

MPS

MATRIX-PRODUCT STATES

TNS

STATE / TENSOR-NETWORK STATES

( DMRG density-matrix renormalization group )

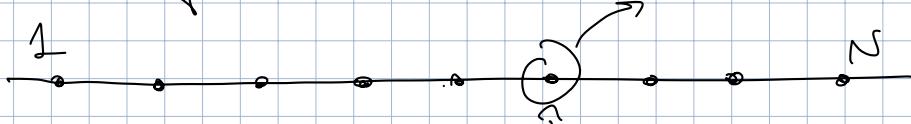
Class of variational quantum many-body states  
approx. of ground states of  $H$   
time-evolved states

Variational MC :  $\tilde{\Psi} = \text{product distribution } |\tilde{\Psi}|^2$

MPS / TNS methods  $\rightarrow$  view a quantum state as a  
tensor  $\tilde{\Psi}$   
 $\sigma_1, \sigma_2, \dots, \sigma_N$   
 $\rightarrow$  information content of  $\tilde{\Psi}$   
( Schmidt decomposition )  
 $\rightarrow$  "compress" the tensor by  
decomposing it

$\Rightarrow$  extremely effective for low-dimensional quantum systems  
esp. one-dimensional

Collection of "modes"



d-dimensional Hilbert space

mode : quantum spin  $\vec{s} \rightarrow |s\rangle$  eig of  $S^z$   
 $(\vec{s})^2 = s(s+1)$   $d = 2s+1$

lowest mode fermionic  $a_\alpha, a_\alpha^\dagger, |n\rangle$

$$d = n_{\max} + 1$$

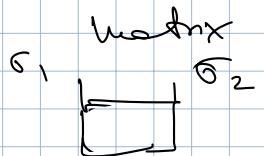
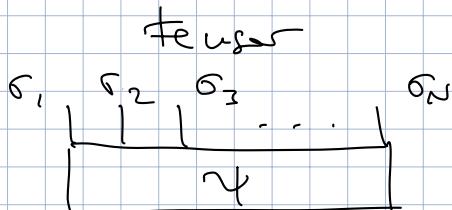
$$n = 0, \dots, n_{\max}$$

(5) : basis of local Hilbert space

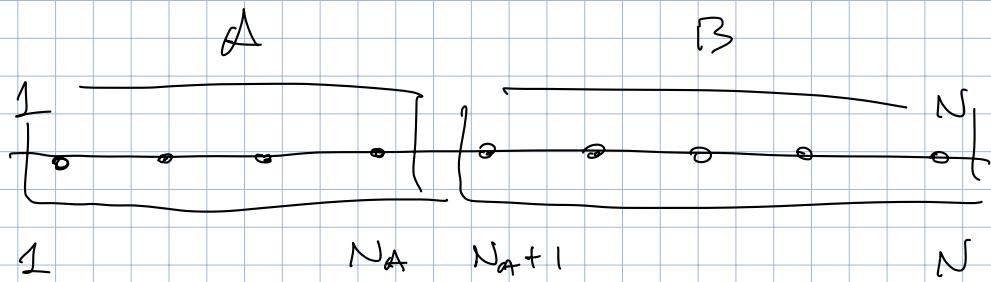
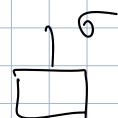
generic state

$\sigma = \sigma_1, \dots, \sigma_N$ , population

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



Vector



$$(\sigma_1, \sigma_2, \dots, \sigma_{N_A}) = |\dot{\gamma}_A\rangle$$

$d^{N_A}$  values

$$(\sigma_{N_A+1}, \dots, \sigma_N) = |\dot{\gamma}_B\rangle$$

$$|\Psi\rangle = \sum_{\dot{\gamma}_A = (\sigma_1, \dots, \sigma_{N_A})} \sum_{\dot{\gamma}_B = (\sigma_{N_A+1}, \dots, \sigma_N)} \psi_{\dot{\gamma}_A, \dot{\gamma}_B} |\dot{\gamma}_A\rangle \otimes |\dot{\gamma}_B\rangle$$

$$|\dot{\gamma}_A\rangle = (\sigma_1 - \sigma_{N_A}), \quad |\dot{\gamma}_B\rangle = (\sigma_{N_A+1} - \sigma_N)$$

$$\sigma_1 \left[ \begin{array}{cccc|c} 1 & 1 & 1 & \dots & \sigma_N \\ \hline \psi & & & & \end{array} \right] \rightarrow \begin{array}{c} |\dot{\gamma}_A\rangle \\ \rightarrow \\ |\dot{\gamma}_B\rangle \end{array} \quad N_B = N - N_A$$

