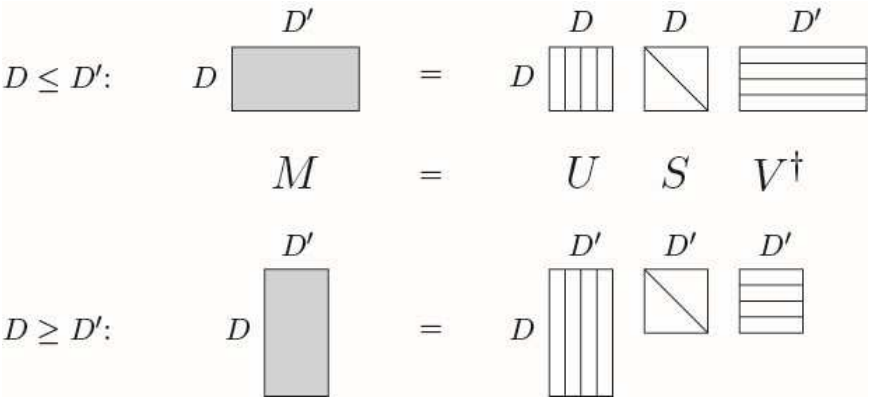
1. Singular value decomposition (SVD)

[Schollwoeck2011, Sec. 4]

Any matrix M of dimension $D \times D'$ can be written as $M = U S V^\dagger$ (1)



Properties of S

- square matrix, of dimension $D_{min} \times D_{min}$, with $D_{min} = \min(D, D')$
- diagonal, with non-negative diagonal elements, called 'singular values' $S_\alpha \equiv S_{\alpha\alpha}$

- 'Schmidt rank' r : number of non-zero singular values
- arrange in descending order: $S_1 \geq S_2 \geq \dots \geq S_r > 0$

$$\Rightarrow \quad S = \mathrm{diag}(s_1, s_2, \dots, s_r, \underbrace{0, \dots, 0}_{D_{min} - r}) \qquad (2)$$

zeros

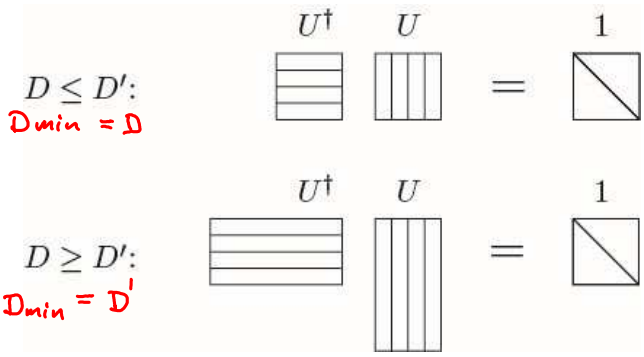
Properties of U:

- matrix of dimension $D \times D_{min}$
- columns are orthonormal:

$$U^\dagger U = \mathbb{1} \qquad (3)$$

but $UU^\dagger \neq \mathbb{1}$

(not unitary)



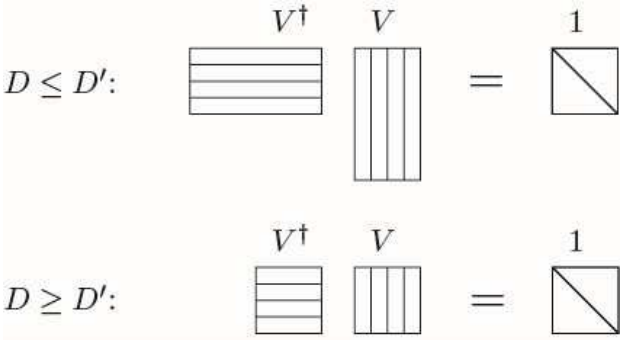
Properties of $V^\dagger$:

- matrix of dimension $D_{min} \times D'$
- rows are orthonormal:

$$V^\dagger V = \mathbb{1} \qquad (4)$$

but $VV^\dagger \neq \mathbb{1}$

(not unitary)



(1), (3), (4) imply:

$$MM^\dagger \overset{(1)}{=} (USV^\dagger)(VSU^\dagger) \overset{(4)}{=} US^2U^\dagger \overset{(3)}{\Rightarrow} MM^\dagger U = US^2 \quad (5)$$

($V^\dagger V = 1$)

$$M^\dagger M \overset{(1)}{=} (VSU^\dagger)(USV^\dagger) \overset{(3)}{=} VS^2V^\dagger \overset{(4)}{\Rightarrow} M^\dagger M V = VS^2 \quad (6)$$

($U^\dagger U = 1$)

So, columns of U are eigenvectors of $MM^\dagger$, and columns of V are eigenvectors of $M^\dagger M$.

