MATRIX-PRODUCT STATES / TENSOR-NETWORK STATES
(MPS / TNS)

(DMRG density-matrix renormalization group)

Class of variational quantum many-body states

approx. of ground states of H

time-evolved states

Variational MC : Ψ = probability distribution $|\Psi|^2$

MPS / TNS methods $\to$ view a quantum state as a tensor $\Psi_{\sigma_1 \sigma_2 \dots \sigma_N}$

$\to$ information content of Ψ

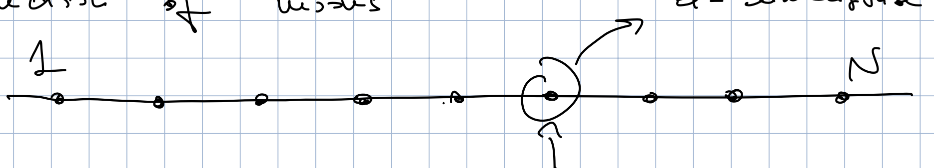
(Schmidt decomposition)

$\to$ "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 $\vec{S} \to |\sigma\rangle$ eig of S^z (local basis)

$|\vec{S}|^2 = S(S+1)$ $d = 2S+1$

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

$d = n_{max} + 1$

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

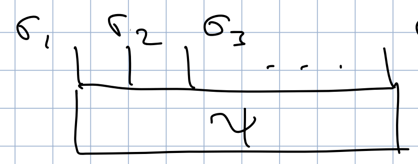
$|\sigma\rangle$: basis of local Hilbert space

σ = spin, population

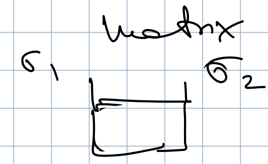
generic state

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

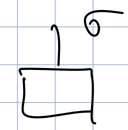
$\in \mathbb{C}$

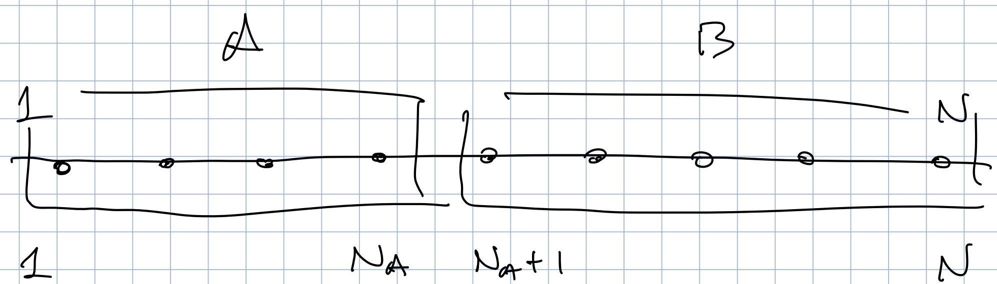


matrix



vector



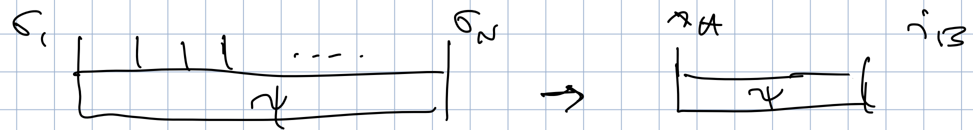


$(\sigma_1, \sigma_2 \dots \sigma_{N_A}) = i_A$ $\qquad (\sigma_{N_A+1} \dots \sigma_N) = i_B$

d^{N_A} values

$$|\Psi\rangle = \sum_{i_A = (\sigma_1 \dots \sigma_{N_A})} \sum_{i_B = (\sigma_{N_A+1} \dots \sigma_N)} \psi_{i_A, i_B} \, |i_A\rangle \otimes |i_B\rangle$$

$|i_A\rangle = |\sigma_1 \dots \sigma_{N_A}\rangle$, $\quad |i_B\rangle = |\sigma_{N_A+1} \dots \sigma_N\rangle$



