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

1. Overlaps and normalization $\langle \tilde\psi | \psi \rangle$

Consider overlap of 2-site MPS:

$$|\beta\rangle = |\sigma_2\rangle|\sigma_1\rangle A^{1\sigma_1}{}_{\alpha} B^{\alpha\sigma_2}{}_{\beta}$$

$$\langle\beta'|\beta\rangle = \overline{A^{1\sigma_1'}{}_{\alpha'}}\ \overline{B^{\alpha'\sigma_2'}{}_{\beta'}}\ \underbrace{\langle\sigma_1'|\overbrace{\langle\sigma_2'|\sigma_2\rangle}^{\delta^{\sigma_2'}{}_{\sigma_2}}|\sigma_1\rangle}_{\delta^{\sigma_1'}{}_{\sigma_1}} A^{1\sigma_1}{}_{\alpha} B^{\alpha\sigma_2}{}_{\beta}$$

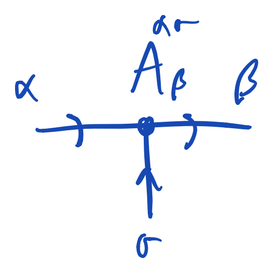
[$'$ → different variable for sum]

introduce $A^\dagger$: $\langle\beta'|\beta\rangle = A^{\dagger\alpha'}{}_{\sigma_1' 1} B^{\dagger\beta'}{}_{\sigma_2'\alpha'} \langle\langle\ \rangle\rangle A^{1\sigma_1}{}_{\alpha} B^{\alpha\sigma_2}{}_{\beta}$

reorder: $B^{\dagger\beta'}{}_{\sigma_2\alpha'} A^{\dagger\alpha'}{}_{\sigma_1 1} A^{1\sigma_1}{}_{\alpha} B^{\alpha\sigma_2}{}_{\beta}$ Messy!

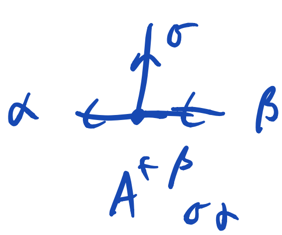
($\sigma_1'=\sigma_1$, $\sigma_2'=\sigma_2$)

Ket: $|\beta\rangle = |\sigma\rangle|\alpha\rangle A^{\alpha\sigma}{}_{\beta}$



Use diagrammatic rules to keep track of contraction patterns:

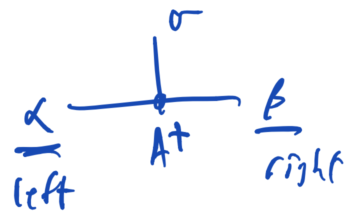
Bra: $\langle\beta| = \langle\alpha|\langle\sigma|\ \overline{A^{\alpha\sigma}{}_{\beta}} \equiv A^{\dagger\beta}{}_{\sigma\alpha}\langle\alpha|\langle\sigma|$



We accommodated complex conjugation via Hermitian conjugation and index transposition:

$$A^{\dagger\beta}{}_{\sigma\alpha} = \overline{A^{\alpha\sigma}{}_{\beta}}$$

left right



This scheme switches upper and lower indices -> inverts all arrows in diagram.

Note that in diagram the vertex α is left, β right, whereas on $A^\dagger$,

β sits left, α right.

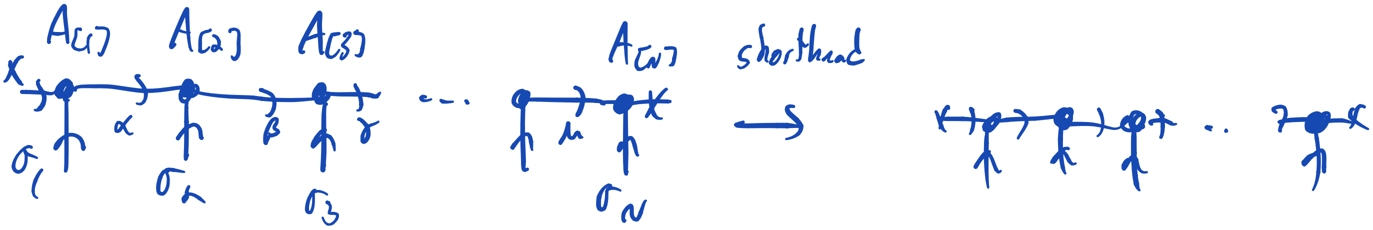
It will simplify the structure of diagrams representing overlaps.

Generalization to many-site MPS:

$$|\psi\rangle = |\vec{\sigma}\rangle_N \, A^{1\sigma_1}_{\underbrace{[1]}_{\text{site \#}}\alpha} \, A^{\alpha\sigma_2}_{[2]\beta} \, A^{\beta\sigma_3}_{[3]\gamma} \cdots A^{\mu\sigma_N}_{[N]\underbrace{1}_{\text{dummy index}}}$$

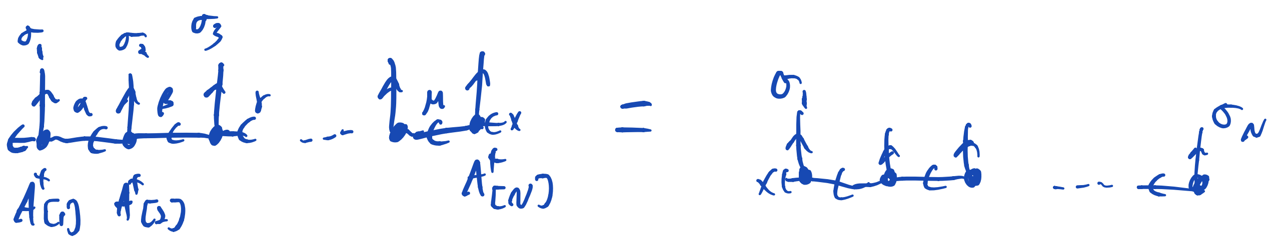
Square brackets indicate that each site has a different A matrix.

We can use shorthand notation and schematic: $A^{\alpha\sigma_\ell}{}_{\beta} \equiv A^{\alpha\sigma_\ell}_{[\ell]\beta}$ (ℓ = site #)



Recipe for ket formula: as chain grows, attach new matrices on the right (in the same order as vertices in diagram) resulting in MPS.

