b_N & a_N \end{array} \qquad (42)$$

Ground state of H_{K_N} satisfies the eigenvalue equation $$(H_{K_N})^i{}_j \, (\psi_g^N)^j = E_g^N (\psi_g^N)^i \qquad (43)$$

Thus $$E_g^N \text{ and } |\psi_g^N\rangle = \sum_{j=0} |v_j\rangle (\psi_g^N)^j \qquad (44)$$

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

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

<u>Summary</u> Construct Krylov space of dimension $N+1$ as follows:

1. Initialization: start with arbitrary (normalized) state $|v_0\rangle$

Then repeat steps 2 to 4 for $n = 0, \ldots, N-1$:

2. Explore new direction in Krylov space by applying H:

$$|\tilde{v}_{n+1}\rangle := H|v_n\rangle \,, \qquad a_n := \langle \tilde{v}_{n+1}|v_n\rangle \qquad (45)$$

3. Orthogonalize w.r.t. the <u>two previous</u> Krylov vectors:

$$|\tilde{v}_{n+1}\rangle \to |\tilde{v}_{n+1}\rangle - \sum_{j=n-1}^{n} |v_j\rangle\langle v_j|\tilde{v}_{n+1}\rangle \qquad (46)$$

3. Orthogonalize w.r.t. the two previous Krylov vectors:

$$|v_{n+1}^{\perp}\rangle := |\tilde{v}_{n+1}\rangle - \sum_{j=n-1}^{n} |v_j\rangle\langle v_j|\tilde{v}_{n+1}\rangle \tag{46}$$

Orthogonalize again, now w.r.t. all previous Krylov vectors (to minimize accumulation of errors, "ghosts"):

$$|v_{n+1}^{\perp\perp}\rangle := |v_{n+1}^{\perp}\rangle - \sum_{j=0}^{n} |v_j\rangle\langle v_j|v_{n+1}^{\perp}\rangle \tag{47}$$

4. Compute norm and normalize: $b_{n+1} := \sqrt{\langle v_{n+1}^{\perp\perp}|v_{n+1}^{\perp\perp}\rangle}$ (48)

If $b_{n+1} \neq 0$, then $|v_{n+1}\rangle := |v_{n+1}^{\perp\perp}\rangle / b_{n+1}$ (49)

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

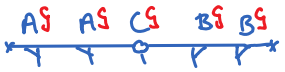
There are other ways of organizing this iteration loop, but the one shown here is numerically the most stable. [Paige1972]

In the resulting Krylov space $K_N = \text{span}\{|v_0\rangle, |v_1\rangle, \ldots, |v_N\rangle\}$ (50)

the Hamiltonian has the representation

$$H_N = \begin{pmatrix} a_0 & b_1 & & & \\ b_1 & a_1 & b_2 & & \\ & b_2 & a_2 & \ddots & \\ & & & a_{N-1} & b_N \\ & & & b_N & a_N \end{pmatrix} \tag{51}$$

DMRG.3 Excited states - block Lanczos

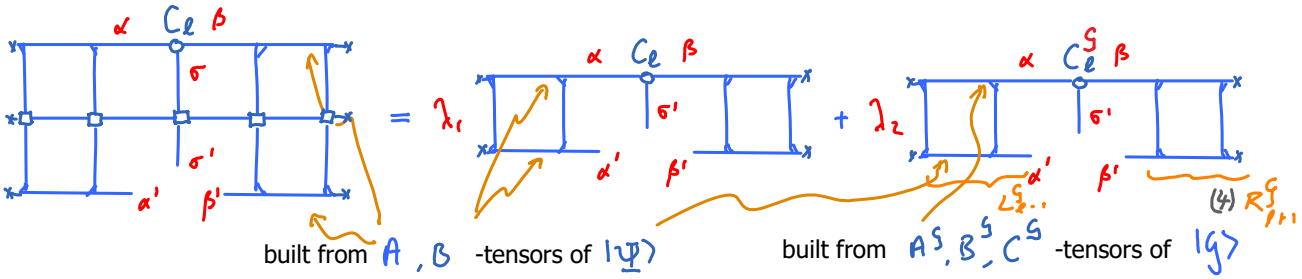
Suppose we have an MPS representation for ground state, $|g\rangle =$  (1)

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



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

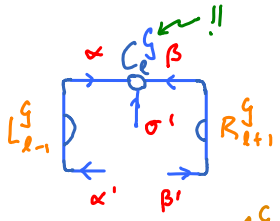
$$H^{(1)}_\ell C_\ell = \lambda_1 C_\ell + \lambda_2 C^g_\ell \quad (5) \qquad \text{with} \quad C^\dagger_\ell \cdot C_\ell \overset{(3)}{=} 1\,, \quad C^\dagger_\ell C^g_\ell \overset{(3)}{=} 0 \quad (6)$$

cf. (DMRG-I.1.7)