$N_B = N - N_A$

ψ_{i_A, i_B} is a rectangular $d^{N_A} \times d^{N_B}$ matrix

d^{N_A} ↑ d_A, $\quad d^{N_B}$ ↑ d_B

Singular value decomposition (SVD)

$$\Psi = U S V^\dagger \qquad d_A \times d_B \qquad d_A < d_B$$

$U =$ unitary $d_A \times d_A$ matrix $\qquad U^\dagger U = \mathbb{1}$

left-singular vectors

$$U = \begin{pmatrix} \vec{u}_1 & \vec{u}_2 & \cdots & \vec{u}_{d_A} \\ | & | & & | \end{pmatrix}$$

$S = d_A \times d_A$ square matrix

diagonal

$$S = \begin{pmatrix} s_1 & & & 0 \\ & s_2 & & \\ & & \ddots & \\ 0 & & & s_{d_A} \end{pmatrix}$$

$$s_\alpha \geq 0$$

singular values

$V^\dagger = d_A \times d_B$

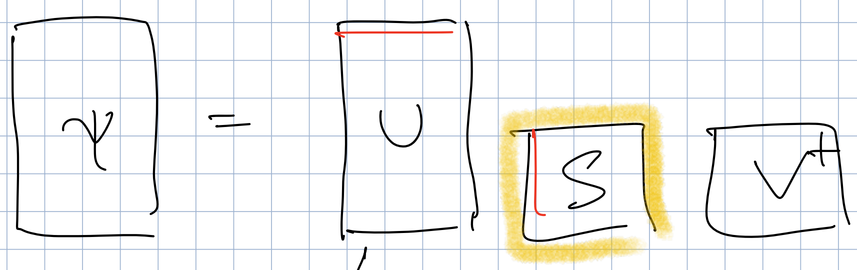
$V = d_B \times d_A$ unitary matrix $\qquad V^\dagger V = \mathbb{1}_{d_A \times d_A}$

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

right-singular vectors

$$\boxed{\Psi} = \boxed{U}\,\boxed{S}\,\boxed{V^\dagger}$$

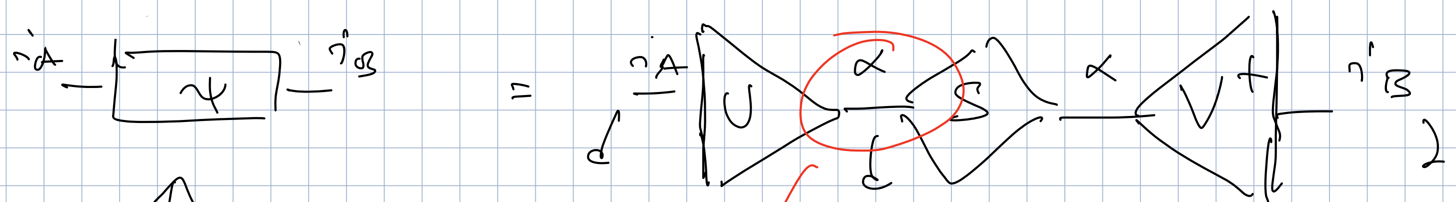
$d_A > d_B$



$d_A \times d_B \qquad d_B \times d_B \qquad d_B \times d_B$

S : $\min(d_A, d_B) \times \min(d_A, d_B)$

graphical representation of SVD



$1, \dots, d_A \qquad \alpha = 1, \dots, \min(d_A, d_B) \qquad 1, \dots, d_B$

contracted index (= summed over)

# of values of index = "bond dimension"

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

SVD applied to a bipartite quantum state

$$|\Psi\rangle = |\Psi_{AB}\rangle = \sum_{i_A i_B} \psi_{i_A i_B} |i_A\rangle \otimes |i_B\rangle$$

$d_A \times d_B$ values

SVD

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

$$= \sum_{\alpha=1} s_\alpha \underbrace{\sum_{i_A} U_{i_A \alpha} |i_A\rangle}_{\sum_{i_A} U^T_{\alpha i_A} |i_A\rangle = |\alpha_A\rangle} \otimes \underbrace{\sum_{i_B} (V^\dagger)_{\alpha i_B} |i_B\rangle}_{|\alpha_B\rangle}$$

Schmidt vectors

$$= \sum_{\alpha=1}^{d_{min}} s_\alpha |\alpha_A\rangle \otimes |\alpha_B\rangle$$