Def: Frobenius norm: $\|M\|_F^2 := \sum_{\alpha\beta} |M_{\alpha\beta}|^2 = \sum_{\alpha\beta} \overline{M_{\alpha\beta}} M_{\alpha\beta} = \sum_{\alpha\beta} M^\dagger_{\beta\alpha} M_{\alpha\beta} = \mathrm{Tr}\, M^\dagger M$ (7)

evaluated via SVD: $= \mathrm{Tr}(VSU^\dagger USV^\dagger) = \mathrm{Tr}(V^\dagger V S^2)$ (8)

($U^\dagger U = 1$; trace is cyclic; $V^\dagger V = 1$)

$\mathrm{Tr}\, S^2$ — singular values determine norm

Truncation

SVD can be used to approximate a rank r matrix M by a rank r' ($< r$) matrix M':

Suppose $M = USV^\dagger$ (7)

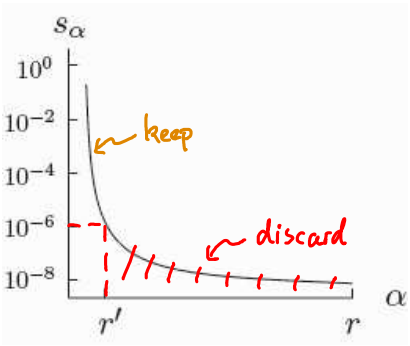
with $S = \mathrm{diag}(s_1, s_2, \ldots, s_r, 0, \ldots, 0)$ (8)

($D_{min} - r$ zeros)

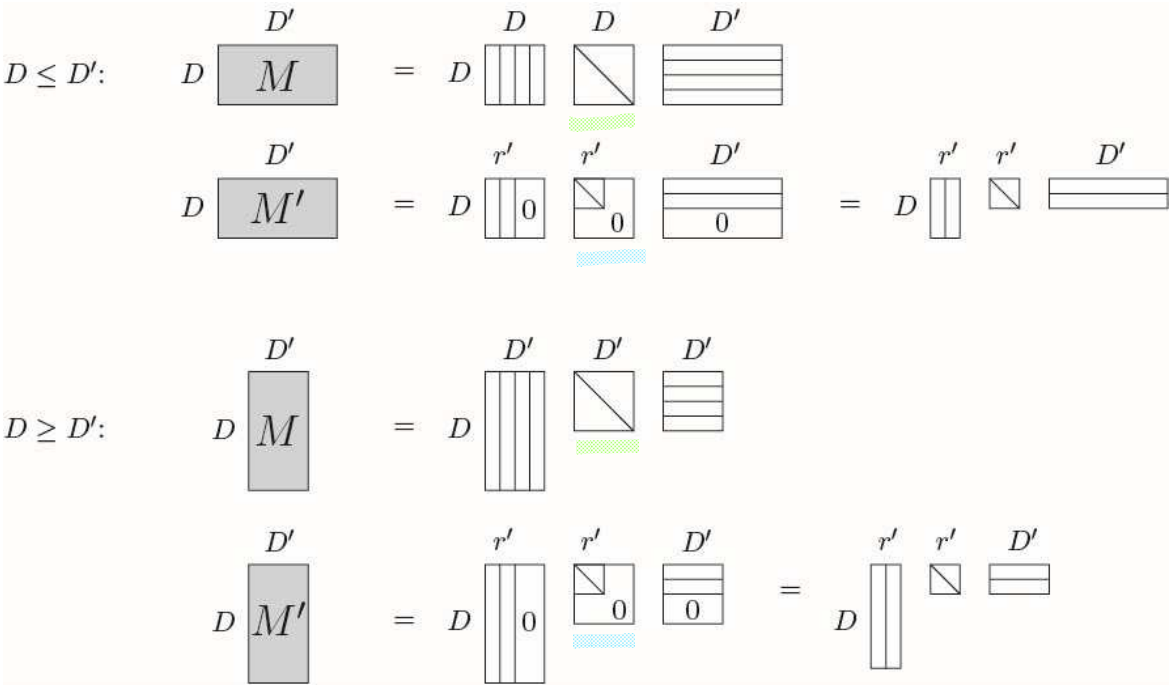
Truncate: $M' := US'V^\dagger$ (9)

