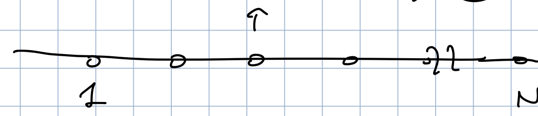
MATRIX PRODUCT STATES

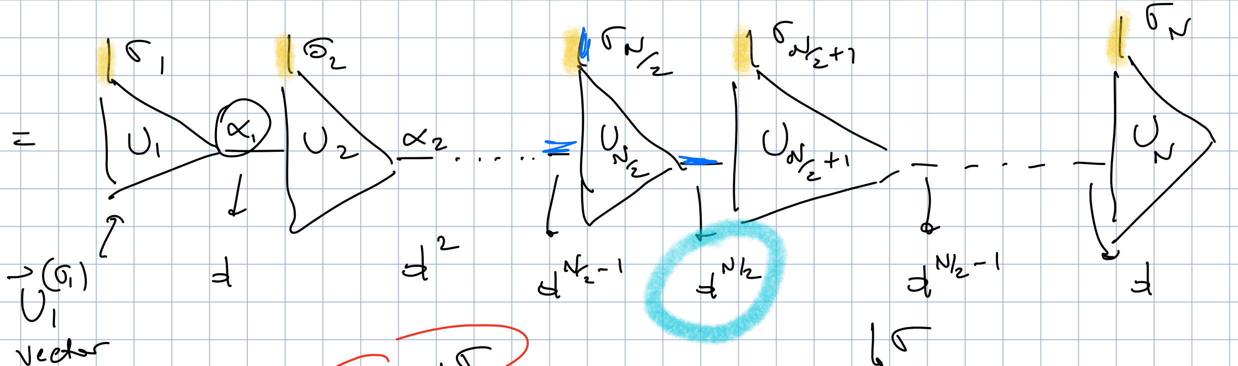
$|\sigma\rangle : \sigma = 1, \dots, d$



$$|\Psi\rangle = \sum_{\sigma_1 \sigma_2 \dots \sigma_N} \psi(\sigma_1, \sigma_2, \dots, \sigma_N)\, |\sigma_1 \sigma_2 \dots \sigma_N\rangle$$

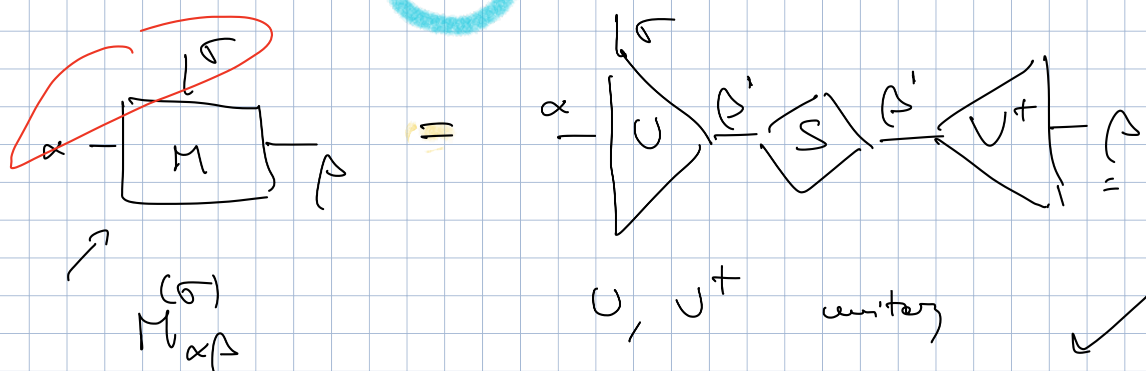
tensor = SVD

left-canonical MPS form



$= \dots S_N e^{i\phi_N}$

SVD :

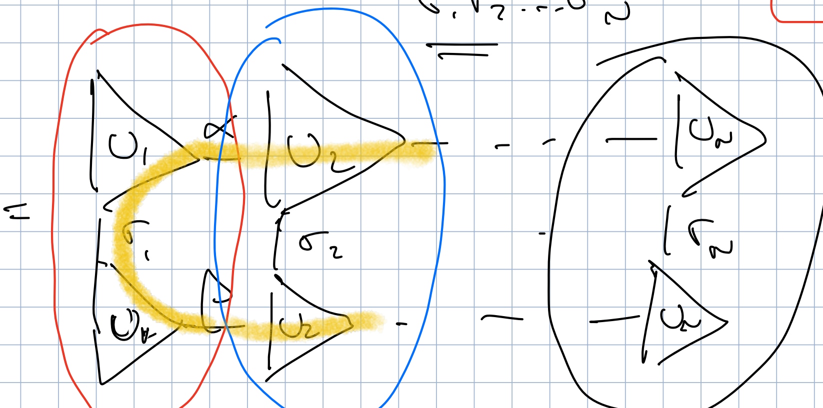


U, U^+ unitary

$$|\Psi\rangle = S_N e^{i\phi_N} \sum_{\sigma_1 \sigma_2 \dots \sigma_N} \vec{U}_1^{(\sigma_1)} U_2^{(\sigma_2)} \cdots U_{N-1}^{(\sigma_{N-1})} \vec{U}_N^{(\sigma_N)} |\sigma_1 \sigma_2 \dots \sigma_N\rangle$$

matrix-product form

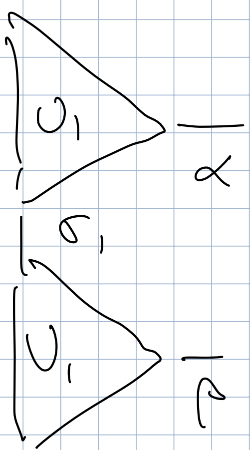
$$\langle\Psi|\Psi\rangle = \sum_{\sigma_1 \sigma_2 \dots \sigma_N} \psi^*(\sigma_1, \sigma_2, \dots, \sigma_N)\, \psi(\sigma_1, \sigma_2, \dots, \sigma_N)$$