$\psi_{\dot{\gamma}_A, \dot{\gamma}_B}$  is a rectangular

$$d_A^{N_A} \times d_B^{N_B} \text{ matrix}$$

## Singular value decomposition (SVD)

$$A = U S V^+ \quad d_A < d_B$$

$U$  = unitary  $d_A \times d_A$  matrix

left - singular vectors

$$U^T U = I$$

$$\begin{pmatrix} \vec{u}_1 & \vec{u}_2 & \dots & \vec{u}_{d_A} \\ | & | & & | \end{pmatrix}$$

$S = d_A \times d_A$  square matrix

diagonal

$$S_{\alpha} \geq 0$$

singular values

$$\begin{pmatrix} S_1 & & & 0 \\ & S_2 & & \\ & & \ddots & \\ 0 & & & S_{d_A} \end{pmatrix}$$

$$V^T = d_A \times d_B$$

$V = d_B \times d_A$  unitary matrix

$$V^T V = I_{d_A \times d_A}$$

$$V = d_B \begin{pmatrix} \vec{v}_1 & \dots & \vec{v}_{d_A} \\ | & & | \end{pmatrix}$$

right - singular vectors

$$A = [A] = [U] [S] [V^T]$$

$$\partial_A > \partial_B$$

The diagram illustrates the decomposition of a density matrix  $\Psi$  into a sum of projectors. On the left, a box labeled  $\Psi$  is shown. An equals sign follows, followed by a box labeled  $U$ , a yellow box labeled  $|S|$  (with a red line through it), and a box labeled  $V^+$ . Below the boxes are three equations:  $\partial_A \times \partial_B$  under the  $U$  box,  $\partial_B \times \partial_B$  under the  $|S|$  box, and  $\partial_B \times \partial_B$  under the  $V^+$  box.

$$S : \min(\partial_A, \partial_B) \times \min(\partial_A, \partial_B)$$

graphical representation of SVD

The diagram shows the graphical representation of the SVD decomposition of a density matrix  $\Psi$ . On the left, a box labeled  $\Psi$  is shown with indices  $i_A$  and  $i_B$ . An equals sign follows, followed by a diagram where  $\Psi$  is decomposed into  $U$ ,  $S$ , and  $V^+$ . The  $S$  matrix is circled in red. A red arrow points from this circle to the text "Contracted (= summed over) index". Another red arrow points from the same circle to the text "# of values of index = bond dimension".

$$\Psi_{i_A i_B} = \sum_{\alpha} U_{i_A \alpha} S_{\alpha \alpha} (V^+)^{\alpha}_{i_B}$$

SVD applied to a bipartite quantum state

$$|\tilde{\Psi}\rangle = |\tilde{\Psi}_{AB}\rangle = \underbrace{|\tilde{\Psi}_{i_A i_B}\rangle}_{\partial_A \times \partial_B \text{ values}} \quad \underbrace{|\tilde{\Psi}_{i_A i_B}\rangle}_{\text{SVD}} \quad (i_A) \otimes (i_B)$$

$$\min(d_A, d_B) = d_{\min}$$

$$= \sum_{\alpha=1}^{\infty} S_\alpha \underbrace{\sum_{i_A} U_{i_A \alpha}^\dagger |i_A\rangle}_{\downarrow} \otimes \underbrace{\sum_{i_B} (V^+)_{\alpha i_B}^\dagger |i_B\rangle}_{\downarrow}$$

$$\sum_{i_A} U_{i_A \alpha}^\dagger |i_A\rangle \xrightarrow{\text{Schmidt vectors}} |\alpha_A\rangle$$

$$= \sum_{\alpha=1}^{\infty} S_\alpha |\alpha_A\rangle \otimes |\alpha_B\rangle$$