Bra:
$$\langle\psi| = \sum_{\bar\sigma} \langle\bar\sigma|\, \overline{A^{1\sigma_1}_{[1]\alpha}}\, \overline{A^{\alpha\sigma_2}_{[2]\beta}}\, A^{\beta\sigma_3}_{[3]\gamma} \cdots \overline{A^{\mu\sigma_N}_{[N]1}}$$
$$= A^{\dagger 1}_{[N]\sigma_N\mu} \cdots A^{\dagger\gamma}_{[3]\sigma_3\beta}\, A^{\dagger\beta}_{[2]\sigma_2\alpha}\, A^{\dagger\alpha}_{[1]\sigma_1 1} \langle\bar\sigma|_N$$

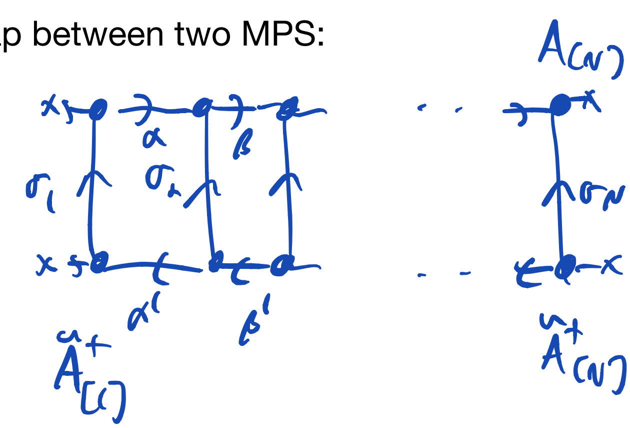


We rewrite using Hermitian conjugates, change schematic by transposing indices and inverting arrows. To recover MPS structure, order Hermitian conjugate matrices to appear in order opposite to vertex order in diagram.

Recipe for bra formula: as chain grows, attach new matrices $A^\dagger$ on the left, *opposite to vertex order in diagram.

Now consider overlap between two MPS:

$$\langle\tilde\psi|\psi\rangle =$$

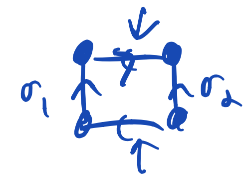


← contracting all physical (σ) indices

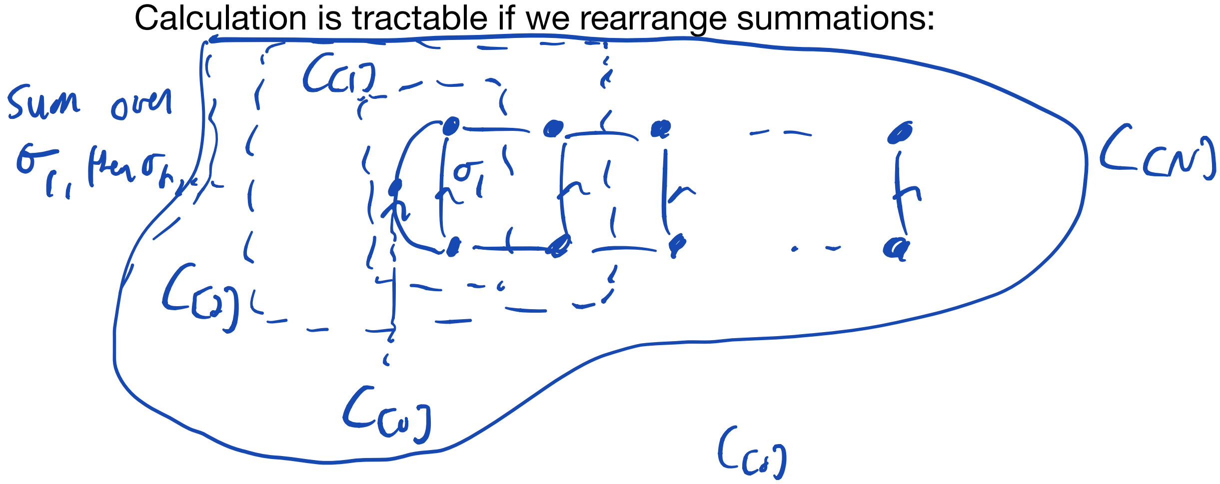
$$= \tilde A^{\dagger 1}_{[N]\sigma_N\mu'} \cdots \tilde A^{\dagger\alpha'}_{[1]\sigma_1 1}\, A^{1\sigma_1}_{[1]\alpha} \cdots A^{\mu\sigma_N}_{[N]1}$$

Exercise: derive result algebraically.

Contraction order matters! If we perform matrix multiplication first, for fixed $\bar{\sigma}$, and then sum over $\bar{\sigma}$, we get d^N terms, each of which is a product of matrices. Exponentially costly!

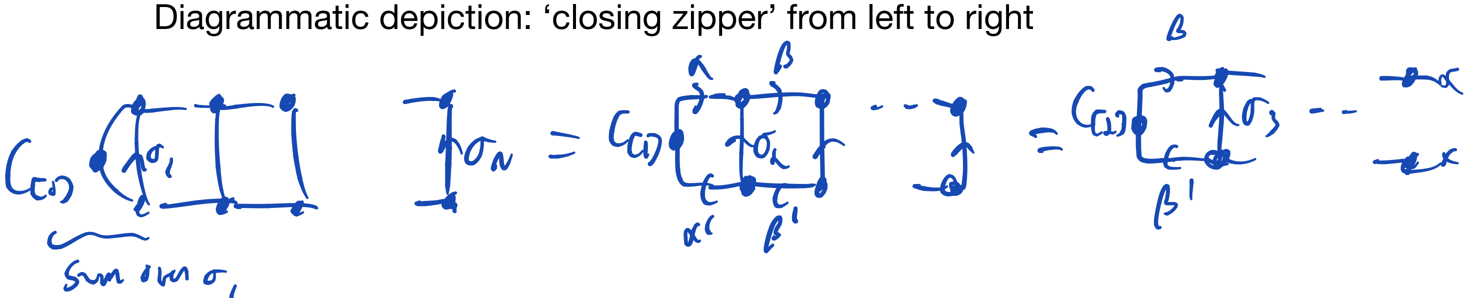


Calculation is tractable if we rearrange summations:



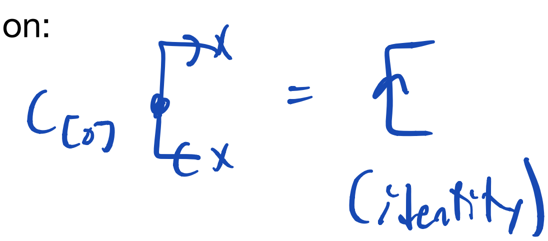
$$= A^{\dagger 1}_{\sigma_N \mu'} \cdots \underbrace{A^{\dagger \alpha'}_{\sigma_1 1} \cdot \overset{C_{[0]}}{\overset{\downarrow}{1}} \cdot A^{1\sigma_1}_{\alpha}}_{C_{[1]}} \cdots A^{\mu \sigma_N}_{1} = C'_{[N]1}$$

Diagrammatic depiction: 'closing zipper' from left to right



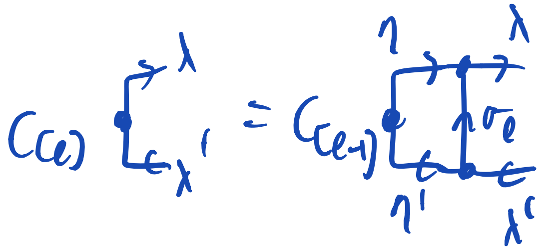
The set of two-leg tensors $C_{[\ell]}$ can be computed iteratively:

Initialization:



$C'_{[0]1} = 1$

Iteration step:



$$C^{\lambda'}_{[\ell]\lambda} = \tilde{A}^{\dagger\lambda'}_{\sigma_\ell \eta'} \, C^{\eta'}_{[\ell-1]\eta} \, A^{\eta\sigma_\ell}_{\lambda}$$

Final answer:

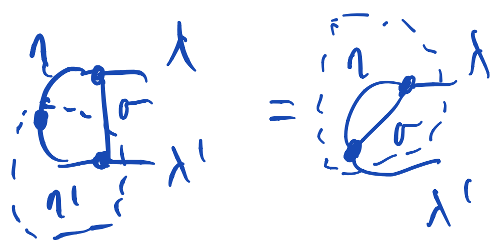
$$\langle \tilde{\psi} | \psi \rangle = C^{1}_{[N]1}$$

Cost estimate (assume all A's are $D \times D$):

One iteration:

$$D^2 \cdot d \cdot D + D^2 \cdot dD$$

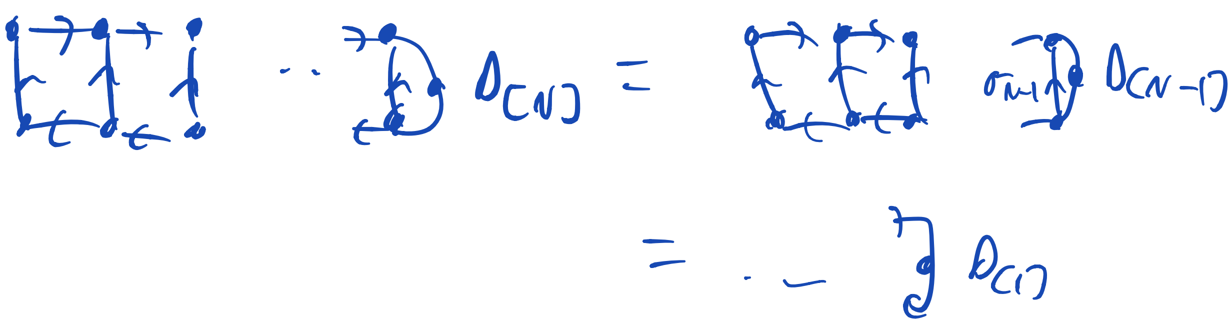
fixed $\lambda'\eta\sigma$, sum η' fixed, sum $\lambda\lambda'$ / $\eta\sigma$



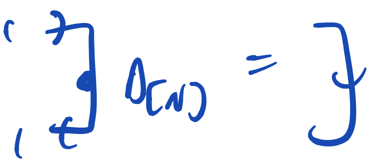
Total cost:

$$\sim D^3 \cdot d \cdot N \ll d^N \, !$$

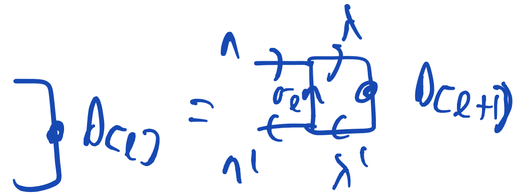
Remark: a similar iteration scheme can be used to 'close zipper' from right to left':



Initialization and iteration step:



Iteration:



Normalization: Try above scheme with $\langle\psi|\psi\rangle$

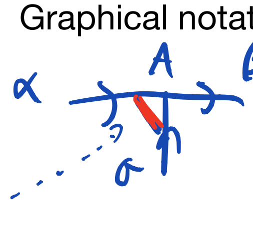
Left-normalization

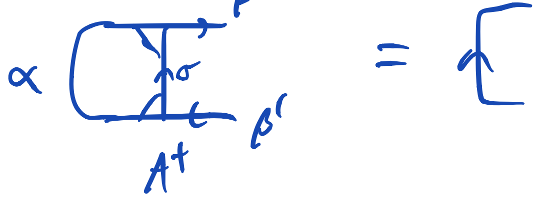
A 3-leg tensor $A^{\alpha\sigma}{}_{\beta}$ is called 'left-normalized' if it satisfies

$$A^{\dagger}A = I \quad \Leftrightarrow \quad (A^{\dagger}A)^{\beta'}{}_{\beta} = A^{\dagger\,\beta'}{}_{\underbrace{\sigma\alpha}_{\text{composite index}}} A^{\alpha\sigma}{}_{\beta} = I^{\beta'}{}_{\beta}$$

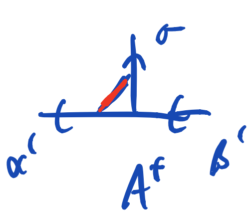
Graphical notation:

Kets:

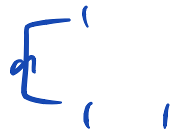
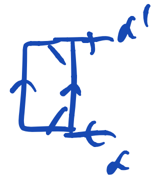
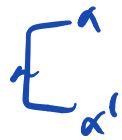




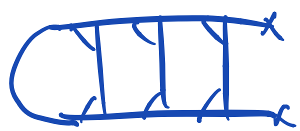
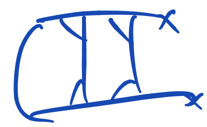
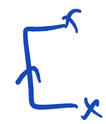
Bra:



When all A's are left-normalized, closing the zipper left-to-right is easy, since all $C_{[\ell]}$ reduce to identity matrices:

$C_{[0]} =$  , $C_{[1]\,\alpha}^{\;\alpha'} =$  $=$ 

Hence:

$\langle\psi|\psi\rangle =$  $=$  $\cdots =$ 

$= 1$

Left-normalized states are automatically normalized to unity.

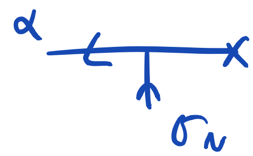
Right-normalization

So far we have viewed an MPS as being built up from left to right, hence used right-pointing arrows on ket diagram. Sometimes it is useful to build it up from right to left, running left-pointing arrows.

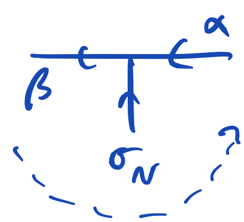
Building blocks:

ket:

$$|\alpha\rangle = |\sigma_N\rangle B_\alpha^{\sigma_N 1}$$

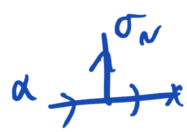


$$|\beta\rangle = |\sigma_N\rangle|\sigma_{N-1}\rangle B_\beta^{\sigma_{N-1}\alpha} B_\alpha^{\sigma_N 1}$$

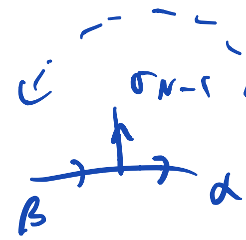


Bra:

$$\langle\alpha| = B^{\dagger\alpha}_{1\sigma_N}\langle\sigma_N|$$

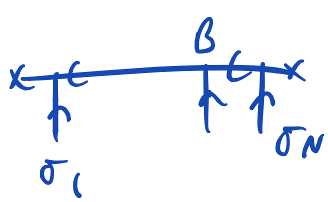


$$\langle\beta| = B^{\dagger\alpha}_{1\sigma_N} B^{\dagger\beta}_{\alpha\sigma_{N-1}} \langle\sigma_{N-1}|\langle\sigma_N|$$