S_N^2

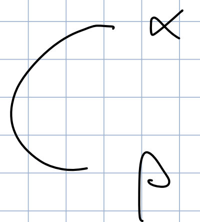
$$= \sum_{\sigma_1 \sigma_2 \cdots \sigma_N} \vec{U}_1^{(\sigma_1)} U_2^{(\sigma_2)} \cdots U_{N-1}^{(\sigma_{N-1})} \vec{U}_N^{(\sigma_N)} \left(\vec{U}_1^{(\sigma_1)} U_2^{(\sigma_2)} \cdots U_{N-1}^{(\sigma_{N-1})} \vec{U}_N^{(\sigma_N)} \right)^{*}$$

$$= \sum_{\sigma_1 \sigma_2 \cdots \sigma_N} \vec{U}_N^{(\sigma_N)\dagger} U_{N-1}^{(\sigma_{N-1})\dagger} \cdots U_2^{(\sigma_2)\dagger} \vec{U}_1^{(\sigma_1)\dagger} \vec{U}_1^{(\sigma_1)} U_2^{(\sigma_2)} \cdots U_{N-1}^{(\sigma_{N-1})} \vec{U}_N^{(\sigma_N)}$$

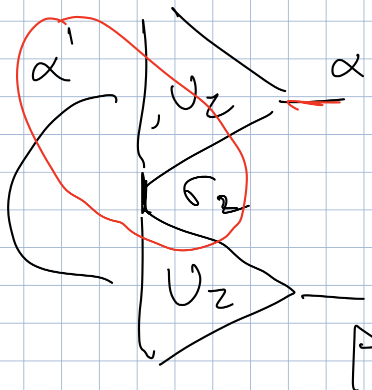


$$= \sum_{\sigma_1} \left(U_1^{(\sigma_1)\dagger} U_1^{(\sigma_1)} \right)_{\alpha\beta} = \delta_{\alpha\beta}$$

↓ unitary

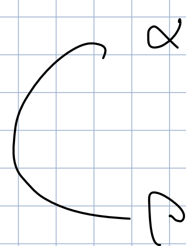
= 

$\delta_{\alpha\beta}$



$$= \sum_{\sigma_2, \alpha'} \left(U_2^{\dagger} \right)_{\alpha, (\sigma_2 \alpha')} \left(U_2 \right)_{(\sigma_2, \alpha'), \beta} = \delta_{\alpha\beta}$$

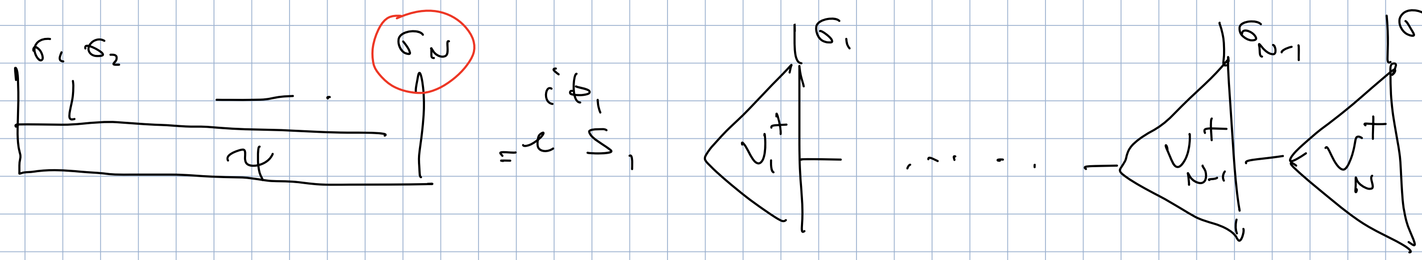
$$= \left(U_2^{\dagger} U_2 \right)_{\alpha\beta} =$$