Schmidt decomposition

Schmidt decomposition

$$\langle \alpha_A' | \alpha_A \rangle = \delta_{\alpha \alpha'}$$

$$S_\alpha = \sqrt{p_\alpha} \geq 0$$

Schmidt values

$$\langle \alpha_B' | \alpha_B \rangle = \delta_{\alpha \alpha'}$$

$$\sum_\alpha S_\alpha^2 = \langle \tilde{\Sigma} | \tilde{\Sigma} \rangle = \sum_\alpha p_\alpha = 1$$

Entanglement : for bipartite systems

$$|\tilde{\Sigma}_{AB}\rangle \neq |\tilde{\Sigma}_A\rangle \otimes |\tilde{\Sigma}_B\rangle$$

entanglement  $\Leftrightarrow$  at least two non-zero Schmidt values  
 $\Rightarrow p_1, p_2 \neq 0$

$$|\tilde{\Sigma}_{AB}\rangle = \sqrt{p_1} |1_A\rangle |1_B\rangle + \sqrt{p_2} |2_A\rangle |2_B\rangle + \dots$$

Entanglement is the root of the information complexity of quantum mechanics

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

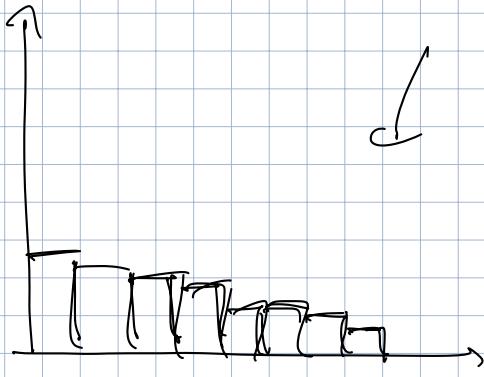
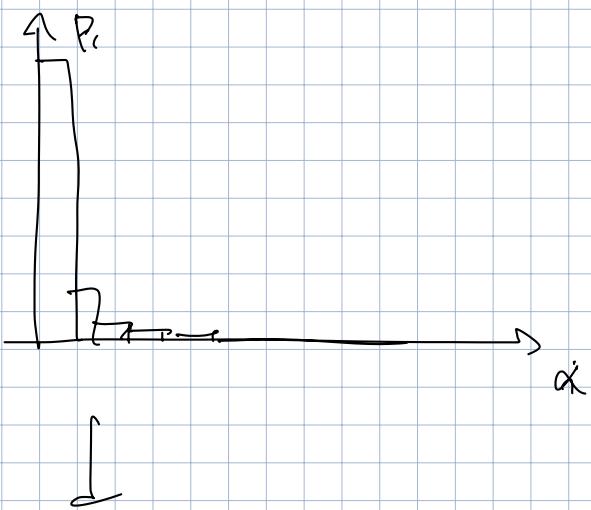
→  $2^N$  coefficients

$\neq |\psi_1\rangle \otimes |\psi_2\rangle \otimes \dots \otimes |\psi_N\rangle$

$\hookrightarrow$   $2^N$  coefficients

To quantify entanglement: maybe count the non-Schmidt values

$$p_1 > p_2 > p_3 > \dots$$



$$|\psi_{\text{AS}}\rangle \approx |1_A\rangle \otimes |1_B\rangle + \dots$$

(Shannon) entropy of the Schmidt values

$$S_A = - \sum_{\alpha \geq 1} p_\alpha \log p_\alpha$$

( Von Neumann ) entanglement entropy

= thermodynamic entropy of the reduced state  
of A (or B)

$$|\psi_{AB}\rangle \rightarrow \rho_{AB} = |\psi_{AB}\rangle \langle \psi_{AB}|$$

$$\rho_A = \text{Tr}_B \rho_{AB}$$

$$= \sum_{|j_B\rangle} \langle j_B | \sum_{\substack{i_A i_B \\ i_A' i_B'}} \chi_{i_A i_B}^* \chi_{i_A' i_B'} |i_A\rangle \langle i_B | \langle i_A' | \langle i_B' | |j_B\rangle$$