with $S' := \mathrm{diag}(s_1, s_2, \ldots, s_{r'}, 0, \ldots, 0, \ldots, 0)$ (10)

($D_{min} - r'$ zeros)



Retain only r' largest singular values! Visualization, with $r = D_{min}$:



SVD truncation yields 'optimal' approximation of a rank r matrix M by a rank r' ($<r$) matrix M',

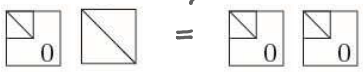
in the sense that it can be shown to minimize the Frobenius norm of the difference, $M - M'$.

$$\|M - M'\|_F^2 = Tr\,(M - M')^\dagger (M - M') = Tr\,(M^\dagger M + M'^\dagger M' - M'^\dagger M - M^\dagger M') \quad (11)$$

similar steps as for (8)

$$= Tr\,(S \cdot S + S' \cdot S' - S' \cdot S - S \cdot S') \quad (12)$$

$S' \cdot S = S' \cdot S'$ $\quad$ $S \cdot S' = S' \cdot S'$



$$= Tr\,(S^2 - S'^2) = \sum_{\alpha=1}^{r} S_\alpha^2 - \sum_{\alpha=1}^{r'} S_\alpha^2 = \sum_{\alpha=r'+1}^{r} S_\alpha^2 \quad (13)$$

'truncated weight'

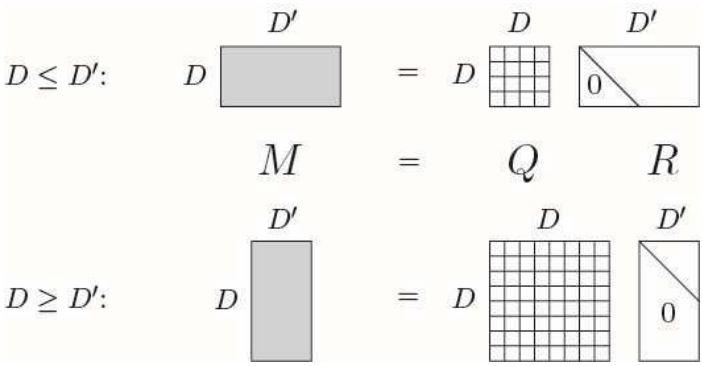
<u>QR-decomposition</u>

If singular values are not needed,

a $D \times D'$ matrix M

has the 'full QR decomposition'

$$M = Q R \quad (14)$$

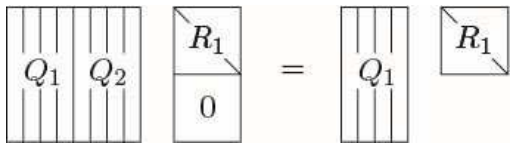


with Q a $D \times D$ unitary matrix, $\quad Q Q^\dagger = Q^\dagger Q = \mathbb{1}$ (15)

and R a $D \times D'$ upper triangular matrix, $\quad R_{\alpha\beta} = 0$ if $\alpha > \beta$ (16)

If D ≥ D', then M has the 'thin QR decomposition'

$$M = (Q_1, Q_2) \cdot \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_1 \cdot R_1 \quad (17)$$



with dim(Q1) = $D \times D'$, dim(R1) = $D' \times D'$, $\quad Q_1^\dagger Q_1 = \mathbb{1}$ but $Q_1 Q_1^\dagger \neq \mathbb{1}$ (18)

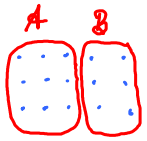
and R1 upper triangular.

QR-decomposition is numerically cheaper than SVD, but has less information (not 'rank-revealing').