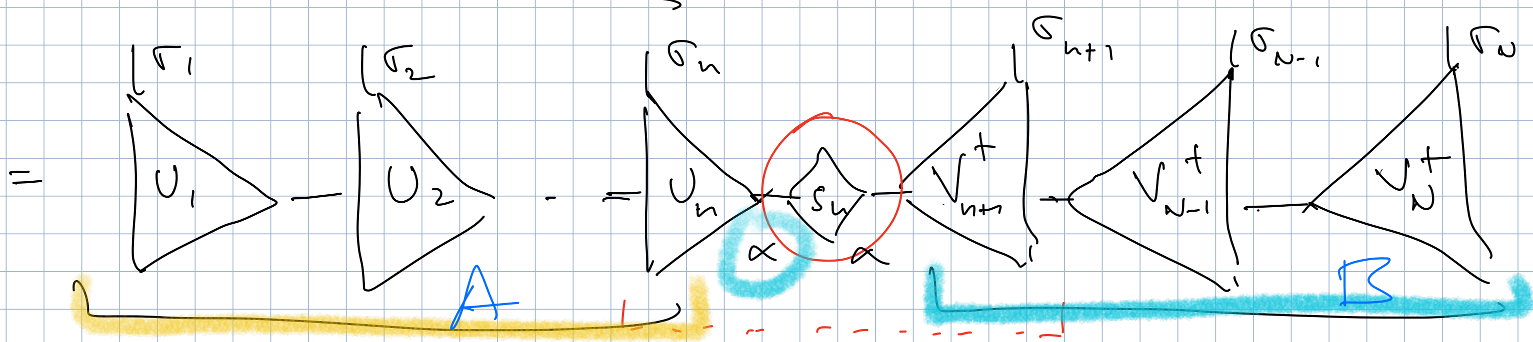
$\delta_{\alpha\beta}$

$$= \cdots = s_N^2 = \langle \Psi | \Psi \rangle = 1$$

Right-canonical form



Mixed canonical form



$|\Psi\rangle$

$|\alpha_n\rangle$

$$= \sum_\alpha \sum_{\sigma_1\sigma_2\cdots\sigma_n} \left(U_1^{(\sigma_1)} U_2^{(\sigma_2)} \cdots U_n^{(\sigma_n)}\right)_\alpha |\sigma_1 \sigma_2 \cdots \sigma_n\rangle$$

$$(S_n)_{\alpha\alpha} \sum_{\sigma_{n+1}\cdots\sigma_N} \left((V_{n+1}^\dagger)^{\sigma_{n+1}} \cdots (V_N^\dagger)^{\sigma_N}\right)_\alpha |\sigma_{n+1}\cdots\sigma_N\rangle$$

$|\alpha_{N-n}\rangle$

$$= \sum_{\alpha=1}^{d_n} (S_n)_{\alpha\alpha} |\alpha_n\rangle \otimes |\alpha_{N-n}\rangle$$

$\downarrow$

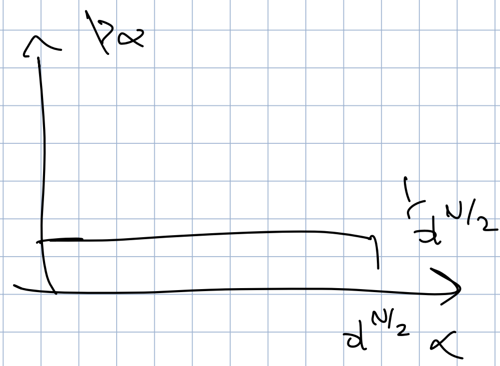
Schmidt decomposition

$$s_\alpha = \sqrt{p_\alpha} \qquad \sum_\alpha p_\alpha = 1$$

$\chi_n \le d^{N/2}$

$$\sum_{\alpha=1}^{d^{N/2}} p_\alpha = 1$$

extreme situation $\rightarrow$ $p_\alpha = \frac{1}{d^{N/2}}$



$S_n = S_A = \frac{N}{2} \log d$ maximally entangled state

To represent general states as MPS, I need to work with matrices as big as $d^{N/2} \times d^{N/2-1}$ (exponentially big in N).

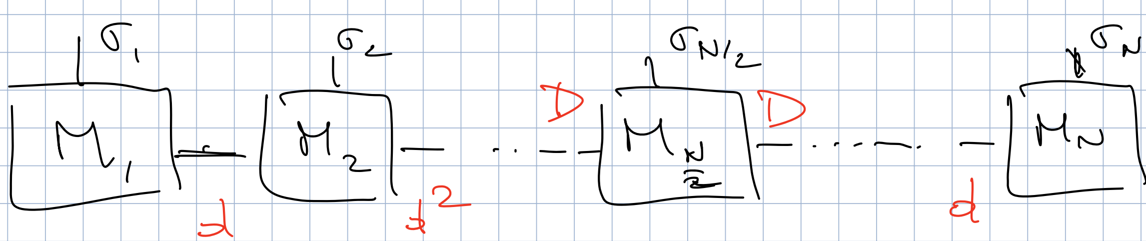
But for special states (ground states of a local Hamiltonian):