Schmidt decomposition

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

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

Schmidt values

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

$$\sum_\alpha s_\alpha^2 = \langle \Psi | \Psi \rangle = \sum_\alpha p_\alpha = 1$$

Entanglement : for bipartite systems

$$|\Psi_{AB}\rangle \neq |\Psi_A\rangle \otimes |\Psi_B\rangle$$

entanglement $\iff$ $\exists$ at least two non-zero Schmidt values

$\exists \; p_1, p_2 \neq 0$

$$|\Psi_{AB}\rangle = \sqrt{p_1} |1_A\rangle |1_B\rangle + \sqrt{p_2} |2_A\rangle |2_B\rangle + \ldots$$

Entanglement is the root of the information complexity of quantum mechanics

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

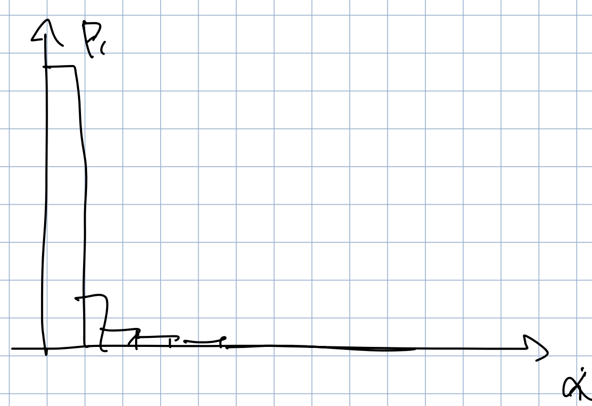
→ d^N coefficients

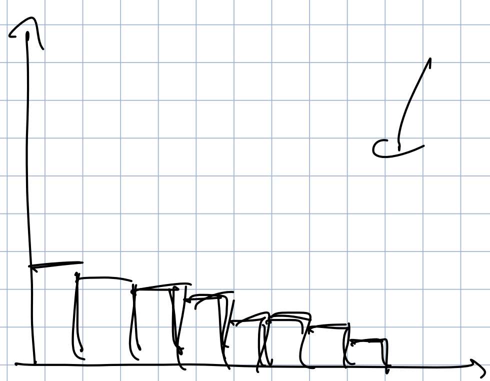
$$\neq |\psi_1\rangle \otimes |\psi_2\rangle \otimes \dots \otimes |\psi_N\rangle$$

↪ $\sim O(N)$ coefficients

To quantify entanglement: maybe count the non zero Schmidt values

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





↓

$$|\Psi_{AB}\rangle \simeq |1_A\rangle \otimes |1_B\rangle + \dots$$

(Shannon) entropy of the Schmidt values

$$S_A = - \sum_{\alpha=1}^{d_{min}} p_\alpha \log p_\alpha$$

(Von Neumann) entanglement entropy

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

$$|\Psi_{AB}\rangle \to \rho_{AB} = |\Psi_{AB}\rangle\langle\Psi_{AB}|$$

$$\rho_A = \mathrm{Tr}_B\, \rho_{AB}$$

$$= \sum_{|j_B\rangle} \langle j_B| \sum_{\substack{i_A i_B \\ i'_A i'_B}} \psi_{i_A i_B} \psi^*_{i'_A i'_B} |i_A\rangle|i_B\rangle\langle i'_A|\langle i'_B| \, |j_B\rangle$$

$$= \sum_{i_A i'_A} \left(\sum_{j_B} \psi_{i_A j_B} \psi^*_{i'_A j_B} \right) |i_A\rangle\langle i'_A|$$

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

$$|\Psi_{AB}\rangle = \sum_\alpha \sqrt{p_\alpha}\, |\alpha_A\rangle \otimes |\alpha_B\rangle$$

$$\rho_A = \sum_\alpha p_\alpha |\alpha_A\rangle\langle\alpha_A| \qquad \rho_B = \sum_\alpha p_\alpha |\alpha_B\rangle\langle\alpha_B|$$

$$S_A = \begin{cases} 0 & p_1 = 1,\ p_{\alpha\neq 1} = 0 \\ \log d_{min} & p_\alpha = \dfrac{1}{d_{min}} \end{cases}$$

$$\log d_{min} = \min(\underline{N_A}, \underline{N_B}) \log d$$

$S_A \sim \min(N_A, N_B)$ extensive entropies (?)