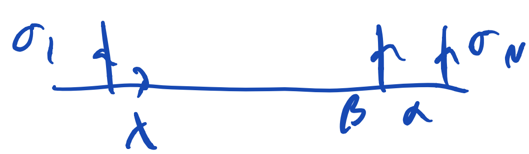


Iterating, we obtain kets and bras of the form

$$|\psi\rangle = |\sigma_N\rangle\ldots|\sigma_1\rangle B_1^{\sigma_1 x}\ldots B_\beta^{\sigma_{N-1}\alpha} B_\alpha^{\sigma_N 1}$$



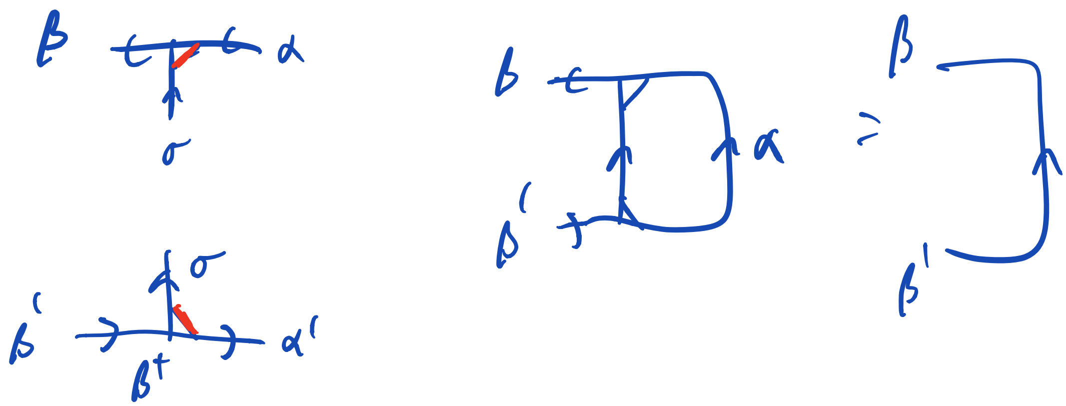
$$\langle\psi| = B^{\dagger\alpha}_{1\sigma_N} B^{\dagger\beta}_{\alpha\sigma_{N-1}}\ldots B^{\dagger 1}_{x\sigma_1}\langle\sigma_1|\ldots\langle\sigma_N|$$



A 3-leg tensor $B_\beta^{\sigma\alpha}$ is called right-normalized if it satisfies

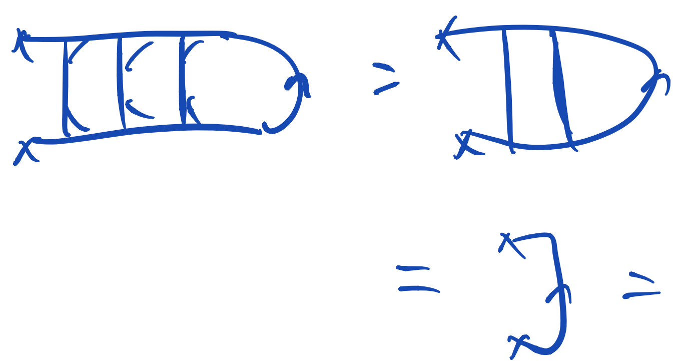
$$BB^\dagger = I, \quad (BB^\dagger)_\beta^{\beta'} = B_\beta^{\sigma\alpha} B^{\dagger\,\beta'}_{\alpha\sigma} = I_\beta^{\beta'}$$

Graphical notation for right-normalization:



When all A's are right-normalized, closing zipper right-to-left is easy

$\langle\psi|\psi\rangle =$

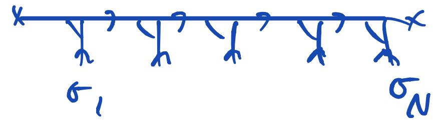


$= 1$

Conclusion: MPS built purely from left-normalized A or purely from right-normalized B are automatically normalized to 1.

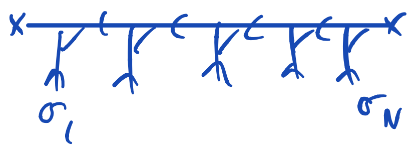
2. Various canonical MPS forms

Left-canonical (lc-) MPS

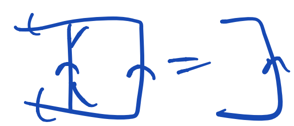


$$|\psi\rangle = |\bar{\sigma}\rangle_N \left(A^{\sigma_1} \ldots A^{\sigma_N}\right) \; ; \quad A^\dagger A = I \; ;$$

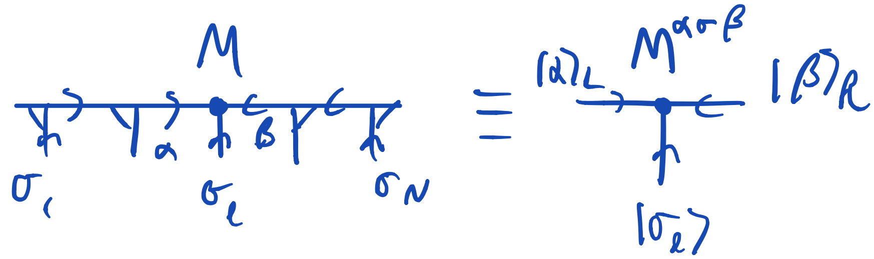
Right-canonical (rc-) MPS:



$$|\psi\rangle = |\bar{\sigma}\rangle_N \left(B^{\sigma_1} \ldots B^{\sigma_N}\right) \; ; \quad B B^\dagger = I \; ;$$

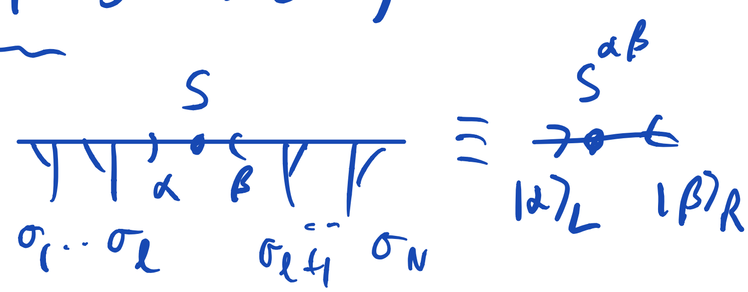


Site-canonical (sc-) MPS:
(expectation values)



$$|\psi\rangle = |\bar{\sigma}_N\rangle \left(A^{\sigma_1} \ldots A^{\sigma_{\ell-1}} \underset{\sim}{M^{\sigma_\ell}} B^{\sigma_{\ell+1}} \ldots B^{\sigma_N}\right)$$

Bond-canonical (bc-) (or mixed) MPS:
(entanglement)



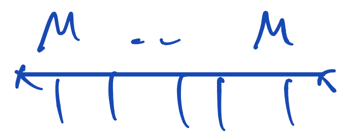
$$|\psi\rangle = |\bar{\sigma}\rangle_N \left(A^{\sigma_1} \ldots A^{\sigma_\ell}\right)_\alpha S^{\alpha\beta} \left(B^{\sigma_{\ell+1}} \ldots B^{\sigma_N}\right)_\beta$$

$$= \sum_{\alpha\beta} |\alpha\rangle_L S^{\alpha\beta} |\beta\rangle_R$$

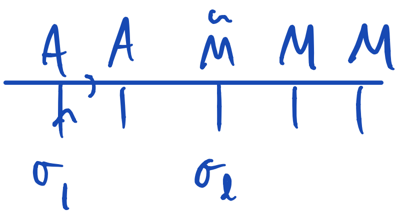
How to bring an arbitrary MPS into one of these forms?