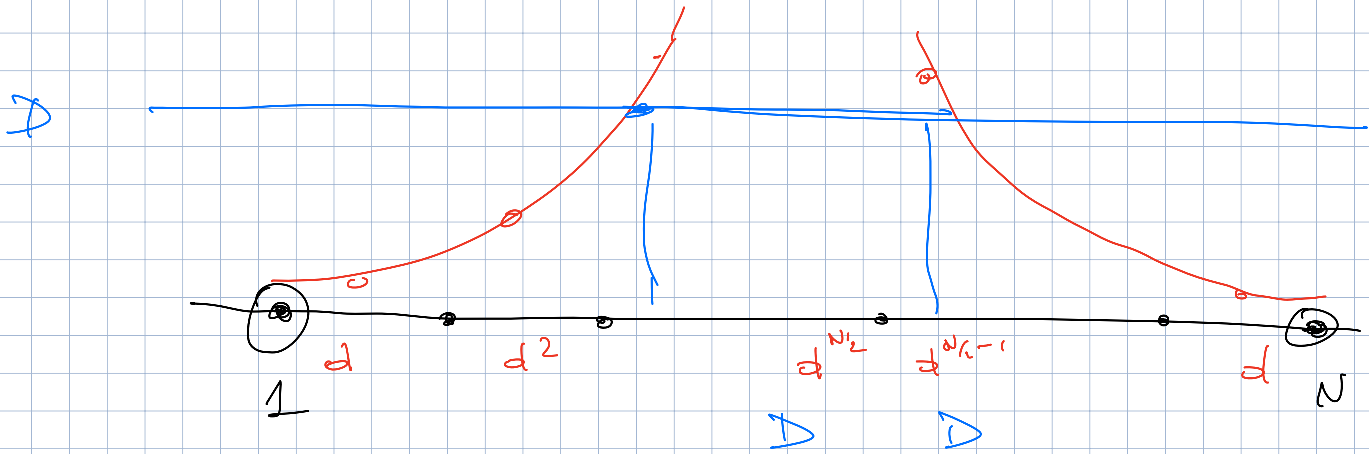
$S_n \sim N^0$ the dimension $D = 1$

$\Rightarrow$ I can truncate the bond dimension of the matrices of the MPS to a finite value

MPS Ansatz with finite bond-dimension D

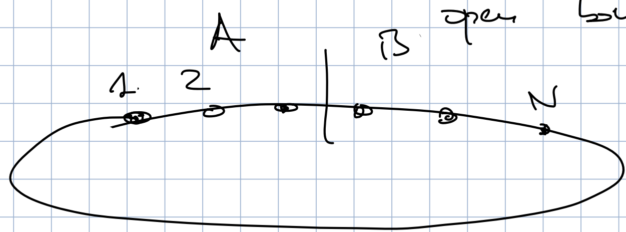
$\psi(\sigma_1 \dots \sigma_N) =$





$$|\Psi\rangle_{MPS} = \sum_{\sigma_1\sigma_2\cdots\sigma_N} \underbrace{\vec{M}_1^{(\sigma_1)}}_{1\times d}\ \underbrace{M_2^{(\sigma_2)}}_{d\times d^2} \cdots \underbrace{\ }_{D\times D} \underbrace{\vec{M}_N^{(\sigma_N)}}_{d\times 1} |\sigma_1\sigma_2\cdots\sigma_N\rangle$$

open boundary conditions



periodic BCs

$$= \sum_{\sigma_1\sigma_2\cdots\sigma_N} \mathrm{Tr}\Big(\underbrace{M_1^{(\sigma_1)}}_{D\times D}\underbrace{M_2^{(\sigma_2)}}_{D\times D} \cdots M_N^{(\sigma_N)}\Big)|\sigma_1\cdots\sigma_N\rangle$$

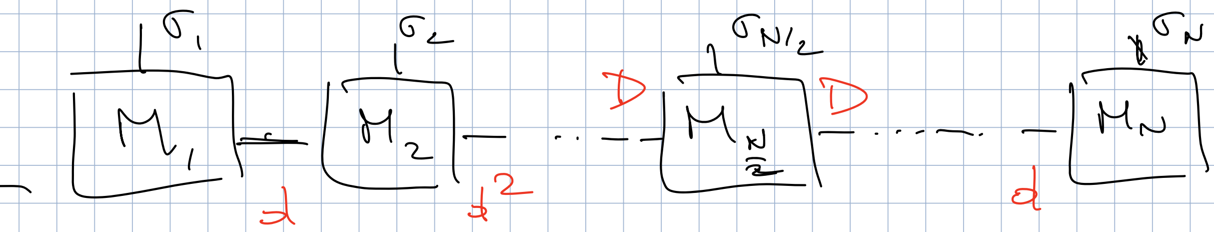
maximal entanglement entropy associated with an MPS of bond dimension D

$\Rightarrow S_A \le \log D$ D fixed

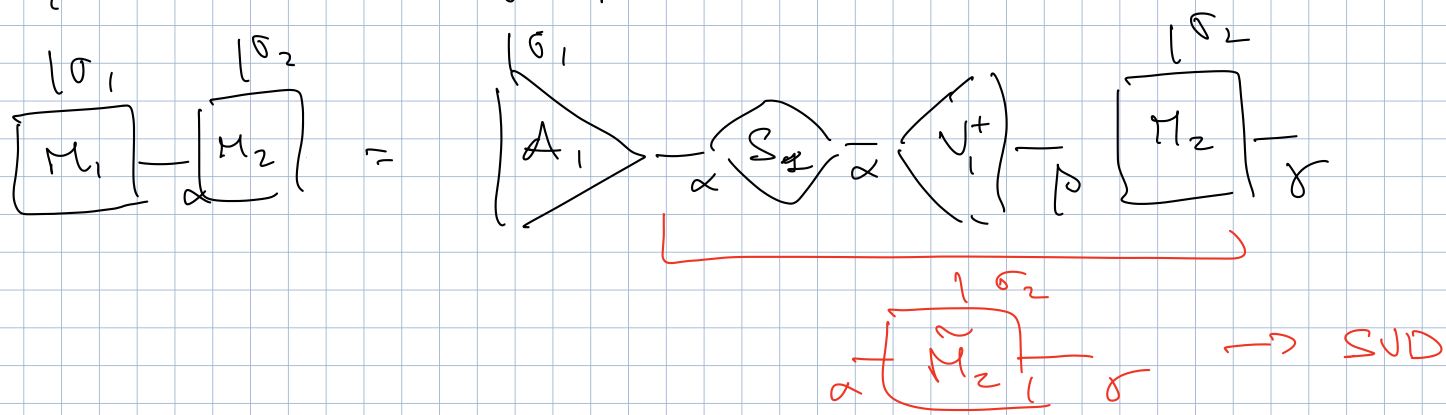
I can use MPS to approximate weakly entangled states