if you extract a random state in Hilbert space

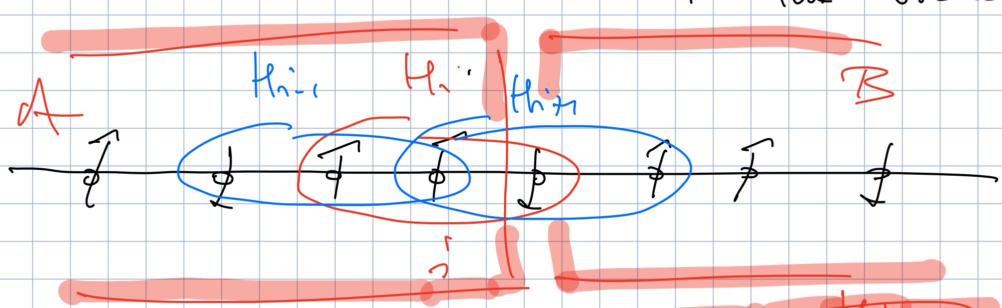
$\psi_{\sigma_1 \sigma_2 \dots \sigma_N}$ are random numbers

$\Rightarrow S_A \sim \min(N_A, N_B)$ "volume law" of scaling

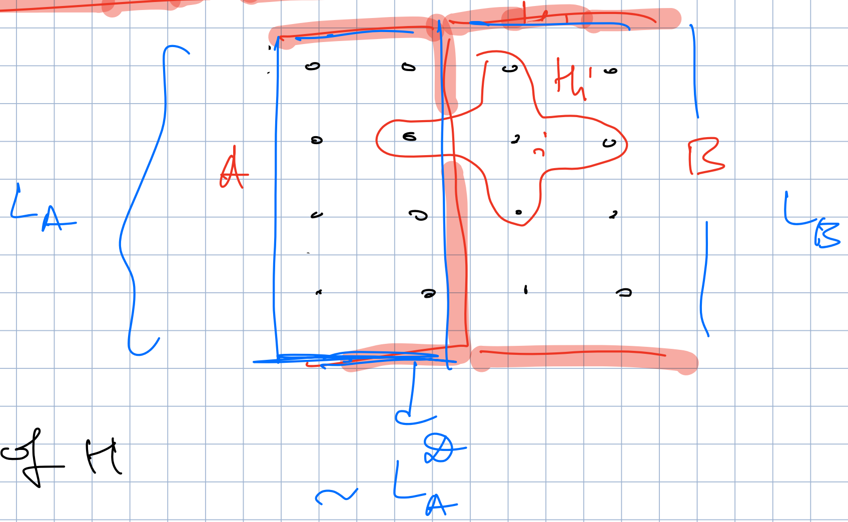
If you look at physically relevant states:

ground states of local Hamiltonians

$H = \sum_i H_i$ H_i contains only degrees of freedom in the vicinity of a mode i



quantum spins



Ground state of H

$S_A \sim L_A^{\mathcal{D}-1}$ "area law" of scaling

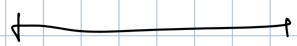
$\mathcal{D}$ = # of spatial dimensions

$L_A^{\mathcal{D}-1} \sim$ perimeter / outer surface of A

$\mathcal{D}=2$ $\mathcal{D}=3$

L_A = linear dimension of A

in $\mathcal{D}=1$ $S_A \sim L_A^0$



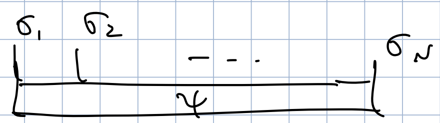
Idea: searching for efficient approximations of "weakly entangled" states (satisfying an area law)

=> Matrix product states (MPS) for $d=1$

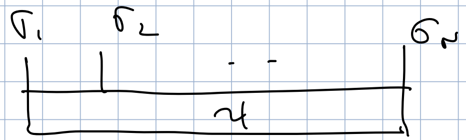
[tensor network states (TNS) for $d>1$]