<u>Transforming to left-normalized form</u>

Given: $|\psi\rangle = |\vec{\sigma}\rangle_N \left(M^{\sigma_1} \ldots M^{\sigma_N}\right)$



Goal: left-normalize $M^{\sigma_1} \to M^{\sigma_{\ell-1}}$

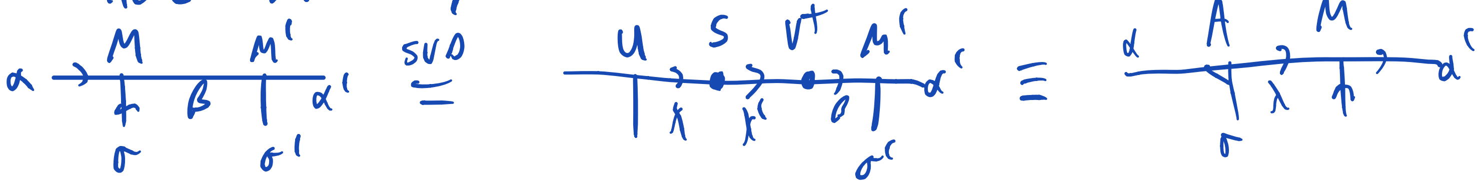


$$\boxed{\begin{aligned} &M^{\alpha\sigma}_{\beta} M^{\beta\sigma'}_{\alpha'} \\ &= U^{\alpha\sigma}_{\lambda}\left(S^{\lambda}_{\lambda'} V^{\dagger\lambda'}_{\beta} M^{\beta\sigma'}_{\alpha'}\right) \\ &= A^{\alpha\sigma}_{\lambda} \tilde{M}^{\lambda\sigma'}_{\alpha'} \end{aligned}}$$

Strategy: take a pair of adjacent tensors, MM', and use SVD:

$$MM' = USV^{\dagger}M' \equiv A\tilde{M}$$

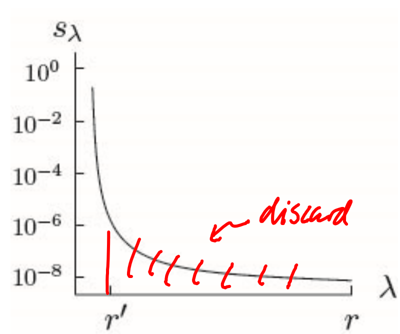
Here $A = U$, $\tilde{M} = SV^{\dagger}M'$.



Left-Normalization assured by: $U^{\dagger}U = I \Leftrightarrow A^{\dagger}A = I$

Truncation can be performed by discarding some of the smallest singular values(remains left-normalized!)

$$\sum_{\lambda=1}^{r} \to \sum_{\lambda=1}^{r'}$$



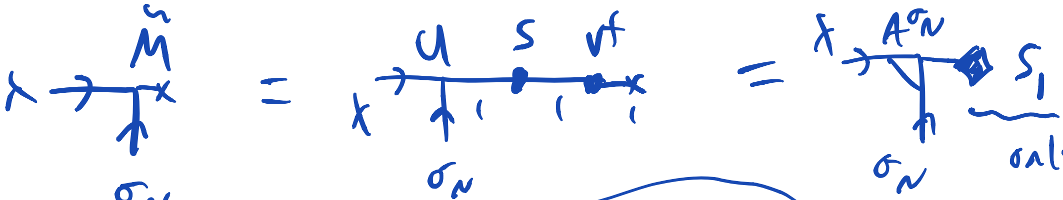
(truncation to decrease bond dimension)

Note: if we don't need to truncate we can use QR (cheaper).

By iterating, starting from $M^{\sigma_1}M^{\sigma_2}$, we left-normalize $M^{\sigma_1} \to M^{\sigma_{\ell-1}}$

To left-normalize the entire MPS, choose $\ell = N$.

As last step, left-normalize last site using SVD on final $\tilde{M}$:



vector

only 1 singular value

$\Rightarrow$ norm of state $= |s_1|^2$

$\equiv$ single number

$$\tilde{M}^{\lambda\sigma_N}_{1} = \underbrace{U^{\lambda\sigma_N}_{1}}_{A^{\lambda\sigma_N}_{1}} S_1 \underbrace{V^{\dagger}_{11}}_{=1}$$

lc-form:

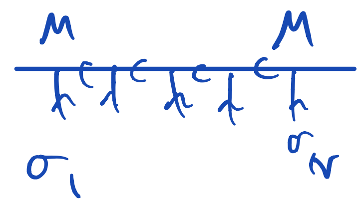
$$|\psi\rangle = |\vec{\sigma}\rangle_N \left(A^{\sigma_1} \cdots A^{\sigma_N}\right) s$$

The final singular value, s_1, determines normalization:

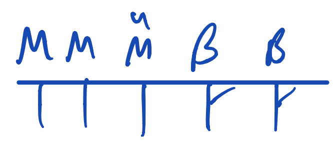
$$\langle\psi|\psi\rangle = |s_1|^2$$

<u>Transforming to right-normalized form</u>

Given: $|\psi\rangle = |\vec{\sigma}\rangle_N \left(M^{\sigma_1} \cdots M^{\sigma_N}\right)$

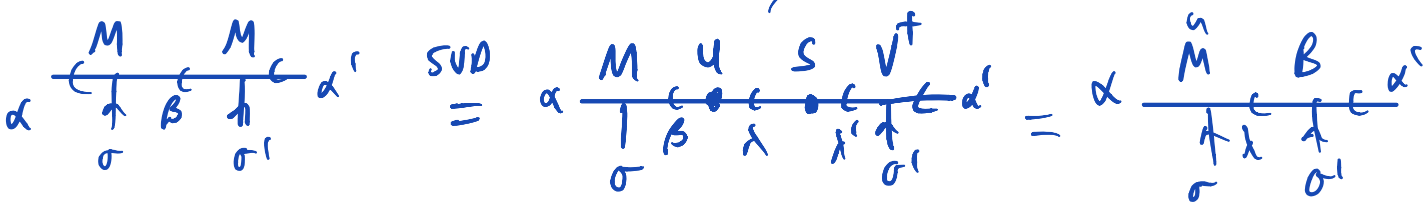


Goal: right normalize $M^{\sigma_N} \to M^{\sigma_{\ell+1}}$



Strategy: take a pair of adjacent tensors, MM', and use SVD:

$$MM' = MUSV^\dagger = \hat{M}B \; ; \quad \hat{M} = MUS, \; B = V^\dagger$$



$$M_\alpha^{\sigma\beta} M_\beta^{\sigma'\alpha'} = \left(M_\alpha^{\sigma\beta} U_\beta^{\lambda} S_\lambda^{\lambda'}\right)\left(V^{\dagger}{}_{\lambda'}^{\sigma'\alpha'}\right) = \hat{M}_\alpha^{\sigma\lambda'} B_{\lambda'}^{\sigma'\alpha'}$$

