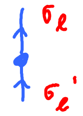
MPS II: Matrix product states

MPS-II.1

## 1. Matrix elements and expectation values

One-site operator

$$\hat{O}_{[\ell]} = |\sigma'_\ell\rangle \, O^{\sigma'_\ell}{}_{\sigma_\ell} \, \langle \sigma_\ell | \qquad (1)$$



E.g. for spin $1/2$ :

$$(S_z)^{\sigma'}{}_{\sigma} = \tfrac{1}{2}\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}, \quad (S_+)^{\sigma'}{}_{\sigma} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad (S_-)^{\sigma'}{}_{\sigma} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad (2)$$

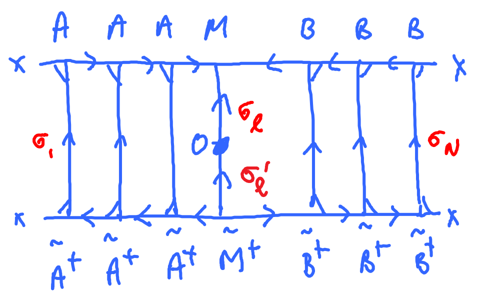
Consider two states in site-canonical form for site $\ell$ :

$$|\psi\rangle = |\sigma_N\rangle \left( A^{\sigma_1} \cdots A^{\sigma_{\ell-1}} M^{\sigma_\ell} B^{\sigma_{\ell+1}} \cdots B^{\sigma_N} \right) \qquad (3)$$

$$|\tilde{\psi}\rangle = |\sigma'_N\rangle \left( \tilde{A}^{\sigma'_1} \cdots \tilde{A}^{\sigma'_{\ell-1}} \tilde{M}^{\sigma'_\ell} \tilde{B}^{\sigma'_{\ell+1}} \cdots \tilde{B}^{\sigma'_N} \right) \qquad (4)$$

Matrix element:

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





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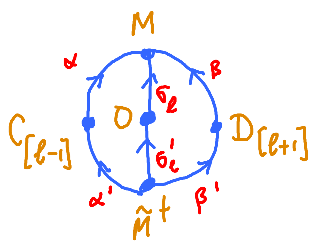



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Close zipper from left using $C_{[\ell-1]}$ from left-normalized $A$'s [see MPS-I.1-(15)],
and from right using $D_{[\ell+1]}$ from right-normalized $B$'s [analogous to MPS-I.1-(20)].

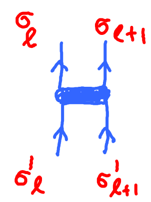
$$= \tilde{M}^\dagger{}_{\beta'\sigma'_\ell\alpha'} \, C_{[\ell-1]}{}^{\alpha'}{}_{\alpha} \, M^{\alpha\sigma_\ell\beta} \, D_{[\ell+1]}{}_{\beta}{}^{\beta'} \, O^{\sigma'_\ell}{}_{\sigma_\ell} \qquad (6)$$

Now consider the expectation value, $\langle\psi|\hat{O}|\psi\rangle$ (i.e. drop all tilde's). The left-normalization of $A$'s guarantees that $C_{[\ell-1]} = \mathbb{1}$ , and right-normalization of $B$'s that $D_{[\ell+1]} = \mathbb{1}$.

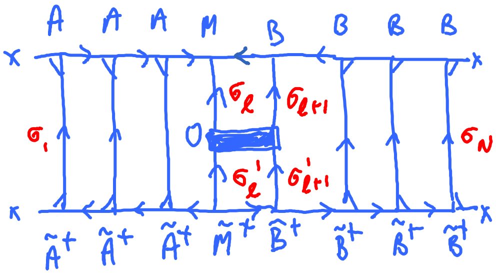
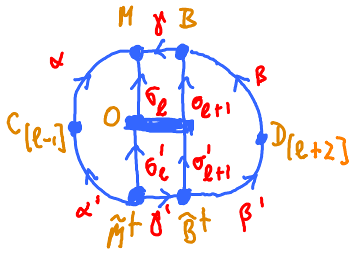
Hence
$$\langle\psi|\hat{O}|\psi\rangle = M^\dagger{}_{\beta\sigma'_\ell\alpha} \, M^{\alpha\sigma_\ell\beta} \, O^{\sigma'_\ell}{}_{\sigma_\ell} \qquad (7)$$