$$= \sum_{i_A i_B} \left( \sum_{j_B} \chi_{i_A j_B}^* \chi_{i_A' j_B'} \right) |i_A\rangle \langle i_A'|$$

$$S_A = -\text{Tr}(\rho_A \log \rho_A) = S_B = -\text{Tr}(\rho_B \log \rho_B)$$

$$|\psi_{AB}\rangle = \sum_{\alpha} p_{\alpha} |\alpha_A\rangle \otimes |\alpha_B\rangle$$

$$\rho_A = \sum_{\alpha} p_{\alpha} |\alpha_A\rangle \langle \alpha_A|$$

$$\rho_B = \sum_{\alpha} p_{\alpha} |\alpha_B\rangle \langle \alpha_B|$$

$$S_A = \begin{cases} 0 & p_2 = 1, p_{\alpha \neq 2} = 0 \\ \log d_{\min} & \end{cases}$$

$$p_{\alpha} = \frac{1}{d_{\min}}$$

$$\log S_{\text{min}} = \min(N_A, N_B) \log d$$

$$S_A \sim \min(N_A, N_B)$$

extreme entropies (?)

If you extract a random state in Hilbert space

$\psi_{\epsilon_1, \epsilon_2, \dots, \epsilon_n}$  are random numbers

$$\Rightarrow S_A \sim \min(N_A, N_B)$$

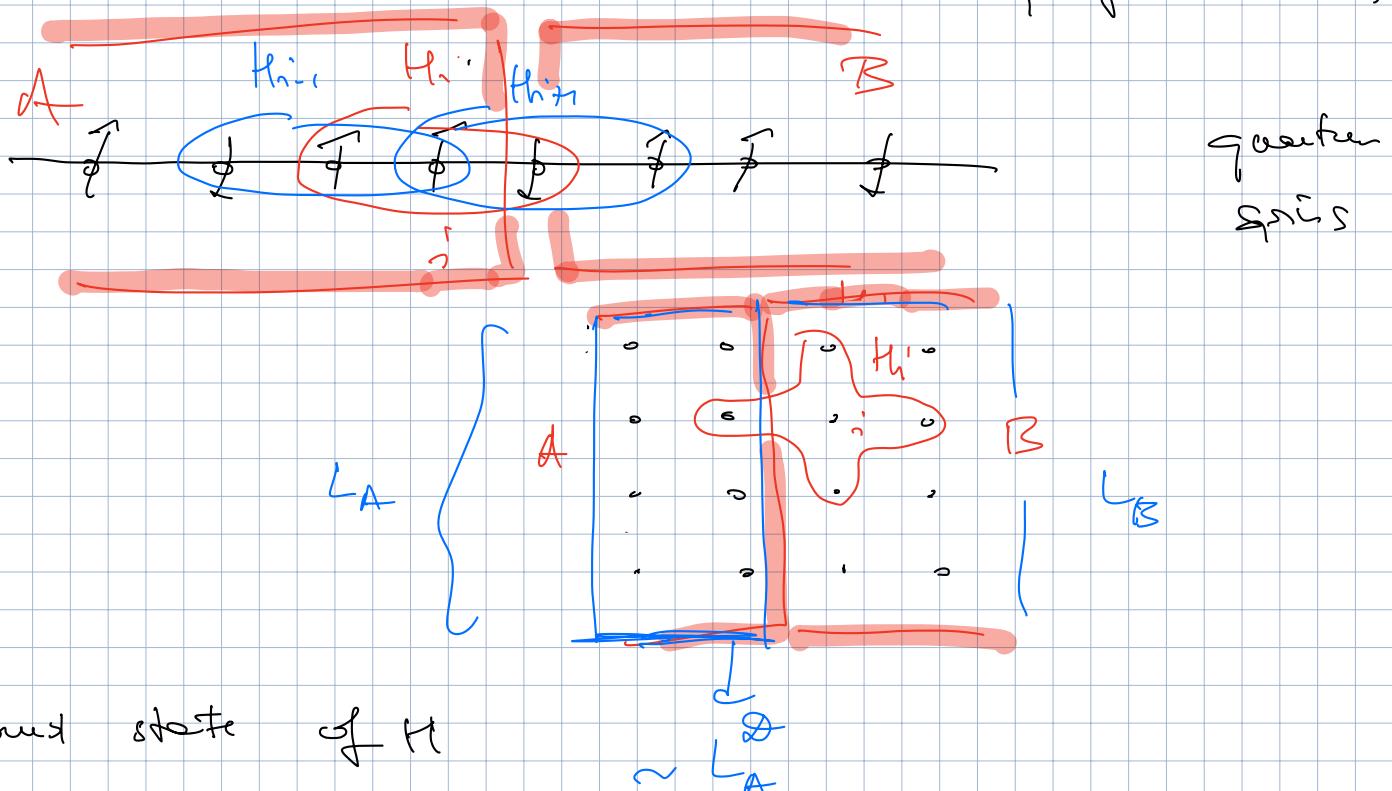
"volume law" of scaling

If you look at physically relevant states:

ground states of local Hamiltonians

$$H = \sum_i H_i$$

$H_i$  contains only degrees of freedom in the vicinity of a node



Ground state of  $H$

$$S_A \sim L_A^{d-1}$$

"area law" of scaling

$d = \#$  of spatial dimensions

$$L_A \sim \text{perimeter} / \text{outer surface} \quad \begin{cases} d=2 \\ d=3 \end{cases}$$

$L_A$  = linear dimension of A

$$\text{in } d=1 \quad S_A \sim L_A^0$$



Idea: searching for efficient approximations of "weakly entangled" states (satisfying an area law)

=> Matrix product states (MPS) for  $d=1$   
[tensor network states (TNS) for  $d>1$ ]

Bringing a generic state into matrix-product form

$$|\psi\rangle \rightarrow \begin{array}{c} \sigma_1 \quad \sigma_2 \\ \boxed{\phantom{...}} \quad \dots \quad \boxed{\phantom{...}} \\ \downarrow \qquad \qquad \qquad \downarrow \\ \sigma_N \end{array}$$