Here, right-normalization is assured by: $V^\dagger V = I \to BB^\dagger = I$ ✓

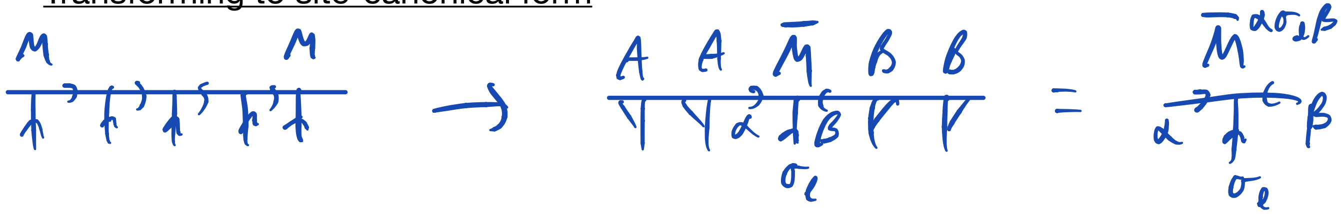
Starting from $M^{\sigma_{N-1}} M^{\sigma_N}$, move left to $M^{\sigma_\ell} M^{\sigma_{\ell+1}}$

To right-normalize entire chain, choose $l = 1$.

$$\underbrace{\tilde{M}_1^{\sigma_1 \lambda}}_{\text{vector}} = \underbrace{U_1^1}_{=1} \underbrace{S_1^1}_{S_1} V_1^{+\sigma_1 \lambda}$$

and as before S_1 determines normalization. $\left(\langle \psi | \psi \rangle = |S_1|^2 \right)$

Transforming to site-canonical form



Left-normalize states $1 \to \ell-1$ starting from site 1.

Then right-normalize states $N \to \ell+1$ starting from site N.

Result:
$$|\psi\rangle = |\sigma_N\rangle \cdots |\sigma_{\ell+1}\rangle \left(B^{\sigma_{\ell+1}} \cdots B^{\sigma_N}\right)_{\beta}^{\,1} |\sigma_\ell\rangle$$
$$\otimes\, |\sigma_{\ell-1}\rangle \cdots |\sigma_1\rangle \left(A^{\sigma_1} \cdots A^{\sigma_{\ell-1}}\right)_{\alpha}^{\,1} \bar{M}^{\alpha\sigma_\ell\beta}$$
$$= |\beta\rangle_R |\sigma_\ell\rangle |\alpha\rangle_L \bar{M}^{\alpha\sigma_\ell\beta}$$

We get an orthonormal set from the states (**Exercise in HW**):

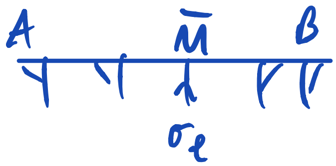
$$|\alpha, \sigma_\ell, \beta\rangle \equiv |\beta\rangle_R |\sigma_\ell\rangle |\alpha\rangle_L$$
$$\langle \alpha', \sigma_\ell', \beta' | \alpha, \sigma_\ell, \beta\rangle = \delta_{\alpha}^{\alpha'} \delta_{\sigma_\ell}^{\sigma_\ell'} \delta_{\beta}^{\beta'}$$

This basis is a 'local site basis' for site ℓ. Its dimension $D_\alpha d D_\beta$ is usually $\ll d^N =$ the dimension of the full Hilbert space.

Transforming to bond-canonical form:

Start from e.g. sc-form, use SVD for $\bar{M}$, combine (1) $V^\dagger$ with neighbor B

(2) U with neighbor A.



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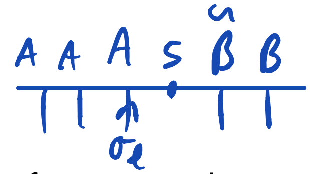


$= |\lambda\rangle_L |\lambda'\rangle_R S^{\lambda\lambda'}$

$$\boxed{\begin{aligned} A &= U \\ \hat{B} &= V^\dagger B \end{aligned}}$$

We get an orthonormal set of states again:

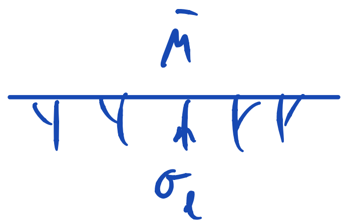
$|\lambda, \lambda'\rangle = |\lambda\rangle_R |\lambda_L\rangle$

$$\Rightarrow \quad \langle \bar{\lambda}, \bar{\lambda}' | \lambda, \lambda' \rangle = \delta^{\bar{\lambda}}_{\lambda} \delta^{\bar{\lambda}'}_{\lambda'}$$

This basis is the 'local bond basis' for bond ℓ (site ℓ & $\ell+1$). It has dimension $r \times r$

where r (= D?) = dimension of singular matrix S.

Option 2:



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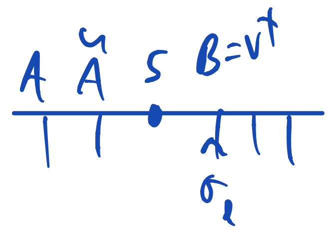


$$= \underbrace{|\lambda\rangle_L}_{1 \to \ell-1} \underbrace{|\lambda'\rangle_R}_{\ell \to N} S^{\lambda\lambda'}$$

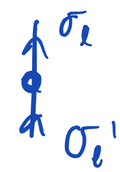
$\tilde{A} = AU$, $\quad B = V^\dagger$

$|\lambda, \lambda'\rangle = |\lambda\rangle_R |\lambda'\rangle_L$ = local bond basis for bond $\underline{\ell - 1}$ (from site $\ell-1, \ell$)

3. Matrix elements and expectation values

<u>One-site operator</u>

$$\hat{O}_{[\ell]} = |\sigma_\ell'\rangle\, O^{\sigma_\ell'}_{\sigma_\ell}\, \langle\sigma_\ell|$$



E.g. for spin 1/2: $(S_z)^{\sigma'}_{\sigma} = \frac{1}{2}\begin{pmatrix}1 & \\ & -1\end{pmatrix}$; $(S_+)^{\sigma'}_{\sigma} = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}$; $(S_-)^{\sigma'}_{\sigma} = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}$

Consider two states in site-canonical form for site ℓ :

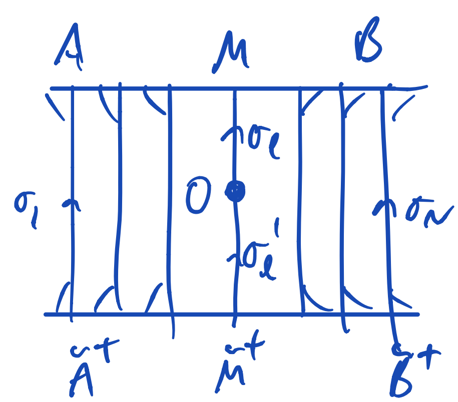
$$|\psi\rangle = |\vec{\sigma}_N\rangle \left(A^{\sigma_1}\cdots A^{\sigma_{\ell-1}} M^{\sigma_\ell} B^{\sigma_{\ell+1}}\cdots B^{\sigma_N}\right)$$

$$|\tilde{\psi}\rangle = |\vec{\sigma}_N'\rangle \left(\tilde{A}^{\sigma_1'}\cdots \tilde{A}^{\sigma_{\ell-1}'} \tilde{M}^{\sigma_\ell'} \tilde{B}^{\sigma_{\ell+1}'}\cdots \tilde{B}^{\sigma_N'}\right)$$