2. Schmidt decomposition [most efficient way of representing entanglement]

MPS-II.2

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



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

Pure state on $\mathcal{A}\cup\mathcal{B}$: $|\psi\rangle = |\beta\rangle_{\mathcal{B}}\,|\alpha\rangle_{\mathcal{A}}\,\psi^{\alpha\beta}$ (1)

Reduced density matrices of subsystems $\mathcal{A}$ and $\mathcal{B}$:

$$\hat{\rho}_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}}|\psi\rangle\langle\psi| = |\alpha\rangle_{\mathcal{A}}\,(\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'}\,{}_{\mathcal{A}}\langle\alpha'|, \qquad (\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} = (\psi\psi^{\dagger})^{\alpha}{}_{\alpha'} \qquad (2)$$

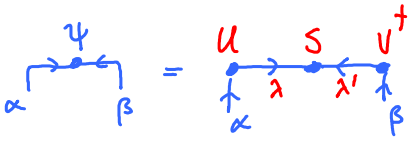
$$\hat{\rho}_{\mathcal{B}} = \mathrm{Tr}_{\mathcal{A}}|\psi\rangle\langle\psi| = |\beta\rangle_{\mathcal{B}}\,(\rho_{\mathcal{B}})^{\beta}{}_{\beta'}\,{}_{\mathcal{B}}\langle\beta'|, \qquad (\rho_{\mathcal{B}})^{\beta}{}_{\beta'} = (\psi^{\dagger}\psi)_{\beta'}{}^{\beta} \qquad (3)$$

Singular value decomposition

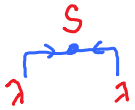
Use SVD to find bases for $\mathcal{A}$ and $\mathcal{B}$ which diagonalizes density matrices:

$$\psi \overset{\text{SVD}}{=} U\,S\,V^{\dagger} \qquad (4)$$

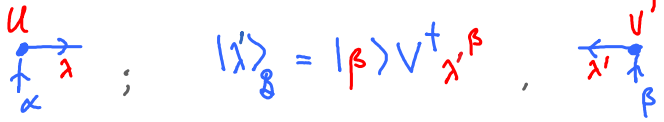
With indices: $\psi^{\alpha\beta} = U^{\alpha}{}_{\lambda}\,S^{\lambda\lambda'}\,V^{\dagger}{}_{\lambda'}{}^{\beta}$, $S^{\lambda\lambda'} = \mathrm{diag}(s_1, s_2, \ldots)$ (5)



Hence $|\psi\rangle = |\lambda'\rangle_{\mathcal{B}}\,|\lambda\rangle_{\mathcal{A}}\,S^{\lambda\lambda'} = \sum_{\lambda}|\lambda\rangle_{\mathcal{B}}\,|\lambda\rangle_{\mathcal{A}}\,s_{\lambda}$ (6)



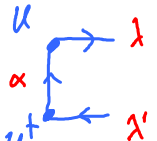
where $|\lambda\rangle_{\mathcal{A}} = |\alpha\rangle_{\mathcal{A}}\,U^{\alpha}{}_{\lambda}$, $|\lambda'\rangle_{\mathcal{B}} = |\beta\rangle V^{\dagger}{}_{\lambda'}{}^{\beta}$ (7)



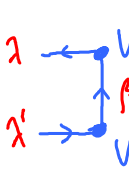
are orthonormal sets of states for $\mathcal{A}$ and $\mathcal{B}$, and can be extended to yield orthonormal bases for $\mathcal{A}$ and $\mathcal{B}$ if needed.

Orthonormality is guaranteed by $U^{\dagger}U = \mathbb{1}$ and $V^{\dagger}V = \mathbb{1}$! (8)

$${}_{\mathcal{A}}\langle\lambda'|\lambda\rangle_{\mathcal{A}} = U^{\dagger\lambda'}{}_{\alpha}\,U^{\alpha}{}_{\lambda} = \mathbb{1}^{\lambda'}{}_{\lambda} \qquad (9)$$



$${}_{\mathcal{B}}\langle\lambda'|\lambda\rangle_{\mathcal{B}} = V^{\dagger}{}_{\lambda}{}^{\beta}\,V_{\beta}{}^{\lambda'} = \mathbb{1}_{\lambda}{}^{\lambda'} \qquad (10)$$



