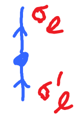
MPS II: Matrix product states

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 $1/2$:

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

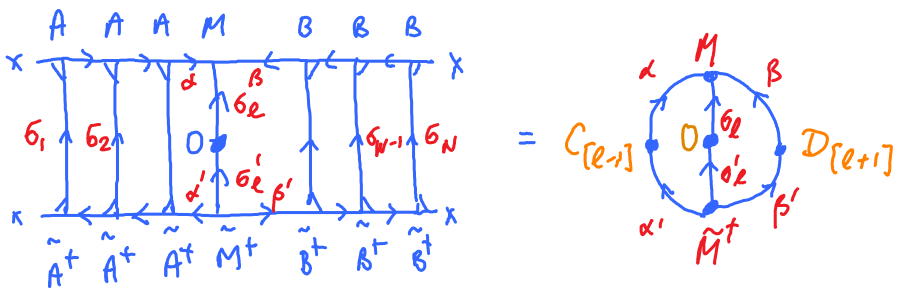
Consider two states in site-canonical form for site ℓ :

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

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

Matrix element:

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



(5)

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)].

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

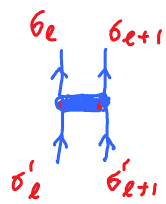
Now consider the expectation value, $\langle\psi|\hat{O}|\psi\rangle$ (i.e. drop all tilde's). The left-normalization of A's guarantees that $C_{[\ell-1]} = \mathbb{1}$, and right-normalization of B's that $D_{[\ell+1]} = \mathbb{1}$.

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

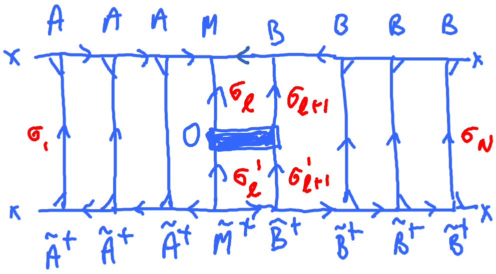
(e.g. for spin chain: $\vec S_\ell \cdot \vec S_{\ell+1}$) $= S^z S^z + S^x S^x + S^y S^y$

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



Matrix elements:

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



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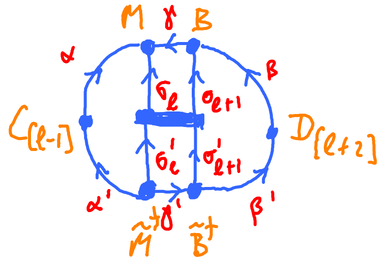
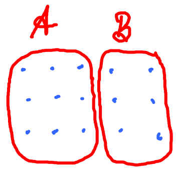


(11)

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

2. Schmidt decomposition



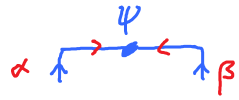
Consider a quantum system composed of two subsystems, $\mathcal{A}$ and $\mathcal{B}$,

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

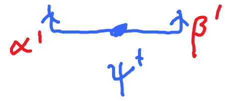
To be specific, think of physical basis: $\quad |\alpha\rangle_{\mathcal{A}} \equiv |\vec{\sigma}_A\rangle, \quad |\beta\rangle_{\mathcal{B}} \equiv |\vec{\sigma}_B\rangle \qquad (1)$

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

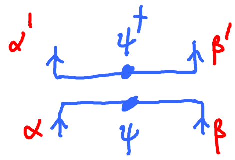
$$|\psi\rangle = |\beta\rangle_{\mathcal{B}} |\alpha\rangle_{\mathcal{A}} \psi^{\alpha\beta} \qquad (2)$$



$$\langle\psi| = \underbrace{\psi^{\dagger}_{\beta'\alpha'}}_{\equiv} \overline{{}_{\mathcal{A}}\langle\alpha'|\,{}_{\mathcal{B}}\langle\beta'|}^{\,\psi^{\alpha'\beta'}} \qquad (3)$$



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



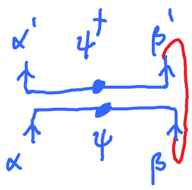
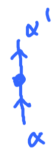
Reduced density matrix of subsystem $\mathcal{A}$:

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

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

with

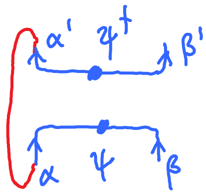
$$(\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} = \sum_{\bar{\beta}} \underbrace{{}_{\mathcal{B}}\langle\bar{\beta}|\beta\rangle_{\mathcal{B}}}_{\delta^{\bar{\beta}}{}_{\beta}}\, \psi^{\alpha\beta}\, \psi^{\dagger}_{\beta'\alpha'}\, \underbrace{{}_{\mathcal{B}}\langle\beta'|\bar{\beta}\rangle_{\mathcal{B}}}_{\delta^{\beta'}{}_{\bar{\beta}}}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

$\hat{\rho}_A =$  $=$  $\psi^{\alpha\beta}\,\psi^{\dagger}_{\beta\alpha'} = (\psi\psi^{\dagger})^{\alpha}{}_{\alpha'} \qquad (7)$

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

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

Diagrammatic derivation:

$\hat{\rho}_B =$  $=$  $\psi^{\alpha\beta}\,\psi^{\dagger}_{\beta'\alpha} = (\psi^{\dagger}\psi)_{\beta}{}^{\beta'} \qquad (9)$