[$'$ $\rightarrow$ different index]

Matrix element:

$\langle\tilde{\psi}|\hat{O}|\psi\rangle =$



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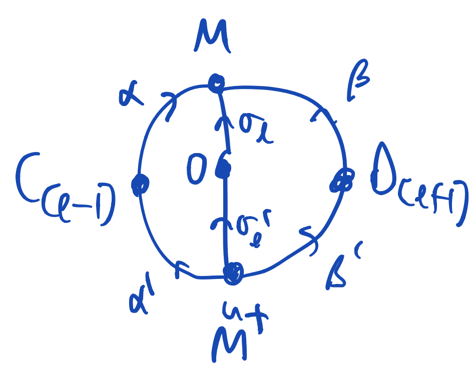


Close zipper from left and right:

$$= \tilde{M}^{\dagger}_{\beta'\sigma_\ell'\alpha'}\, C^{\alpha'}_{(\ell-1)\alpha}\, M^{\alpha\sigma_\ell\beta}\, D^{\beta'}_{(\ell+1)\beta}\, O^{\sigma_\ell'}_{\sigma_\ell}$$

Consider expectation value: $\langle \psi | \hat{O} | \psi \rangle$

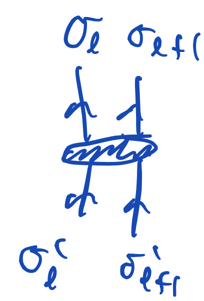
Left-normalization means: $C_{[l-1]} = I$

Right-normalization means $D_{[l+1]} = I$

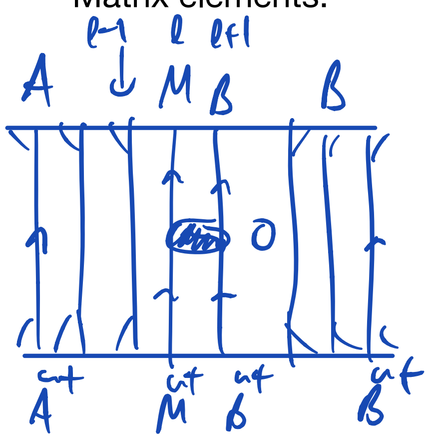
Hence,
$$\langle \psi | \hat{O} | \psi \rangle = M^{\dagger}_{\beta \sigma_l' \alpha} M^{\alpha \sigma_l \beta} O^{\sigma_l'}_{\sigma_l}$$

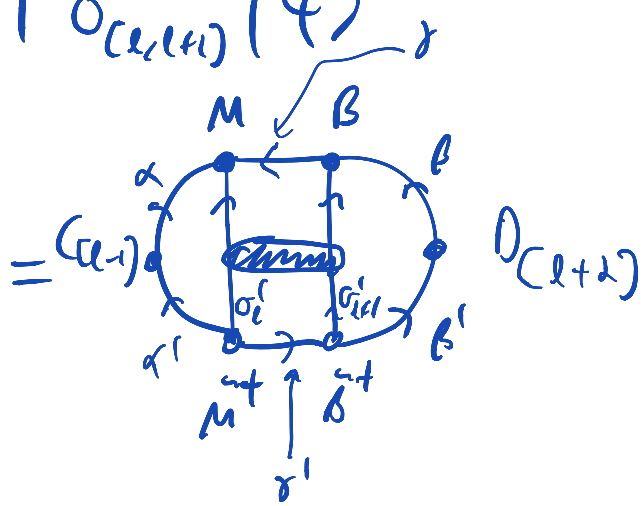
<u>Two-site operator</u> (e.g. for spin chain Hamiltonian term $\bar{S}_l \cdot \bar{S}_{l+1}$)

$$\hat{O}_{[l,l+1]} = |\sigma_{l+1}'\rangle |\sigma_l'\rangle \, O^{\sigma_l' \sigma_{l+1}'}_{\sigma_l \sigma_{l+1}} \langle \sigma_l | \langle \sigma_{l+1} |$$



Matrix elements: $\langle \psi | \hat{O}_{[l,l+1]} | \psi \rangle$



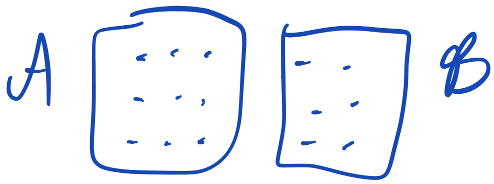


$$= B^{\dagger\,\gamma'}_{\beta' \sigma_{l+1}'} M^{\dagger}_{\gamma' \sigma_l' \alpha'} C^{\alpha'}_{[l-1]\alpha} M^{\alpha \sigma_l \gamma} B_{\gamma}^{\sigma_{l+1} \beta} D^{\beta'}_{[l+2]\beta} O^{\sigma_l' \sigma_{l+1}'}_{\sigma_l \sigma_{l+1}}$$

4. Schmidt decomposition

Consider a quantum system composed of two subsystems $\mathcal{A}, \mathcal{B}$

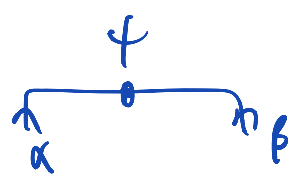
with dimensions D, D' and orthonormal bases $\{|\alpha\rangle_A\}$ & $\{|\beta\rangle_B\}$



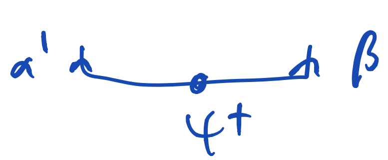
To be specific, think of physical basis: $|\alpha\rangle_{\mathcal{A}} \equiv |\bar{\sigma}_A\rangle$; $|\beta\rangle_{\mathcal{B}} \equiv |\bar{\sigma}_B\rangle$

General form of pure state on joint set $\mathcal{A} \cup \mathcal{B}$

$$|\psi\rangle = |\beta\rangle_{\mathcal{B}} |\alpha\rangle_{\mathcal{A}} \psi^{\alpha\beta}$$

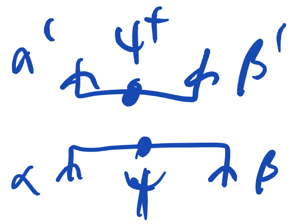


$$\langle\psi| = \psi^{\dagger}_{\beta'\alpha'} \, {}_{\mathcal{A}}\langle\alpha'| \, {}_{\mathcal{B}}\langle\beta'|$$



Density matrix:

$$\hat{\rho} = |\psi\rangle\langle\psi|$$



$\boxed{\bar{\mathcal{B}} = \text{complete set for } \mathcal{B}}$

Reduced density matrix of subsystem $\mathcal{A}$:

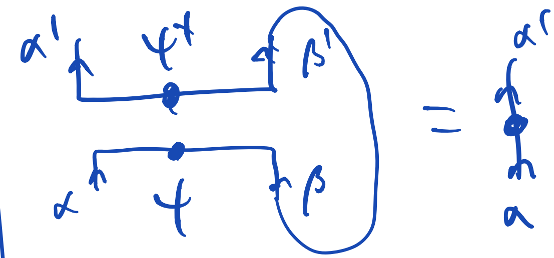
$$\hat{\rho}_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}} |\psi\rangle\langle\psi| = \sum_{\bar{\beta}} {}_{\mathcal{B}}\langle\bar{\beta}|\beta\rangle_{\mathcal{B}} |\alpha\rangle_{\mathcal{A}} \psi^{\alpha\beta} \psi^{\dagger}_{\beta'\alpha'} \, {}_{\mathcal{A}}\langle\alpha'| \, {}_{\mathcal{B}}\langle\beta'|\bar{\beta}\rangle_{\mathcal{B}}$$

$$= |\alpha\rangle_{\mathcal{A}} (\rho_A)^{\alpha}{}_{\alpha'} \, {}_{\mathcal{A}}\langle\alpha'|$$

$$(\rho_A)^{\alpha}{}_{\alpha'} = \sum_{\bar\beta} \underbrace{\langle\bar\beta|\beta\rangle}_{\delta^{\bar\beta}{}_{\beta}} \psi^{\alpha\beta}\psi^{\dagger}{}_{\beta'\alpha'} \underbrace{\langle\beta'|\bar\beta\rangle}_{\delta^{\beta'}{}_{\bar\beta}}$$

with

$$= \psi^{\alpha\beta}\psi^{\dagger}{}_{\beta\alpha'} = (\psi\psi^{\dagger})^{\alpha}{}_{\alpha'}$$

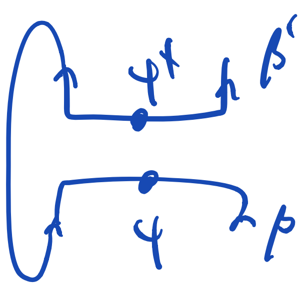


Analogously, RDM of subsystem $\mathcal{B}$:

Diagrammatic derivation:

$$\hat\rho_{B} = \mathrm{Tr}_A |\psi\rangle\langle\psi| = |\beta\rangle(\rho_B)^{\beta}{}_{\beta'}\langle\beta'|$$

$$(\rho_B)^{\beta}{}_{\beta'} = (\psi^{\dagger}\psi)^{\beta}{}_{\beta'}$$



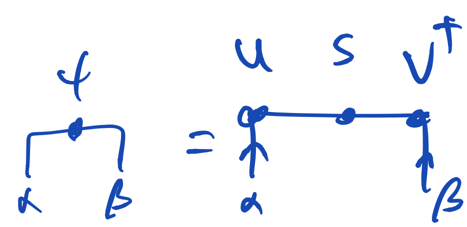
Algebraic derivation:

<u>Singular value decomposition:</u>

Use SVD to find basis for $\mathcal{A}$ & $\mathcal{B}$ that diagonalizes ψ

SVD of $\psi = U S V^\dagger$

With indices: $\psi^{\alpha\beta} = U^{\alpha}{}_{\lambda} S^{\lambda\lambda'} V^{\dagger}_{\lambda'}{}^{\beta}$



Hence $$|\psi\rangle = |\lambda\rangle_{\mathcal{A}} |\lambda'\rangle_{\mathcal{B}} \underbrace{S^{\lambda\lambda'}}_{\text{diagonal}} = \sum_{\lambda} |\lambda\rangle_{\mathcal{A}} |\lambda\rangle_{\mathcal{B}} s_{\lambda}$$

where $$|\lambda\rangle_{\mathcal{A}} = |\alpha\rangle U^{\alpha}{}_{\lambda}$$

$$|\lambda\rangle_{\mathcal{B}} = |\beta\rangle V^{\dagger}_{\lambda}{}^{\beta}$$

are orthonormal sets of states for A & B, and can be extended to yield orthonormal bases if needed.

Orthonormality is guaranteed by $U^\dagger U = I$, $V^\dagger V = I$.

Restrict Σ_λ to the r non-zero singular values to get a

<u>Schmidt decomposition:</u>

$$|\psi\rangle = \sum_{\lambda=1}^{r} s_\lambda |\lambda\rangle_A |\lambda\rangle_B$$

Classical state: $r = 1$

Entangled state: $r > 1$

$r \equiv$ Schmidt number

$$\rho_A = \sum_{\lambda\lambda'} \langle\beta| s_\lambda |\lambda\rangle_A |\lambda\rangle_B \, s_{\lambda'} \, {}_A\langle\lambda'| \, {}_B\langle\lambda'|\beta\rangle$$

$$= \sum_\lambda s_\lambda^2 \, |\lambda\rangle_A \, {}_A\langle\lambda|$$

In this representation, RDMs are diagonal:

$$\hat{\rho}_A = \sum_\lambda |\lambda\rangle_A (s_\lambda)^2 \langle\lambda|_A \; ; \quad \hat{\rho}_B = \sum_\lambda |\lambda\rangle_B (s_\lambda)^2 \langle\lambda|_B$$

Entanglement entropy: $$S_{A|B} = -\sum_{\lambda=1}^{r} (s_\lambda)^2 \ln (s_\lambda)^2$$

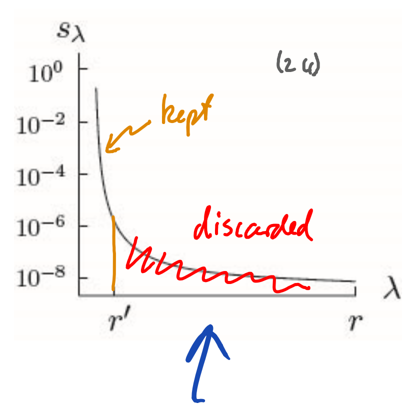
How can one approximate ψ by a cheaper $\tilde{\psi}$?

$$\| |\psi\rangle \|^2 \equiv \langle\psi|\psi\rangle = \sum_{\alpha\beta} |\psi_{\alpha\beta}|^2 = \|\psi\|^2 = \text{Frobenius norm}$$

Define truncated state using $r' < r$ singular values:

$$|\tilde{\psi}\rangle \equiv \sum_{\lambda=1}^{r'} |\lambda\rangle_A |\lambda\rangle_B s_\lambda$$

(If a normalized state is needed, rescale s_λ by $\sum_{\lambda=1}^{r'} s_\lambda^2$)



Truncation error: sum of squares of discarded singular values

$$\| |\psi\rangle - |\tilde{\psi}\rangle \|^2 = \langle\psi|\psi\rangle + \langle\tilde{\psi}|\tilde{\psi}\rangle - 2\,\mathrm{Re}(\langle\tilde{\psi}|\psi\rangle)$$

$$= \sum_{\lambda=1}^{r} (s_\lambda)^2 + \sum_{\lambda=1}^{r'} (s_\lambda)^2 - 2\sum_{\lambda=1}^{r'} (s_\lambda)^2$$

$$= \sum_{\lambda=r'+1}^{r} (s_\lambda)^2$$

Useful to obtain 'cheap' representation of if singular values decay rapidly.