Put MPS in a left or right (or mixed) canonical form

$\psi(\sigma_1 \dots \sigma_N) =$

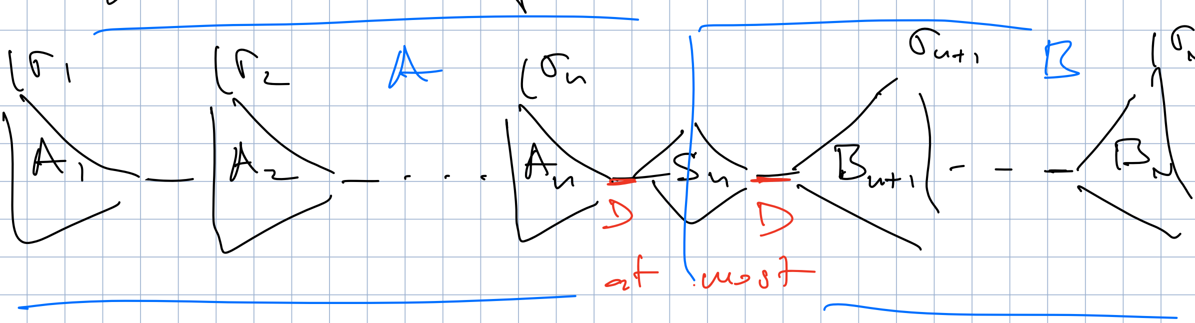


by SVDs starting from the left



Mixed left-right canonical form : MPS with maximal bond dimension D

$\psi(\sigma_1 \dots \sigma_N) =$



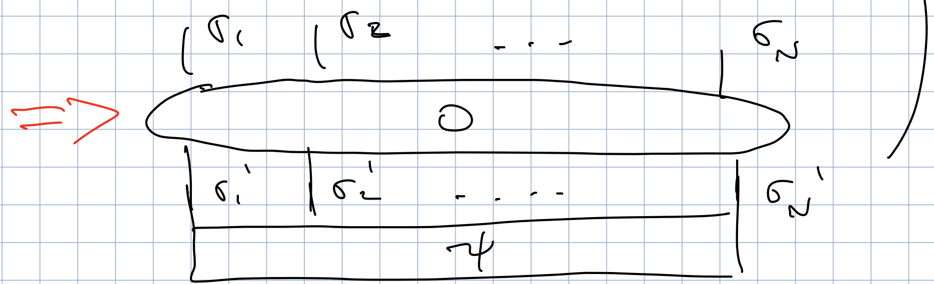
$$S_A \leq \log D$$

Operators $\Rightarrow$ matrix product operators (MPOs)

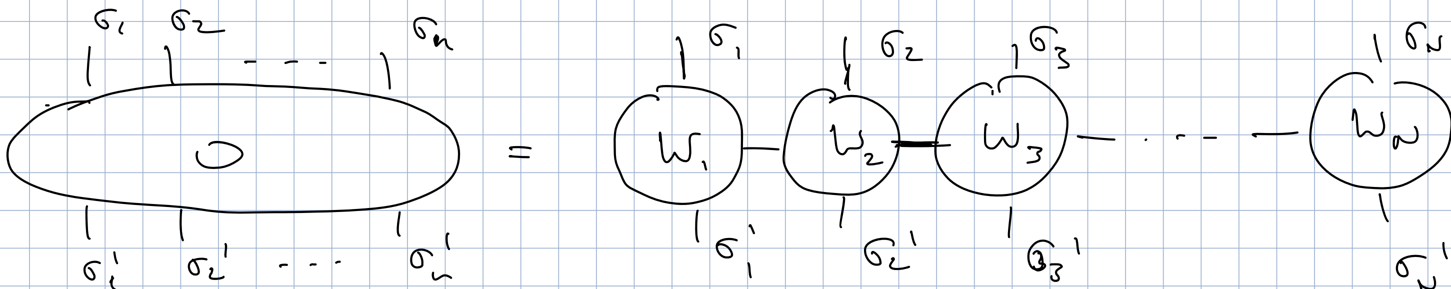
$$\hat{O} = \sum_{\sigma_1\sigma_2\ldots\sigma_N} \sum_{\sigma_1'\sigma_2'\ldots\sigma_N'} O^{\sigma_1\sigma_2\ldots\sigma_N}_{\sigma_1'\sigma_2'\ldots\sigma_N'} |\sigma_1\sigma_2\ldots\sigma_N\rangle\langle\sigma_1'\sigma_2'\ldots\sigma_N'|$$