Two-site operator (e.g. for spin chain: $\vec{S}_\ell \cdot \vec{S}_{\ell+1}$ )

$$\hat{O}_{[\ell,\ell+1]} = |\sigma'_{\ell+1}\rangle|\sigma'_\ell\rangle \, O^{\sigma'_\ell\sigma'_{\ell+1}}{}_{\sigma_\ell\sigma_{\ell+1}} \, \langle\sigma_\ell|\langle\sigma_{\ell+1}| \qquad (10)$$



Matrix elements:

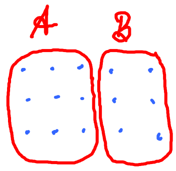
$\langle\tilde\psi|\hat O_{[\ell,\ell+1]}|\psi\rangle =$  $=$  (11)



$$= \tilde B^{\dagger}{}_{\beta'\sigma'_{\ell+1}}{}^{\gamma'}\, \tilde M^{\dagger}{}_{\gamma'\sigma'_\ell\alpha'}\, C_{[\ell-1]}{}^{\alpha'}{}_{\alpha}\, M^{\alpha\sigma_\ell\gamma}\, B_{\gamma}{}^{\sigma_{\ell+1}\beta} D_{[\ell+2]}{}_{\beta}{}^{\beta'}\, O^{\sigma'_\ell\sigma'_{\ell+1}}{}_{\sigma_\ell\sigma_{\ell+1}} \qquad (12)$$

## 2. Schmidt decomposition





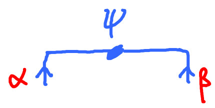

Consider a quantum system composed of two subsystems, $\mathcal{A}$ and $\mathcal{B}$,

with dimensions $D$ and $D'$, and orthonormal bases $\{|\alpha\rangle_{\mathcal{A}}\}$ and $\{|\beta\rangle_{\mathcal{B}}\}$.

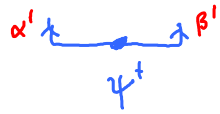
To be specific, think of physical basis: $|\alpha\rangle_{\mathcal{A}} \equiv |\vec{\sigma}_{\mathcal{A}}\rangle$, $|\beta\rangle_{\mathcal{B}} \equiv |\vec{\sigma}_{\mathcal{B}}\rangle$ (1)

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

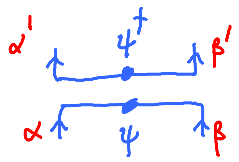
$$|\psi\rangle = |\beta\rangle_{\mathcal{B}} |\alpha\rangle_{\mathcal{A}} \psi^{\alpha\beta} \tag{2}$$




$$\langle\psi| = \underbrace{\psi^\dagger_{\beta'\alpha'}}_{\equiv\,\overline{\psi^{\alpha'\beta'}}}\ {}_{\mathcal{A}}\langle\alpha'|\,{}_{\mathcal{B}}\langle\beta'| \tag{3}$$




Density matrix: $\hat{\rho} = |\psi\rangle\langle\psi|$ (4)




Reduced density matrix of subsystem :

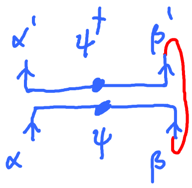
$$\hat{\rho}_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}} |\psi\rangle\langle\psi| = \sum_{\bar\beta} {}_{\mathcal{B}}\langle\bar\beta|\beta\rangle_{\mathcal{B}} |\alpha\rangle_{\mathcal{A}} \psi^{\alpha\beta}\, \psi^\dagger_{\beta'\alpha'}\, {}_{\mathcal{A}}\langle\alpha'|\, {}_{\mathcal{B}}\langle\beta'|\bar\beta\rangle_{\mathcal{B}} \tag{5}$$

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

with

$$(\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} = \sum_{\bar\beta} \underbrace{{}_{\mathcal{B}}\langle\bar\beta|\beta\rangle_{\mathcal{B}}}_{\delta^{\bar\beta}{}_{\beta}} \psi^{\alpha\beta}\, \psi^\dagger_{\beta'\alpha'} \underbrace{{}_{\mathcal{B}}\langle\beta'|\bar\beta\rangle_{\mathcal{B}}}_{\delta^{\beta'}{}_{\bar\beta}} = \psi^{\alpha\beta}\underbrace{\psi^\dagger_{\beta\alpha'}}_{} \equiv (\psi\psi^\dagger)^{\alpha}{}_{\alpha'} \tag{6}$$

$\hat{\rho}_A =$

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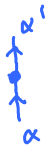