Restrict Σ_{λ} to the r non-zero singular values:

$$|\psi\rangle = \sum_{\lambda=1}^{r}|\lambda\rangle_{\mathcal{B}}\,|\lambda\rangle_{\mathcal{A}}\,s_{\lambda} \quad \text{'Schmidt decomposition'} \qquad (11)$$

If $r = 1$, 'classical' state: $|\psi\rangle = |i\rangle_B |i\rangle_A$. If $r \geq 1$: 'entangled state'

In this representation, reduced density matrices are diagonal:

$$\hat{\rho}_A = \mathrm{Tr}_B |\psi\rangle\langle\psi| = \sum_\lambda |\lambda\rangle_A (s_\lambda)^2 \langle\lambda| \quad (12)$$

$$(\psi\psi^\dagger)\cdot(\psi^\dagger\psi) \text{ with } \psi^{\lambda\lambda'} = s_\lambda \mathbb{1}^{\lambda\lambda'} \quad (13)$$

$$\hat{\rho}_B = \mathrm{Tr}_A |\psi\rangle\langle\psi| = \sum_\lambda |\lambda\rangle_B (s_\lambda)^2 \langle\lambda| \quad (14)$$

Entanglement entropy: $$S_{A/B} = -\sum_{\lambda=1}^{r} (s_\lambda)^2 \log_2 (s_\lambda)^2 \quad (15)$$

Note: for given r, entanglement is maximal if all singular values are equal, $s_\lambda = r^{-1/2}$ (16)

How can one approximate $|\psi\rangle = \sum_{\alpha\beta} |\beta\rangle_B |\alpha\rangle_A \psi^{\alpha\beta}$ by cheaper $|\tilde{\psi}\rangle$?

$$\| |\psi\rangle \|_2^2 \equiv |\langle\psi|\psi\rangle|^2 = \sum_{\alpha\beta} |\psi^{\alpha\beta}|^2 = \|\psi\|_F^2 \quad (17)$$

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

$$|\tilde{\psi}\rangle \equiv \sum_{\lambda=1}^{r'} |\lambda\rangle_B |\lambda\rangle_A \, s_\lambda \quad (18)$$

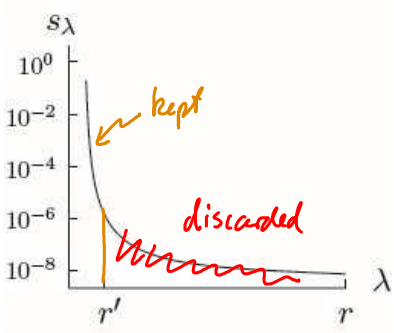
If $|\tilde{\psi}\rangle$ should be normalized, rescale, i.e. replace s_λ by $s_\lambda \left[\sum_{\lambda'=1}^{r'} (s_{\lambda'})^2 \right]^{-1/2}$ (19)

Truncation error:

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

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

= sum of squares of discarded singular values

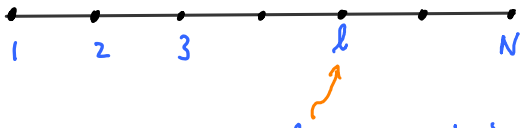


Useful to obtain 'cheap' representation of $|\psi\rangle$ if singular values decay rapidly.

The truncation strategy (18) minimizes the truncation error.
It is used over and over again in tensor network numerics.

3. Iterative Diagonalization [generates a 1d tensor network]

Consider a spin-s chain, with Hamiltonian $H^N = J \sum_{l=1}^{N-1} \vec{S}_l \cdot \vec{S}_{l+1} + \sum_{l=1}^{N} \vec{S}_l \cdot \vec{h}_l$ (1)



local state space for site l : $|\sigma_l\rangle$, $\sigma_l = 1, \dots, d = 2s+1$

We seek eigenstates of H^N : $H^N |E^N_\alpha\rangle = E^N_\alpha |E^N_\alpha\rangle$, $|E^N_\alpha\rangle \in \mathcal{H}^N$ (2)

$\alpha = 1, \dots, d^N$

Diagonalize Hamiltonian iteratively, adding one site at a time:

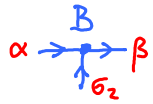
N=1: Start with first site, diagonalize H^1 in Hilbert space $\mathcal{H}^1$. Eigenstates have form