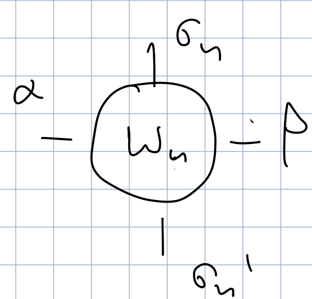
$$\hat{O}|\Psi\rangle = \sum_{\sigma_1\ldots\sigma_N} \underbrace{\left(\sum_{\sigma_1'\ldots\sigma_N'} O^{\sigma_1\sigma_2\ldots\sigma_N}_{\sigma_1'\ldots\sigma_N'}\,\psi(\sigma_1'\ldots\sigma_N')\right)}_{\psi'(\sigma_1\ldots\sigma_N)} |\sigma_1\ldots\sigma_N\rangle$$

$\Rightarrow$



MPO form





$\alpha = 1, \ldots, D_W$

D_W : bond dimension of the MPO

D_W does not scale with the size N of the system

$$O^{\sigma_1\sigma_2\cdots\sigma_N}_{\sigma_1'\sigma_2'\cdots\sigma_N'} = \vec{W}_1^{(\sigma_1\sigma_1')}\, W_2^{(\sigma_2\sigma_2')} \cdots \vec{W}_N^{(\sigma_N\sigma_N')}$$

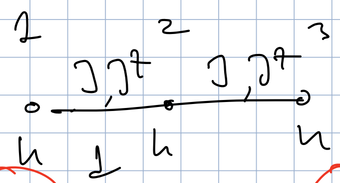
W_n matrix of $d \times d$ matrices

contain only operators acting on site n

Example : XXZ model S - spin

$$H = \sum_{i=1}^{N-1}\left[\frac{J}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + J_z S_i^z S_{i+1}^z\right] - h\sum_i S_i^z$$

$= O$



$N=3$

$$\frac{J}{2}\left(S_1^+ S_2^- + S_1^- S_2^+\right) + J_z S_1^z S_2^z - h S_1^z \times \mathbb{1}_2$$

$$\frac{J}{2}\left(S_2^+ S_3^- + S_2^- S_3^+\right) + J_z S_2^z S_3^z - h S_2^z \otimes \mathbb{1}_1 - h S_3^z \times \mathbb{1}_2$$

$5 = D_W$

$$\begin{pmatrix} -h\hat{S}_1^z \\ \frac{J}{2}\hat{S}_1^+ \\ \frac{J}{2}\hat{S}_1^- \\ J_z\hat{S}_1^z \\ \mathbb{1}_2 \end{pmatrix}^T \begin{pmatrix} \mathbb{1} & & & & \\ S_2^- & & & & \\ S_2^+ & & & & \\ S_2^z & & & & \\ -hS_2^z & \frac{J}{2}S_2^- & \frac{J}{2}S_2^+ & J^z S_2^z & \mathbb{1} \end{pmatrix} \begin{pmatrix} \mathbb{1} \\ S_3^+ \\ S_3^- \\ S_3^z \\ -hS_3^z \end{pmatrix}$$

W_1

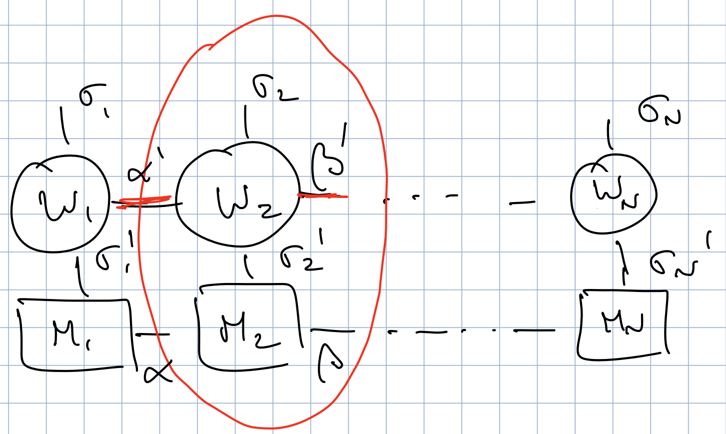
(1) (2) (3)

nearest - neighbor interactions $D_W = 5$

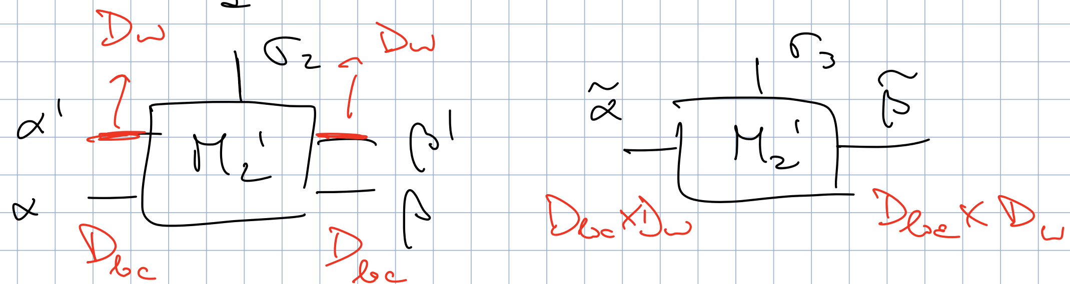
Longer range interactions $\Rightarrow$ bigger bond dimensions D_W