Displaying indices: $a' = (\alpha', \sigma', \beta')$, = ground state wave-function in local basis

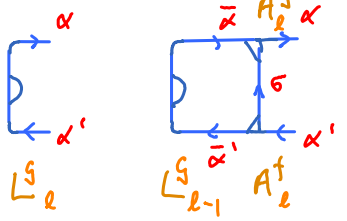
$$[H^{(1)}_\ell]^{a'}{}_a [C_\ell]^a = \lambda_1 [C_\ell]^{a'} + \lambda_2 [C^g_\ell]^{a'} \qquad [C^\dagger_\ell]_a [C_\ell]^a = 1\,, \quad [C^{\dagger g}_\ell]_a [C^g_\ell]^a = 1 \quad (7)$$

$$[C^g_\ell]^{a'} = [C^g_\ell]^{\alpha'\sigma'\beta'} = [L^g_{\ell-1}]^{\alpha'}{}_\alpha [A^g_\ell]^{\alpha\sigma'\beta} [R^g_{\ell+1}]_\beta{}^{\beta'} \quad (8)$$



with L and R computed iteratively,

$$[L^g_\ell]^{\alpha'}{}_\alpha = [A^\dagger_\ell]^{\alpha'}{}_{\sigma\bar\alpha'} [L^g_{\ell-1}]^{\bar\alpha'}{}_{\bar\alpha} [A^g_\ell]^{\bar\alpha\sigma}{}_\alpha \quad (9)$$



Index-free notation for (5): $H|c\rangle = \lambda_1|c\rangle + \lambda_2|g\rangle\,, \quad \langle c|g\rangle = 0$ (10)

Projector onto subspace orthogonal to $|g\rangle$: $\bar P_g = 1 - |g\rangle\langle g|\,, \quad \bar P_g|g\rangle = 0$ (11)

with indices: $\bar P_g{}^{a'}{}_a = \mathbb{1}^{a'}{}_a - g^{a'} g^\dagger_a\,,$ so that $\bar P_g{}^{a'}{}_a\, g^a = 0$ (12)

[with indices: $\bar{P}_g{}^{a'}{}_a = \mathbb{1}^{a'}{}_a - g^{a'} g^{\dagger}_a$, so that $\bar{P}_g{}^{a'}{}_a \, g^a = 0$] (12)

Project (10) onto this subspace: $\bar{P}_g H (\bar{P}_g + |g\rangle\langle g|) |C\rangle \overset{(10)}{=} \lambda_1 \bar{P}_g |C\rangle + \bar{P}_g \lambda_2 |g\rangle$ (13)

($\mathbb{1}$ from (11); $|g\rangle\langle g|C\rangle = 0$ from (10); $\bar{P}_g |g\rangle = 0$)

$$\bar{P}_g H \bar{P}_g |C\rangle = \lambda_1 P_g |C\rangle \quad (14)$$

This is simply an eigenvalue problem, for $\bar{P}_g H$, 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, $|v_0'\rangle = \bar{P}_g |v_0\rangle$ (15)

and construct new Krylov vectors using

$$|v_{n+1}^{\perp}\rangle = \bar{P}_g H |v_{n+1}\rangle - |v_n\rangle a_n - |v_{n-1}\rangle b_n \quad (16)$$

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 $j \leq n-2$, $\langle v_n | v_j \rangle \simeq 10^{-12} - 10^{-16}$ rather than 0. (17)

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 in (15).

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

Standard Lanczos: represent action of H as

$$H |v_0\rangle = |v_0\rangle a_0 + |v_1\rangle b_1 \Rightarrow \begin{pmatrix} a_0 & b_1 & & \\ b_1 & a_1 & b_2 & \\ & b_2 & \ddots & \end{pmatrix} \quad (18)$$

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

$|v_{0,i}\rangle$, $i = 1, \ldots, M$, and represent action of H as (19)

$$H |v_{0,i}\rangle = |v_{0,j}\rangle \mathbb{1}^j_i (a_0)^j{}_i + |v_{1,j}\rangle (b_1)^j{}_i \quad (20)$$

with $\langle v_{0,j} | v_{1,i} \rangle = 0$, $\langle v_{1,j} | v_{1,i} \rangle = \mathbb{1}^j_i$ (21)

and $(a_0)^j{}_i = \langle v_{0,j} | H | v_{0,i} \rangle$, $(b_1)^j{}_i = \langle v_{1,j} | H | v_{0,i} \rangle$ (22)

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

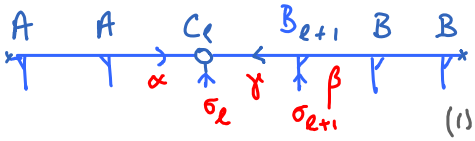
$$\begin{pmatrix} [a_0] & [b_1^{\dagger}] & & \\ [b_1] & [a_1] & [b_2^{\dagger}] & \\ & [b_2] & \ddots & \end{pmatrix} \quad (23)$$

DMRG.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.