$|\alpha\rangle \equiv |E^1_\alpha\rangle = |\sigma_1\rangle A^{\sigma_1}{}_\alpha$ $(\alpha = 1, \dots, d)$ (3)

(sum over σ_1 implied) coefficient matrix combine 'incoming' σ_1 into 'outgoing' α

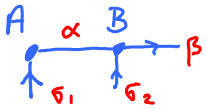
N=2: Add second site, diagonalize H^2 in Hilbert space $\mathcal{H}^2$:

$|\beta\rangle \equiv |E^2_\beta\rangle = |\sigma_2\rangle \otimes |\alpha\rangle B^{\alpha\sigma_2}{}_\beta$ $(\beta = 1, \dots, d^2)$ (4)



(sum over α, σ_2 implied) coefficient tensor combine 'incoming' α, σ_2 into 'outgoing' β

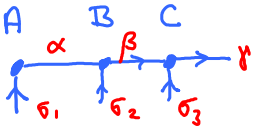
$= \underbrace{|\sigma_2\rangle \otimes |\sigma_1\rangle}_{|\vec{\sigma}\rangle_2} A^{\sigma_1}{}_\alpha B^{\alpha\sigma_2}{}_\beta$ 'matrix multiplication' for 'contracted' index α



N=3: Add third site, diagonalize H^3 in Hilbert space $\mathcal{H}^3$:

$|\gamma\rangle = |\sigma_3\rangle \otimes |\beta\rangle C^{\beta\sigma_3}{}_\gamma$ $(\gamma = 1, \dots, d^3)$ (5)

$= \underbrace{|\sigma_3\rangle \otimes |\sigma_2\rangle \otimes |\sigma_1\rangle}_{|\vec{\sigma}\rangle_3} A^{\sigma_1}{}_\alpha B^{\alpha\sigma_2}{}_\beta C^{\beta\sigma_3}{}_\gamma$



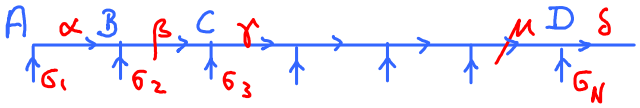
contracted indices α, β

Continue similarly until having added site N. Eigenstates of H^N in $\mathcal{H}^N$ have following structure:

$$|E^N_\delta\rangle = |\delta\rangle = |\sigma_N\rangle \otimes \cdots \otimes |\sigma_3\rangle \otimes |\sigma_2\rangle \otimes |\sigma_1\rangle \underbrace{A^{\sigma_1}{}_{\alpha} B^{\alpha\sigma_2}{}_{\beta} C^{\beta\sigma_3}{}_{\gamma} \cdots D^{\mu\sigma_N}{}_{\delta}}_{\equiv C^{\vec{\sigma}}{}_{\delta}}$$

$$= |\vec{\sigma}\rangle_N \, C^{\vec{\sigma}}{}_{\delta} \qquad \text{'matrix product state' (MPS)}$$

$$(\delta = 1, \ldots, d^N)$$



Nomenclature: σ_ℓ = physical indices, $\alpha, \beta, \gamma, \ldots$ = (virtual) bond indices

Alternative, widely-used notation: 'reshape' the coefficient tensors as

$$\tilde{A}^{\sigma_1}_{\alpha} \equiv A^{\sigma_1}{}_{\alpha}, \quad \tilde{B}^{\sigma_2}_{\alpha\beta} \equiv B^{\alpha\sigma_2}{}_{\beta}, \quad \tilde{C}^{\sigma_3}_{\beta\gamma} \equiv C^{\beta\sigma_3}{}_{\gamma}$$

to highlight 'matrix product' structure in noncovariant notation:

$$|\delta\rangle = |\sigma_1\rangle \otimes \cdots \otimes |\sigma_3\rangle \otimes |\sigma_2\rangle \otimes |\sigma_1\rangle \, \tilde{A}^{\sigma_1}_{\alpha} \tilde{B}^{\sigma_2}_{\alpha\beta} \tilde{C}^{\sigma_3}_{\beta\gamma} \cdots \tilde{D}^{\sigma_N}_{\mu\delta}$$

Comments

1. Iterative diagonalization of ID chain generates eigenstates whose wave functions are tensors that are expressed as matrix products.