Bring a generic state into matrix-product form

$|\Psi\rangle \to$



$\Psi(\sigma_1, \sigma_2, \ldots, \sigma_N) \to \Psi_{i_A i_B}$



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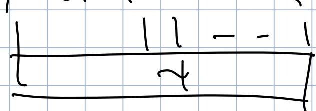
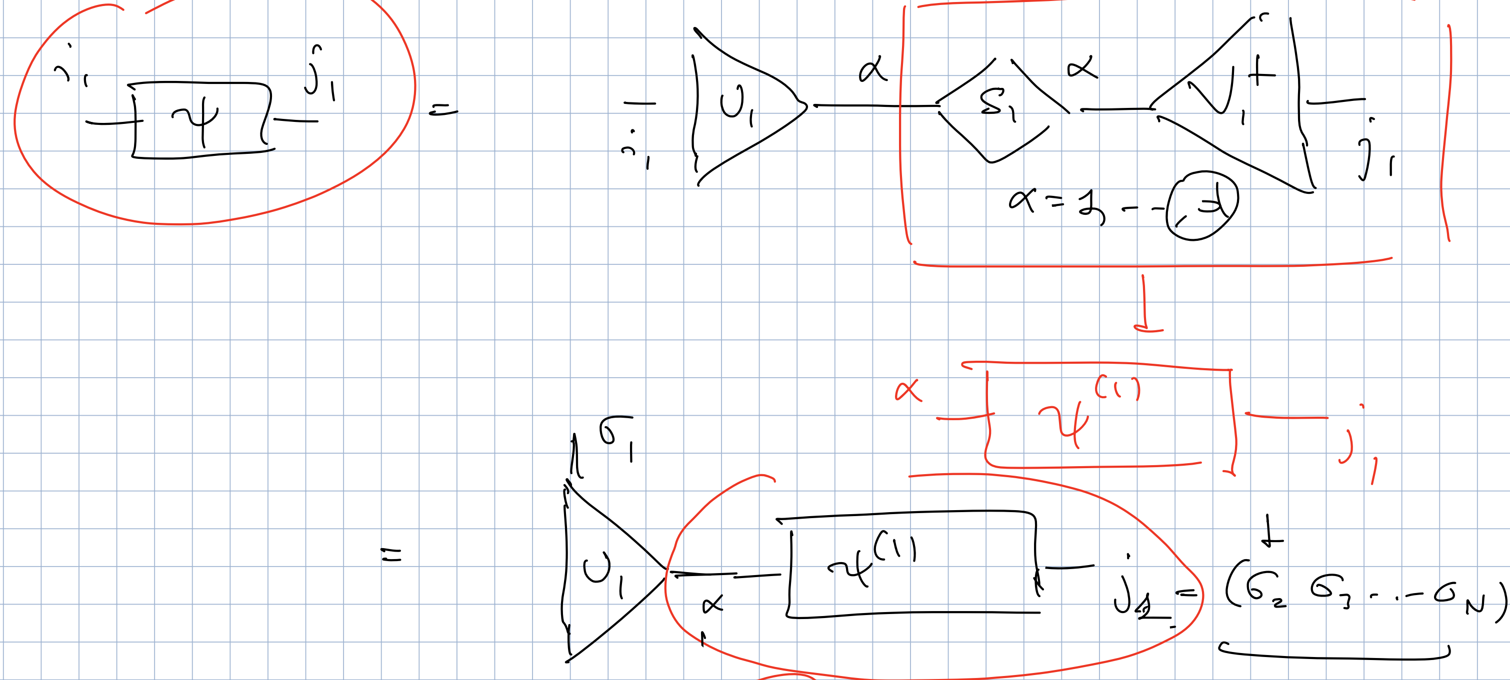
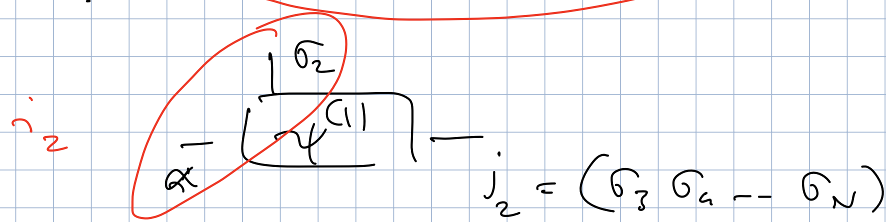