Algebraic derivation:

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

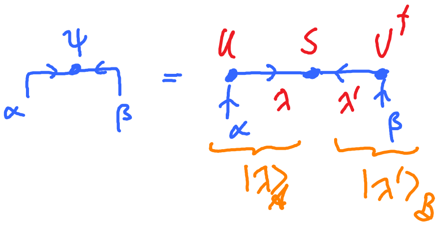
<u>Singular value decomposition</u>

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

SVD of ψ:
$$\psi = U S V^{\dagger}$$

With indices:
$$\psi^{\alpha\beta} = U^{\alpha}{}_{\lambda} S^{\lambda\lambda'} V^{\dagger}{}_{\lambda'}{}^{\beta} \quad (11)$$

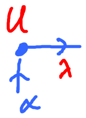
$S^{\lambda\lambda'}$: $\mathrm{diag}(s_1, s_2, \dots)$

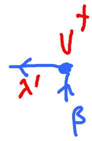


Hence

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

where
$$|\lambda\rangle_A = |\alpha\rangle_A U^{\alpha}{}_{\lambda}, \qquad |\lambda\rangle_B = |\beta\rangle V^{\dagger}{}_{\lambda}{}^{\beta} \quad (13)$$

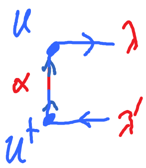




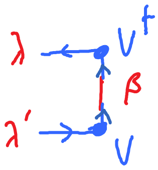
are orthonomal sets of states for $\mathcal{A}$ and $\mathcal{B}$, and can be extended to yield orthonormal bases for $\mathcal{A}$ and $\mathcal{B}$ if needed.

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

$${}_A\langle\lambda'|\lambda\rangle_A = U^{\dagger\lambda'}{}_{\alpha} U^{\alpha}{}_{\lambda} = \mathbb{1}^{\lambda'}{}_{\lambda} \quad (14)$$



$${}_B\langle\lambda'|\lambda\rangle_B = V^{\dagger}_{\lambda}{}^{\beta} V_{\beta}{}^{\lambda'} = \mathbb{1}_{\lambda'}{}^{\lambda} \quad (15)$$



Restrict $\sum_{\lambda}$ to the r non-zero singular values:

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

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

In this representation, reduced density matrices are diagonal:

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

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

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

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

$|\psi\rangle = |\beta\rangle|\alpha\rangle \psi^{\alpha\beta}$

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

$$\| |\psi\rangle \|_2^2 \equiv |\langle\psi|\psi\rangle|^2 = \sum |\psi^{\alpha\beta}|^2 = \|\psi\|_F^2 \qquad (20)$$

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

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

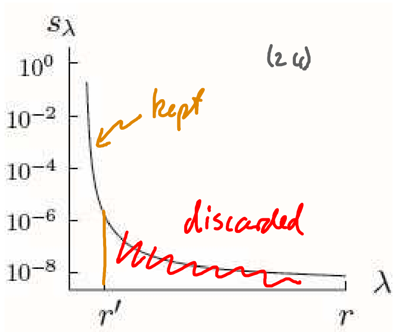
(If $|\tilde\psi\rangle$ should be normalized, rescale s_λ by $\sum_{\lambda=1}^{r'}(s_\lambda)^2$.)

Truncation error:

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

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

= 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 ℓ 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 $\mathcal{B}$.

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

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

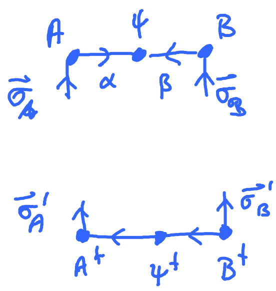
when A and B are unitary,

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

Consider the pure state

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

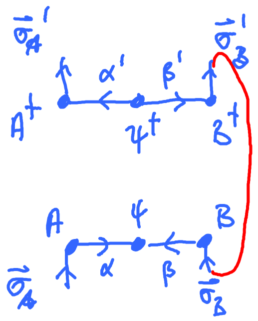
$$\langle\psi| = \psi^{\dagger}{}_{\beta'\alpha'}\; {}_{\mathcal{A}}\langle\alpha'|\; {}_{\mathcal{B}}\langle\beta'| = B^{\dagger}{}_{\vec{\sigma}_{\mathcal{B}}}{}^{\beta}\; \psi^{\dagger}{}_{\beta'\alpha'}\; A^{\dagger\alpha'}{}_{\vec{\sigma}'_{\mathcal{A}}} \langle\vec{\sigma}'_{\mathcal{A}}|\langle\vec{\sigma}'_{\mathcal{B}}|$$



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:



$$= \begin{array}{c} {}_{\mathcal{A}}\langle\alpha'| \\ \uparrow \\ \bullet \\ \uparrow \\ |\alpha\rangle_{\mathcal{A}} \end{array} \psi^{\alpha\beta} \underbrace{B_{\beta}{}^{\vec{\sigma}_{\mathcal{B}}} B^{\dagger}{}_{\vec{\sigma}_{\mathcal{B}}}{}^{\beta'}}_{\mathbb{1}_{\beta}{}^{\beta'}} \psi^{\dagger}{}_{\beta'\alpha'} = (\psi\psi^{\dagger})^{\alpha}{}_{\alpha'}$$

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

Solution:

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

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

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

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