$$\psi(\sigma_1, \sigma_2, \dots, \sigma_N) \rightarrow \psi_{i_1 i_2 \dots i_N}$$

$$\begin{array}{c} \sigma_1 \quad \sigma_2 \\ \boxed{\phantom{...}} \quad \dots \quad \boxed{\phantom{...}} \\ \downarrow \qquad \qquad \qquad \downarrow \\ \sigma_N \end{array} = \begin{array}{c} i_1 = \sigma_1 \quad \sim \quad i_N = (\sigma_2 \dots \sigma_N) \\ \boxed{\phantom{...}} \quad \boxed{\phantom{...}} \quad \dots \quad \boxed{\phantom{...}} \\ \downarrow \qquad \qquad \qquad \downarrow \\ \end{array} = \underbrace{\psi_{i_1 i_2 \dots i_N}}$$

SVD on  $\psi_{i_1 i_2 \dots i_N}$   $d \times d^{N-1}$  matrix

$$\boxed{\psi} = \alpha \left( \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_d \end{array} \right) - j_1$$

$$\alpha = \frac{1}{\sqrt{d}} \quad \text{---} \quad \boxed{j_1}$$

$$= \alpha \left( \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_d \end{array} \right) - j_1$$

$$= \alpha \left( \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_d \end{array} \right) - j_1 = (\sigma_2 \ \sigma_3 \ \dots \ \sigma_N)$$

Reshaping the matrix

$$\boxed{j_2} = \alpha \left( \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_d \end{array} \right) - j_2 = (\sigma_3 \ \sigma_4 \ \dots \ \sigma_N)$$

$$d \times d = d^2$$

$$\boxed{\psi} = \left| \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_d \end{array} \right| = \alpha_1 \left( \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_d \end{array} \right) - j_1$$

$$\alpha_1 = \frac{1}{\sqrt{d}}$$

$$\alpha_1 \left( \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_d \end{array} \right) - j_1$$