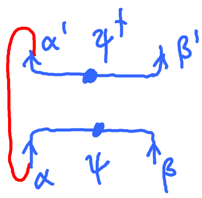

$$\psi^{\alpha\beta}\,\psi^\dagger_{\beta\alpha'} = (\psi\psi^\dagger)^{\alpha}{}_{\alpha'} \tag{7}$$

Analogously: reduced density matrix of subsystem $\mathcal{B}$ :

$$\hat{\rho}_{\mathcal{B}} = \mathrm{Tr}_{\mathcal{A}} |\psi\rangle\langle\psi| = |\beta\rangle_{\mathcal{B}} (\rho_{\mathcal{B}})^{\beta}{}_{\beta'}\, {}_{\mathcal{B}}\langle\beta'| \quad \text{with} \quad (\rho_{\mathcal{B}})^{\beta}{}_{\beta'} = (\psi^\dagger\psi)_{\beta'}{}^{\beta} \tag{8}$$

Diagrammatic derivation:

$\hat{\rho}_B =$

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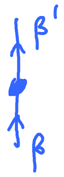



$$\psi^{\alpha\beta}\,\psi^\dagger_{\beta'\alpha} = (\psi^\dagger\psi)_{\beta}{}^{\beta'} \tag{9}$$

Algebraic derivation:

$$(\rho_B)^{\beta}{}_{\beta'} = \sum_{\bar\alpha} \underbrace{{}_A\langle\bar\alpha|\alpha\rangle_A}_{\delta^{\bar\alpha}{}_{\alpha}} \psi^{\alpha\beta}\, \psi^\dagger_{\beta'\alpha'} \underbrace{{}_A\langle\alpha'|\bar\alpha\rangle_A}_{\delta^{\alpha'}{}_{\bar\alpha}} = \psi^\dagger_{\beta'\alpha}\psi^{\alpha\beta} \equiv (\psi^\dagger\psi)_{\beta'}{}^{\beta} \qquad (10)$$

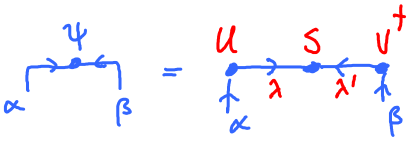
## Singular value decomposition

Use SVD to find basis for $\mathcal{A}$ and $\mathcal{B}$ which diagonalizes $\psi$ :

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

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

$S^{\lambda\lambda'}$: diag$(s_1, s_2, \dots)$

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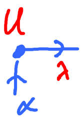
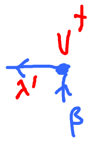
Hence $\qquad |\psi\rangle = |\lambda'\rangle_B |\lambda\rangle_A\, S^{\lambda\lambda'} = \sum_\lambda |\lambda\rangle_B |\lambda\rangle_A\, s_\lambda \qquad (12)$

where $\qquad |\lambda\rangle_A = |\alpha\rangle_A U^{\alpha}{}_{\lambda}$ ,




$|\lambda\rangle_B = |\beta\rangle V^{\dagger}{}_{\lambda}{}^{\beta}$

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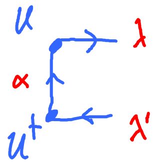
are orthonomal sets of states for $\mathcal{A}$ and $\mathcal{B}$ , and can be extended to yield orthonormal bases for $\mathcal{A}$ and $\mathcal{B}$ if needed.

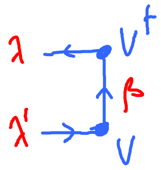
Orthonormality is guaranteed by $\qquad U^\dagger U = \mathbb{1}$ and $V^\dagger V = \mathbb{1}$ !

$${}_A\langle\lambda'|\lambda\rangle_A =$$




$$= U^{\dagger\lambda'}{}_{\alpha} U^{\alpha}{}_{\lambda} = \mathbb{1}^{\lambda'}{}_{\lambda} \qquad (14)$$

$${}_B\langle\lambda'|\lambda\rangle_B =$$




$$= V^{\dagger}{}_{\lambda}{}^{\beta} V_{\beta}{}^{\lambda'} = \mathbb{1}_{\lambda'}{}^{\lambda} \qquad (15)$$

Restrict $\Sigma_\lambda$ to the $r$ non-zero singular values:

$$|\psi\rangle = \sum_{\lambda=1}^{r} |\lambda\rangle_B |\lambda\rangle_A \qquad \text{'Schmidt decomposition'} \qquad (16)$$