Applying a MPO to an MPS

$$\underset{\text{MPO} \;\to\; \text{MPS}}{\hat{O}\,|\Psi\rangle} = \sum_{\sigma_1 \dots \sigma_N} \underbrace{\psi'(\sigma_1 \dots \sigma_N)}_{\downarrow} \, |\sigma_1 \dots \sigma_N\rangle$$



$\downarrow$



$D_{loc} \leq D$

Application of an MPO with BD D_W onto an MPS with max BD D $\to$ MPS with max BD $D \times D_W$ =

$$O^2\,|\Psi\rangle \to D \times D_W^2$$

Compression of an MPS

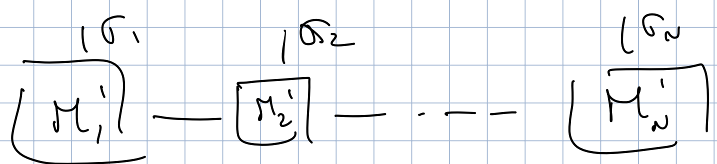
reducing an MPS of BD D' to an MPS of BD $D < D'$

→ SVD compression

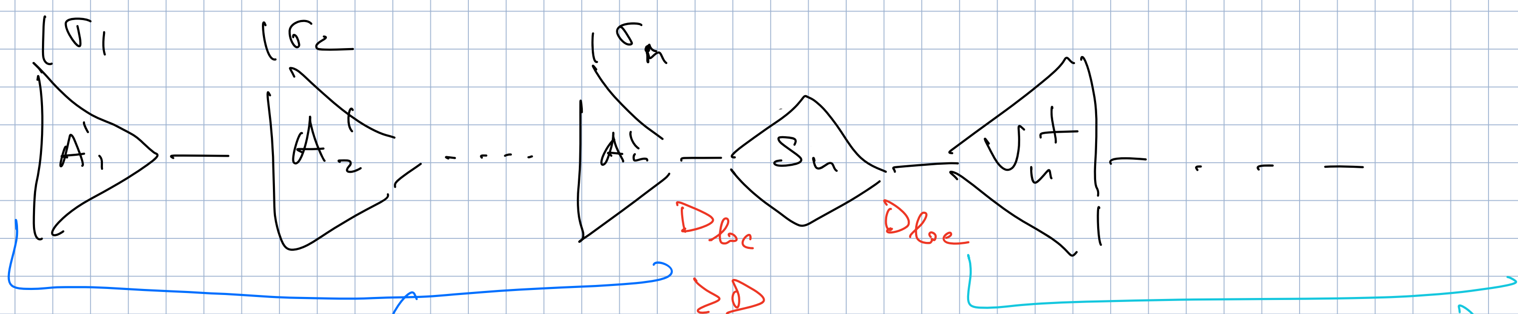
→ variational compression (minimize $\| |\psi_D\rangle - |\psi_{D'}\rangle \|^2$)

SVD compression

MPS with max bond dimension D'



put it in canonical form (left or right)



$$\begin{pmatrix} (S_n)_{11} & & & & & \\ & (S_n)_{22} & & & & \\ & & \ddots & & & \\ & & & (S_n)_{DD} & & \\ & & & & \ddots & \\ & & & & & (S_n)_{D_{loc}D_{loc}} \end{pmatrix}$$

Same as

$$|\Psi\rangle = \sum_{\alpha=1}^{D_{bc}} (S_n)_{\alpha\alpha} \, |\alpha_n\rangle \otimes |\alpha_{N-n}\rangle$$

$$\simeq \sum_{\alpha=1}^{D} (S_n)_{\alpha\alpha} \, |\alpha_n\rangle \otimes |\alpha_{n-N}\rangle \times \mathcal{N}$$

truncation error $\underline{\sum_{\alpha=D+1}^{D_{bc}}} (S_n)^2_{\alpha\alpha} = \epsilon \ll 1$

Use MPS as variational states

$$E_\Psi = \frac{\langle\Psi| H |\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

minimize with respect to $\underline{M^{(\sigma)}_{\alpha\beta}}$

DMRG

S. White (1992) $\rightarrow$ Language of MPS $\underline{\simeq 2004}$

$\underline{\text{or}}$ imaginary time evolution

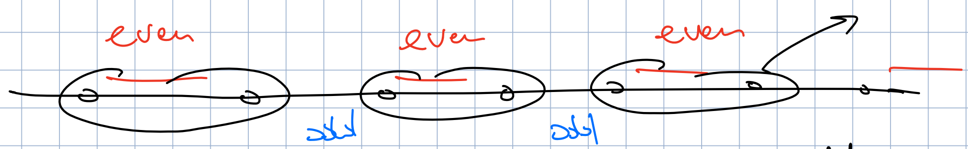
$$\frac{e^{-\tau H} |\Psi\rangle}{\| e^{-\tau H} |\Psi\rangle \|} \xrightarrow[\tau\to\infty]{} |\Psi_0\rangle$$

$$e^{-\tau H} |\Psi\rangle_D \underset{\text{truncation}}{\simeq} |\Psi'_D\rangle$$

$e^{-\tau H}$ $\rightarrow$ MPO $\rightarrow$ apply onto $|\Psi_D\rangle$ $\rightarrow$ truncate