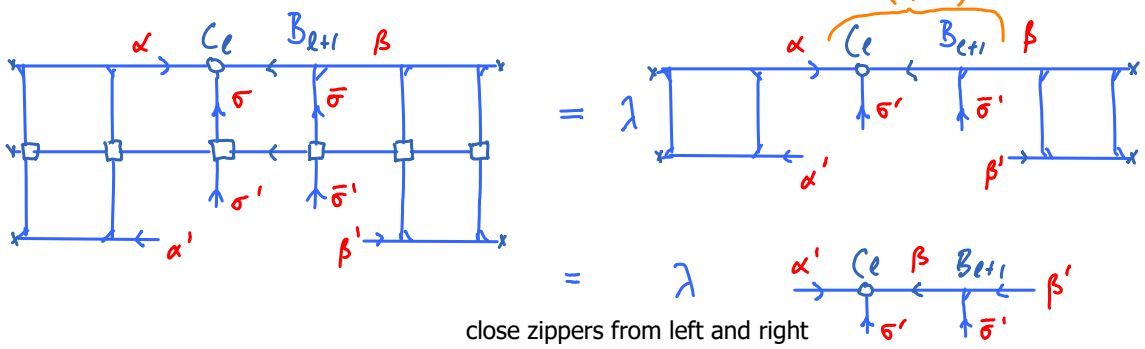
Represent MPS in site-canonical two-site basis:

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



Then extremize simultaneously w.r.t. $C^\dagger_\ell$ and $B^\dagger_{\ell+1}$

$$\frac{\partial}{\partial B^\dagger_{\ell+1}}\,\frac{\partial}{\partial C^\dagger_\ell}\left[\langle\Psi|\hat{H}|\Psi\rangle - \lambda\langle\Psi|\Psi\rangle\right] = 0 \qquad (2)$$



(3)

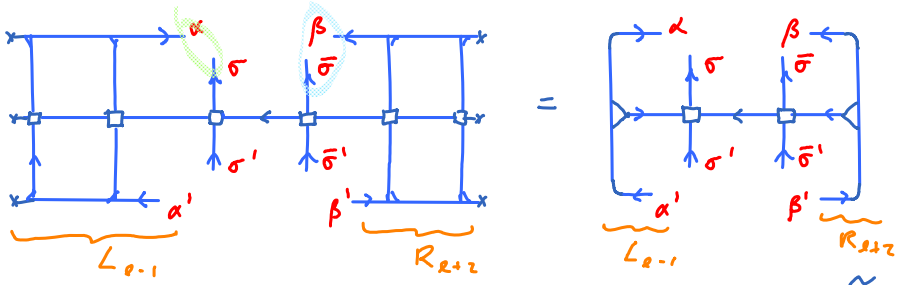
(4)

close zippers from left and right

Compact notation: $[H^{(2)}_\ell]^{a'}{}_{a}\,[\psi^{(2)}_\ell]^{a} = \lambda\,[\psi^{(2)}_\ell]^{a'}$ with composite index $a = (\alpha, \sigma, \bar\sigma, \beta)$ (5)

and

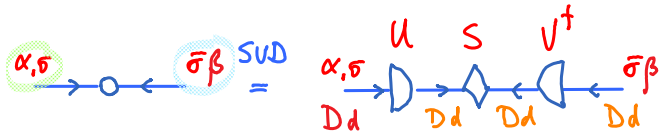
$[H^{(2)}_\ell]^{a'}{}_{a} =$



(6)

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

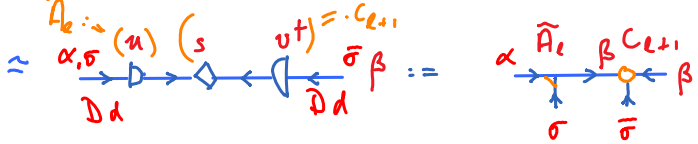
updated $[\tilde\psi^{(2)}_\ell]^{a}$ reshape =



(7)

Key point: S has Dd singular values, larger than the virtual bond dimension D of C_ℓ and $B_{\ell+1}$
Hence, it explores a larger state space, in general also including more symmetry sectors!

Truncate down to D and reshape:
This get rid of 'bad' symmetry sectors.



(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 (i.e. ground state energy converges).

Cost of 1-site DMRG: $O(D^3 d w + D^2 d^2 w^2)$ Cost of 2-site DMRG: $O(D^3 d^3 + D^3 d^2 w)$ (9)