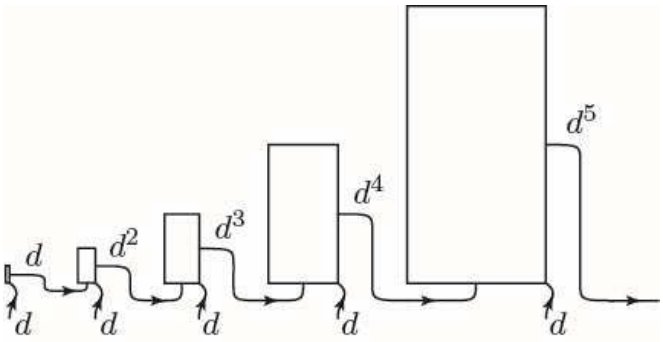
Such states an called 'matrix product states' (MPS)

Matrix size grows exponentially:

for given σ_1, $A^{\sigma_1}{}_{\alpha}$ has dimension $1 \times d$ (vector)

for given σ_2, $B^{\alpha\sigma_2}{}_{\beta}$ has dimension $d \times d^2$ (rectangular matrix)

for given σ_3, $C^{\beta\sigma_3}{}_{\gamma}$ has dimension $d^2 \times d^3$ (larger rectangular matrix)

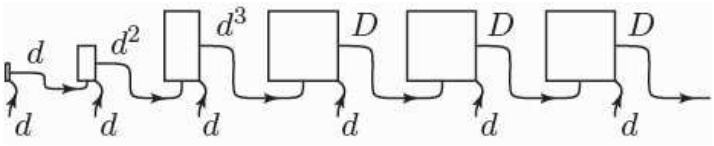


'Hilbert space is a large place'

Numerical costs explode with increasing N, so truncation schemes will be needed...

Truncation can be done in controlled way using tensor network methods!

Standard truncation scheme: use $\alpha, \beta, \gamma, \ldots \leq D$ for all virtual bonds



2. Number of parameters available to encode state:

$\mathcal{N}_{MPS} \leq N \cdot D^2 \cdot d$

would be '=' if all virtual bonds have the same dimension, D :

$D_h \sim d$

$A^{\mu}{}_{\sigma\lambda} \sim D$

$\mathcal{N}_{MPS}$ scales linearly with system size, N

If N is large: $\mathcal{N}_{MPS} \ll d^N$

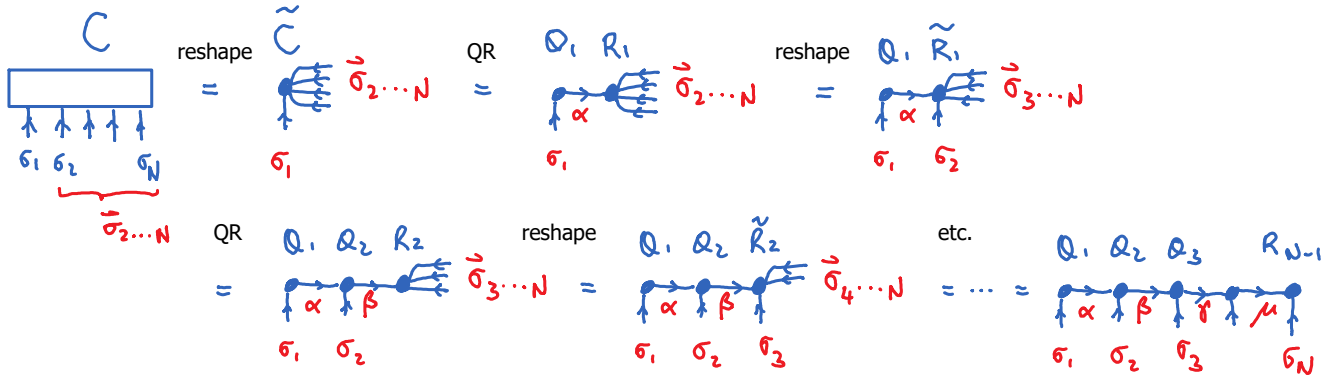
Why should this have any chance of working? Remarkable fact: for 1d Hamiltonians with local interactions and a gapped spectrum, ground state can be accurately represented by MPS!