MPS

$$H = \overbrace{\sum_{even} H_{even}}^{H_e} + \overbrace{\sum_{odd} H_{odd}}^{H_o}$$



$\prod_{even} e^{-\tau H_{even}}$

$$e^{-\delta\tau H} = e^{-\delta\tau H_e} \, e^{-\delta\tau H_o} + O(\delta\tau^2)$$

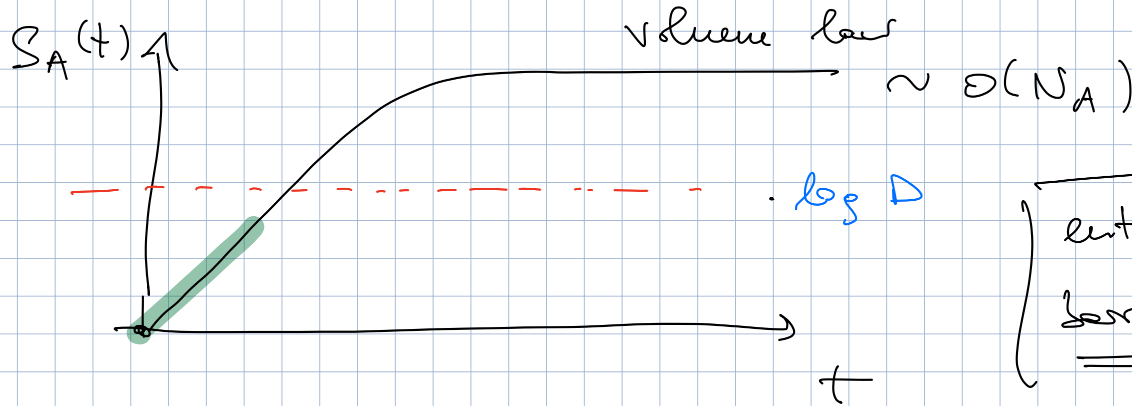
Trotter decomposition

real-time evolution

$\tau \rightarrow it$

$$|\psi(0)\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \qquad S_A = 0$$

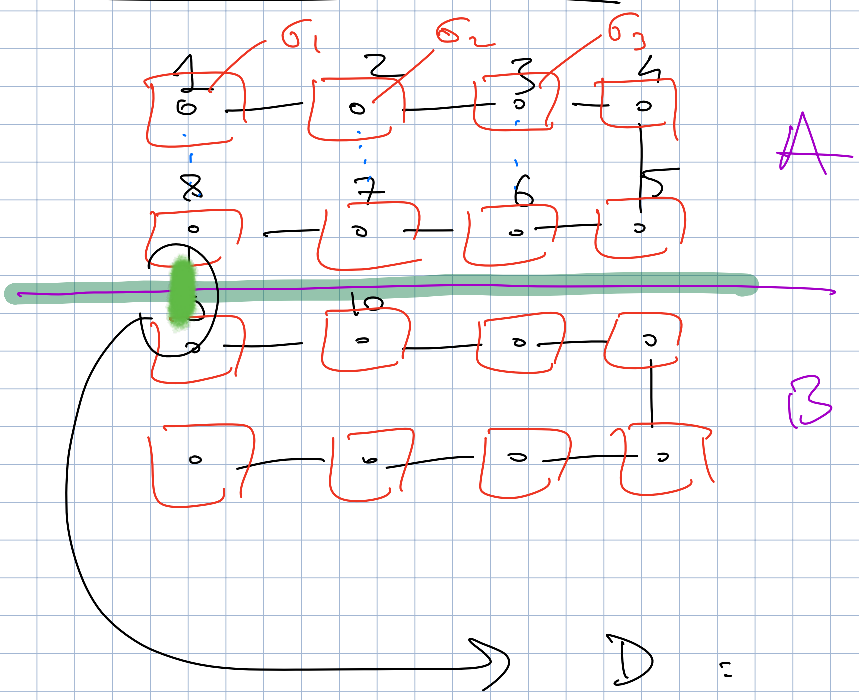
generically $\quad e^{-iHt}|\psi(0)\rangle = |\psi(t)\rangle$



$\boxed{\text{entanglement barrier}}$

Higher dimensions

$d = 2$



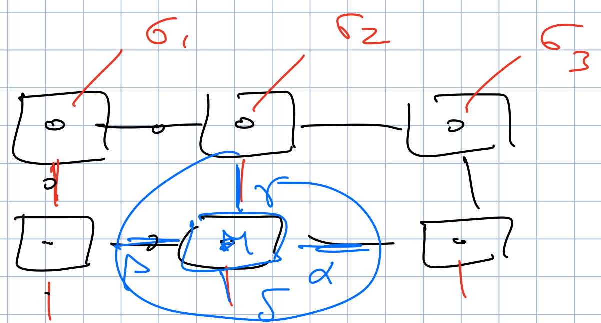
$S_A \sim L_A$

$D: \quad \log D = S_A \sim L_A$

$$D \sim e^{L_A}$$

2D MPS approaches (2D-DMRG)

other approaches : tensor network states



$$M^{(\sigma_n)}_{\alpha\beta\gamma\delta}$$

Problem : contracting a tensor network to calculate $\psi(\sigma_1, \sigma_2, \ldots, \sigma_N)$

r's exponentially costly. $\sim \exp(N)$

<u>matrix product</u> : cost $\sim ND^3$