$$\alpha_2 = \frac{1}{\sqrt{d}}$$

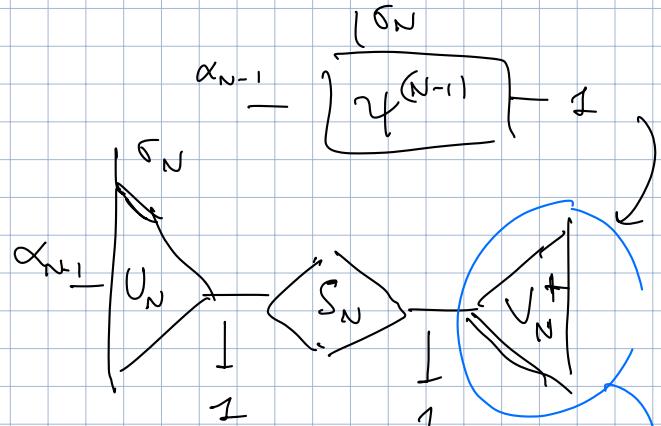
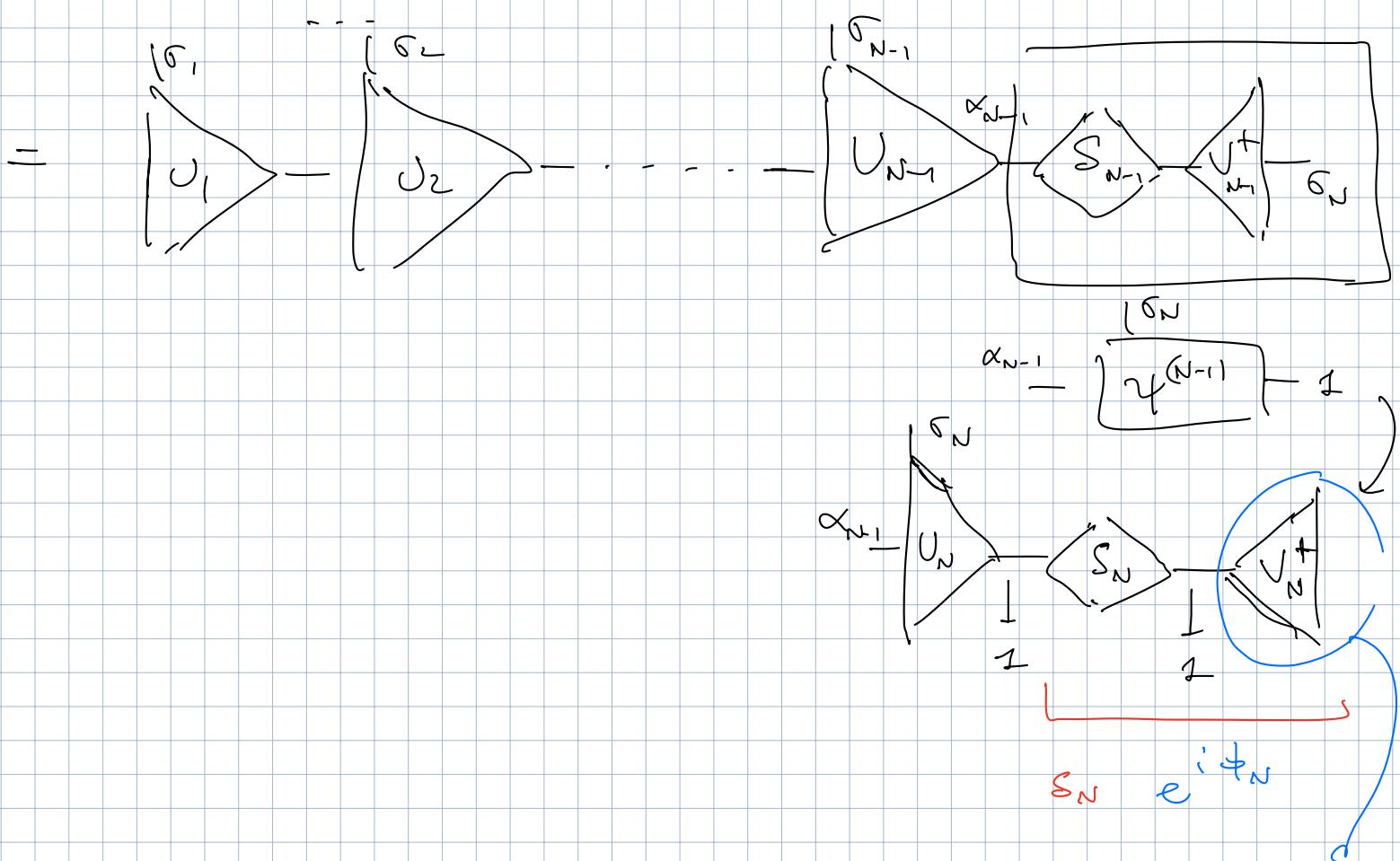
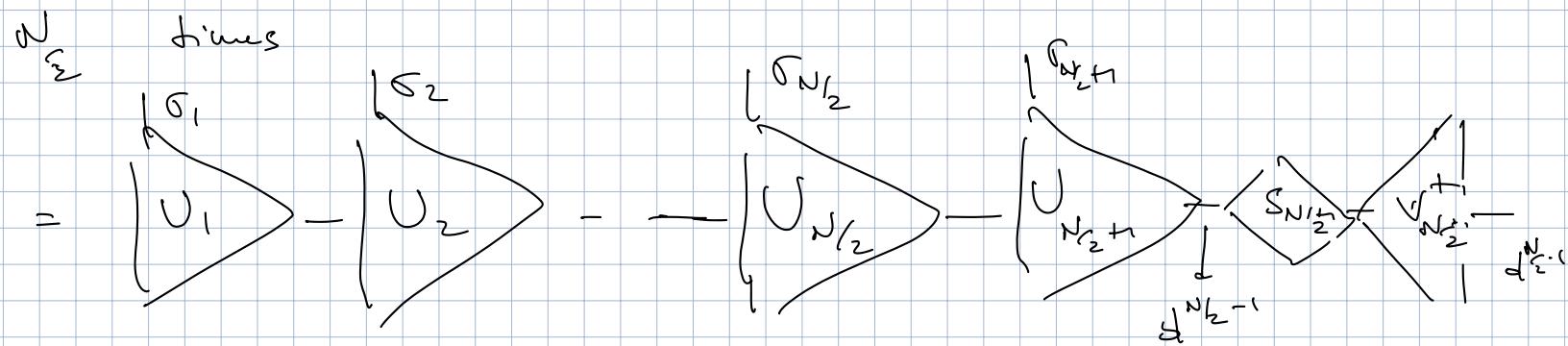