If $r = 1$ : 'classical' state. If $r \geq 1$ : 'entangled state'

In this representation, reduced density matrices are diagonal:

$$\hat\rho_A = \mathrm{Tr}_B |\psi\rangle\langle\psi| = \sum_\lambda |\lambda\rangle_A (s_\lambda)^2\, {}_A\langle\lambda| \qquad (17)$$

$(\psi\psi^\dagger)$, $(\psi^\dagger\psi)$ with $\psi^{\lambda\lambda} = s^\lambda \mathbb{1}^{\lambda\lambda}$

$$\hat{\rho}_B = \mathrm{Tr}_A |\psi\rangle\langle\psi| = \sum_\lambda |\lambda\rangle_B (s_\lambda)^2 {}_B\langle\lambda| \tag{18}$$

Entanglement entropy:

$$S_{A|B} = -\sum_{\lambda=1}^{r} (s_\lambda)^2 \ln_2 (s_\lambda)^2 \tag{19}$$

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

$$\| |\psi\rangle \|_2^2 \equiv |\langle\psi|\psi\rangle|^2 = \sum_{\alpha\beta} |\psi^{\alpha\beta}|^2 = \|\psi\|_F^2 \tag{20}$$

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

$$|\tilde{\psi}\rangle \equiv \sum_{\lambda=1}^{r'} |\lambda\rangle_B |\lambda\rangle_A \, s_\lambda \tag{21}$$

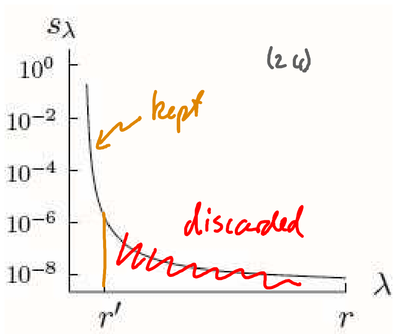
(If $|\tilde{\psi}\rangle$ should be normalized, rescale $s_\lambda$ by $\sum_{\lambda=1}^{r'} (s_\lambda)^2$ .)

Truncation error:

$$\| |\psi\rangle - |\tilde{\psi}\rangle \|_2^2 = \langle\psi|\psi\rangle + \langle\tilde{\psi}|\tilde{\psi}\rangle - 2\,\mathrm{Re}\langle\tilde{\psi}|\psi\rangle \tag{23}$$

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

= sum of squares of discarded singular values




Useful to obtain "cheap" representation of $|\psi\rangle$ if singular values decay rapidly.

## Exercise: Reduced density matrix revisited

Consider a quantum system, subdivided into parts $\mathcal{A}$ and $\mathcal{B}$, defined on sites $1$ to $\ell$ and $\ell+1$ to $N$. Let $\{|\alpha\rangle_{\mathcal{A}}\}$ be a general basis for $\mathcal{A}$, and $\{|\beta\rangle_{\mathcal{B}}\}$ a general basis for $\mathcal{B}$.

$$|\alpha\rangle_{\mathcal{A}} = |\vec{\sigma}_{\mathcal{A}}\rangle A^{\vec{\sigma}_{\mathcal{A}}}{}_{\alpha} ,$$

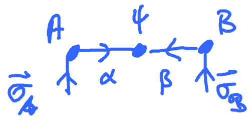
$$|\beta\rangle_{\mathcal{B}} = |\vec{\sigma}_{\mathcal{B}}\rangle B_{\beta}{}^{\vec{\sigma}_{\mathcal{B}}}$$


when $A$ and $B$ are unitary,

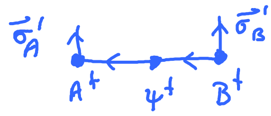
$$(A^\dagger A)^{\alpha'}{}_{\alpha} = \mathbb{1}^{\alpha'}{}_{\alpha} , \quad (B B^\dagger)_{\beta}{}^{\beta'} = \mathbb{1}_{\beta}{}^{\beta'}$$

Consider the pure state

$$|\psi\rangle = |\beta\rangle_{\mathcal{B}} |\alpha\rangle_{\mathcal{A}} \psi^{\alpha\beta} = |\vec{\sigma}_{\mathcal{B}}\rangle|\vec{\sigma}_{\mathcal{A}}\rangle A^{\vec{\sigma}_{\mathcal{A}}}{}_{\alpha} \psi^{\alpha\beta} B_{\beta}{}^{\vec{\sigma}_{\mathcal{B}}}$$