Why? 'Area laws'! Tensor Network Basics I.2.

4. Reshaping generic tensor into MPS form

TNB-II.4

A generic tensor of arbitrary rank can be expressed as a MPS by repeatedly performing SVDs.



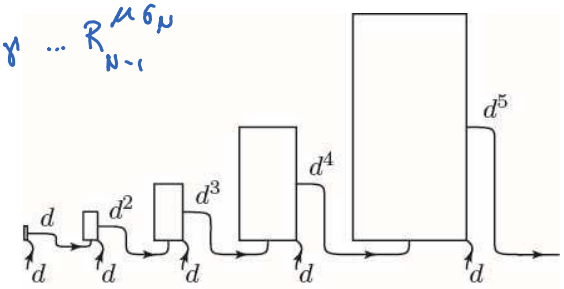
In formulas ('reshape' means regroup indices):

$$C^{\sigma_1 \cdots \sigma_N} \overset{\text{reshape}}{=} \tilde{C}^{\sigma_1, \sigma_2 \cdots \sigma_N} \overset{\text{QR}}{=} Q_1^{\sigma_1 \alpha} R_1^{\alpha, \sigma_2 \cdots \sigma_N} \overset{\text{reshape}}{=} Q_1^{\sigma_1 \alpha} \tilde{R}_1^{\alpha \sigma_2, \sigma_3 \cdots \sigma_N}$$

$$\overset{\text{QR}}{=} Q_1^{\sigma_1 \alpha} Q_2^{\alpha \sigma_2 \beta} R_2^{\beta, \sigma_3 \cdots N} \overset{\text{reshape}}{=} Q_1^{\sigma_1 \alpha} Q_2^{\alpha \sigma_2 \beta} \tilde{R}_2^{\beta \sigma_3, \sigma_4 \cdots N} \overset{\text{etc.}}{=} \cdots$$

$$= Q_1^{\sigma_1 \alpha} Q_2^{\alpha \sigma_2 \beta} Q_3^{\beta \sigma_3 \gamma} \cdots R_{N-1}^{\mu \sigma_N}$$

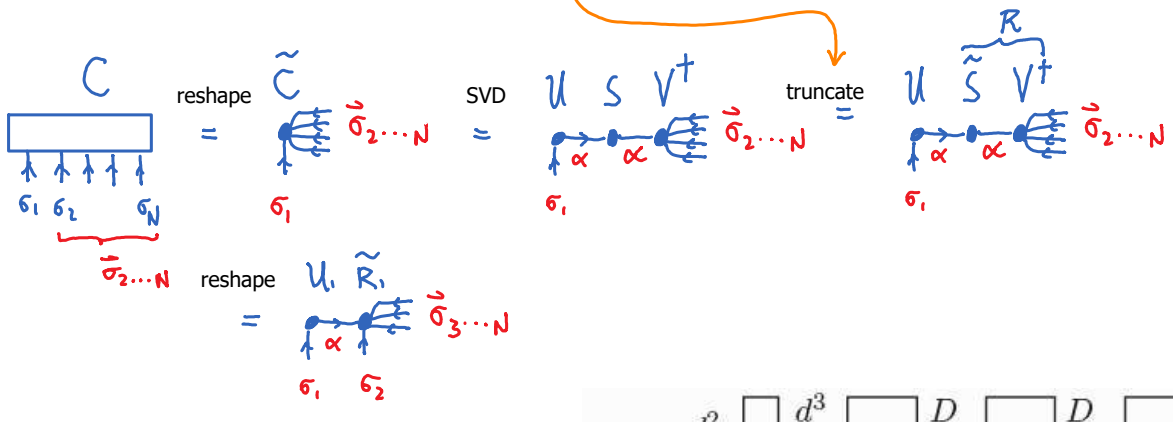
Again, the dimensions grow as



$\cdots \; d^N$

If a maximal bond dimension of $D_\alpha < D$ is desired, this can be achieved using SVD instead of QR decompositions, and retaining only the largest D singular values at each step:

$$\tilde{S}_\alpha = \begin{cases} S_\alpha & \text{for} \quad \alpha \leq D \\ 0 & \text{otherwise} \end{cases}$$



This yields truncated respresentation: $C \simeq$