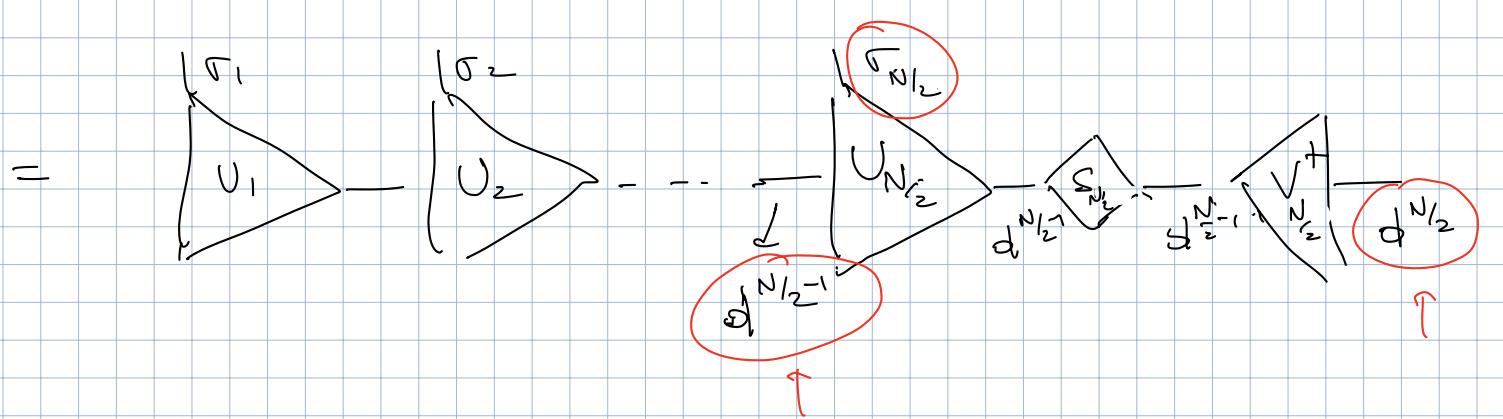
$$\alpha_2 \left( \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_d \end{array} \right) - j_2 = (\sigma_3 \ \sigma_4 \ \dots \ \sigma_N)$$