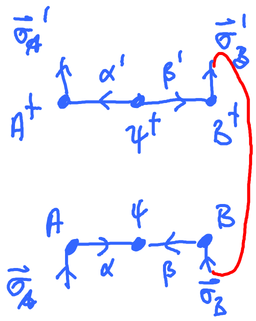

$$\langle\psi| = \psi^\dagger_{\beta'\alpha}\; {}_{\mathcal{A}}\langle\alpha'|\; {}_{\mathcal{B}}\langle\beta'| = B^\dagger_{\vec{\sigma}_{\mathcal{B}}}{}^{\beta} \psi^\dagger_{\beta'\alpha'} A^{\dagger\alpha'}{}_{\vec{\sigma}'_{\mathcal{A}}} \langle\vec{\sigma}'_{\mathcal{A}}|\langle\vec{\sigma}'_{\mathcal{B}}|$$




The reduced density matrix of $\mathcal{A}$ is given by

$$(\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} = (\psi B^\dagger B \psi^\dagger)^{\alpha}{}_{\alpha'} = (\psi\psi^\dagger)^{\alpha}{}_{\alpha'} \qquad \text{(as before).}$$

Diagrammatic derivation:

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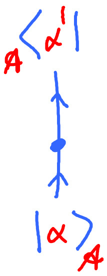


$$\psi^{\alpha\beta} \underbrace{B_{\beta}{}^{\vec{\sigma}_{\mathcal{B}}} B^\dagger_{\vec{\sigma}_{\mathcal{B}}}{}^{\beta'}}_{\mathbb{1}_{\beta}{}^{\beta'}} \psi^\dagger_{\beta'\alpha'} = (\psi\psi^\dagger)^{\alpha}{}_{\alpha'}$$

Exercise: derive this result algebraically. Convince yourself that the above diagrams provide a concise summary of your deviation!

Solution:

$$\hat{\rho} = |\psi\rangle\langle\psi| = |\vec{\sigma}_{\mathcal{B}}\rangle|\vec{\sigma}_{\mathcal{A}}\rangle A^{\vec{\sigma}_{\mathcal{A}}}{}_{\alpha}\, \psi^{\alpha\beta}\, B_{\beta}{}^{\vec{\sigma}_{\mathcal{B}}}\, B^{\dagger}{}_{\vec{\sigma}_{\mathcal{B}}'}{}^{\beta'}\, \psi^{\dagger}_{\beta'\alpha'}\, A^{\dagger\alpha'}{}_{\vec{\sigma}_{\mathcal{A}}'} \langle\vec{\sigma}_{\mathcal{A}}'|\langle\vec{\sigma}_{\mathcal{B}}'|$$

$$\hat{\rho}_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}}|\psi\rangle\langle\psi| = |\vec{\sigma}_{\mathcal{A}}\rangle A^{\vec{\sigma}_{\mathcal{A}}}{}_{\alpha}\, (\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'}\, A^{\dagger\alpha'}{}_{\vec{\sigma}_{\mathcal{A}}'}\langle\vec{\sigma}_{\mathcal{A}}'|$$

$$(\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} = \sum_{\vec{\sigma}_{\mathcal{B}}''} \underbrace{\langle\vec{\sigma}_{\mathcal{B}}''|\vec{\sigma}_{\mathcal{B}}\rangle}_{\delta^{\vec{\sigma}_{\mathcal{B}}''}{}_{\vec{\sigma}_{\mathcal{B}}}}\, \psi^{\alpha\beta}\, B_{\beta}{}^{\vec{\sigma}_{\mathcal{B}}}\, B^{\dagger}{}_{\vec{\sigma}_{\mathcal{B}}'}{}^{\beta'}\, \psi^{\dagger}_{\beta'\alpha'}\, \underbrace{\langle\vec{\sigma}_{\mathcal{B}}'|\vec{\sigma}_{\mathcal{B}}''\rangle}_{\delta^{\vec{\sigma}_{\mathcal{B}}'}{}_{\vec{\sigma}_{\mathcal{B}}''}}$$

$$= \psi^{\alpha\beta}\, \underbrace{(BB^{\dagger})_{\beta}{}^{\beta'}}_{\mathbb{1}_{\beta}{}^{\beta'}}\, \psi^{\dagger}{}_{\beta'\alpha'} = (\psi\psi^{\dagger})^{\alpha}{}_{\alpha'}$$