$$\alpha_2 = \frac{1}{\sqrt{d}}$$

$$\alpha_2 \left( \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_d \end{array} \right) - j_2 = (\sigma_3 \ \sigma_4 \ \dots \ \sigma_N)$$

$$n = N_{1/2} - 1 \quad \text{times}$$

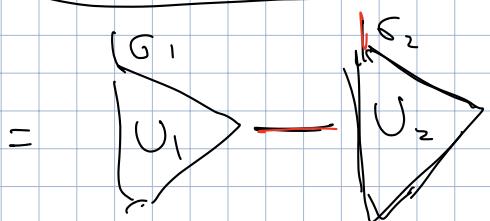
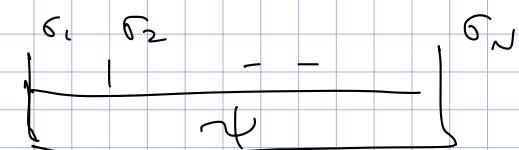
$$\alpha_{N_{1/2}-1} \left( \begin{array}{c} \sigma_1 \\ \vdots \\ \sigma_d \end{array} \right) - j_{N_{1/2}} = (\sigma_{N_{1/2}+1} \ \dots \ \sigma_N)$$



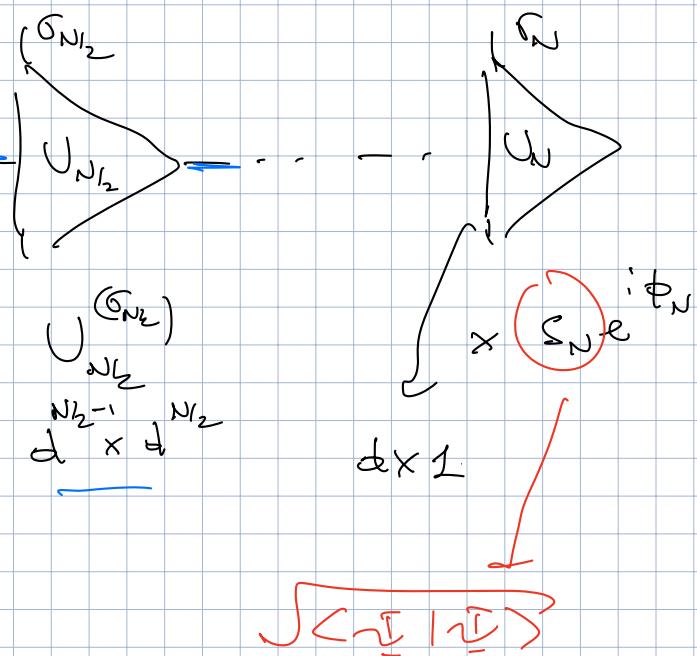
$$S_N e^{i \phi_N}$$

$1 \times 1$  unitary  
matrix

Result : left-canonical matrix-product form



$$= \underbrace{\begin{array}{c} U_1 \\ \vdots \\ U_d \end{array}}_{d \times d} \underbrace{\begin{array}{c} \epsilon_1 \\ \vdots \\ \epsilon_d \end{array}}_{d \times d^2}$$



$$\underbrace{\begin{array}{c} U_{Nl_2} \\ \vdots \\ U_{Nl_2}^{(Nl_2)} \end{array}}_{d \times d^{Nl_2-1}} \underbrace{\begin{array}{c} \epsilon_{Nl_2} \\ \vdots \\ \epsilon_N \end{array}}_{d \times 1}$$

$$\times \underbrace{\begin{array}{c} \epsilon_N \\ \vdots \\ \epsilon_N \end{array}}_{d \times 1} = \underbrace{\sqrt{\sum_{i=1}^N \epsilon_i^2}}_{d \times 1}$$