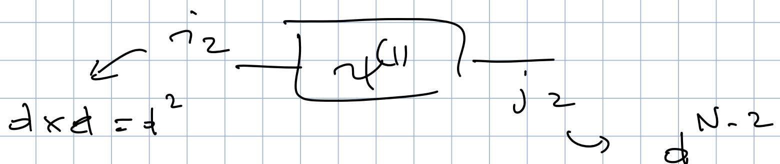
$= \underbrace{\Psi_{i_1 j_1}}_{d \times d^{N-1} \text{ matrix}}$

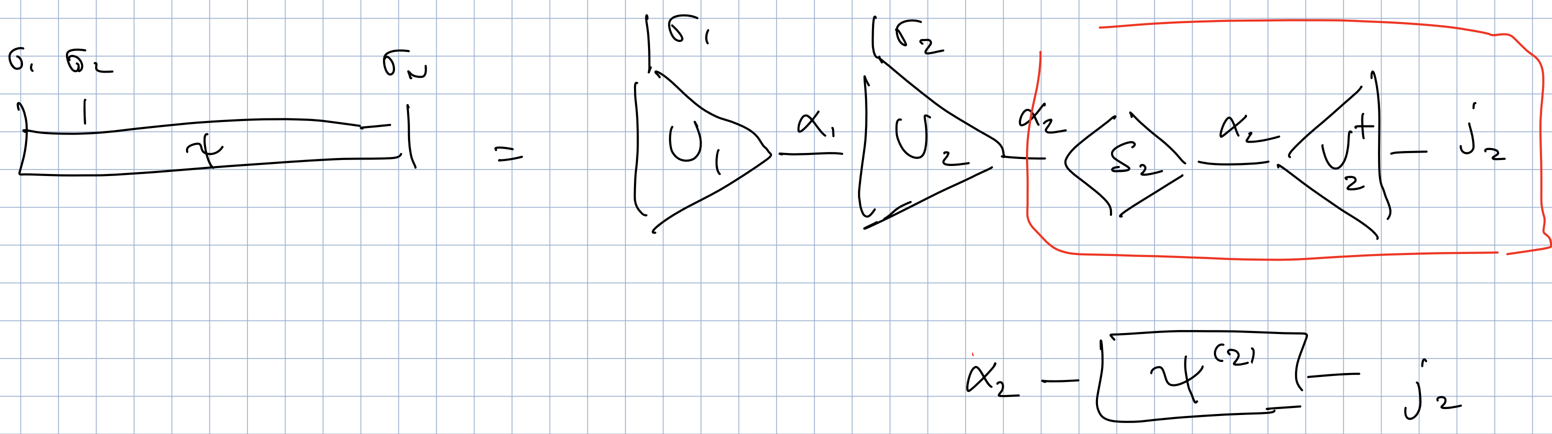
SVD on $\Psi_{i_1 j_1}$



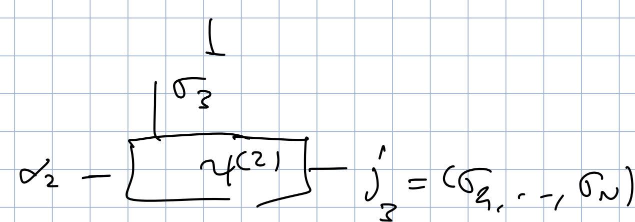
reshaping the matrix





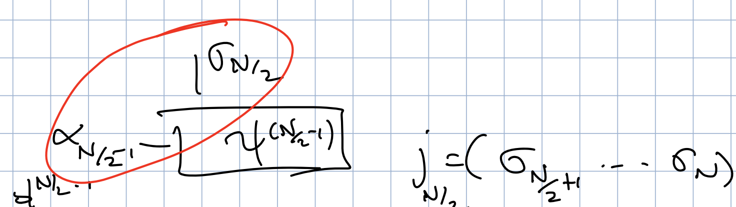


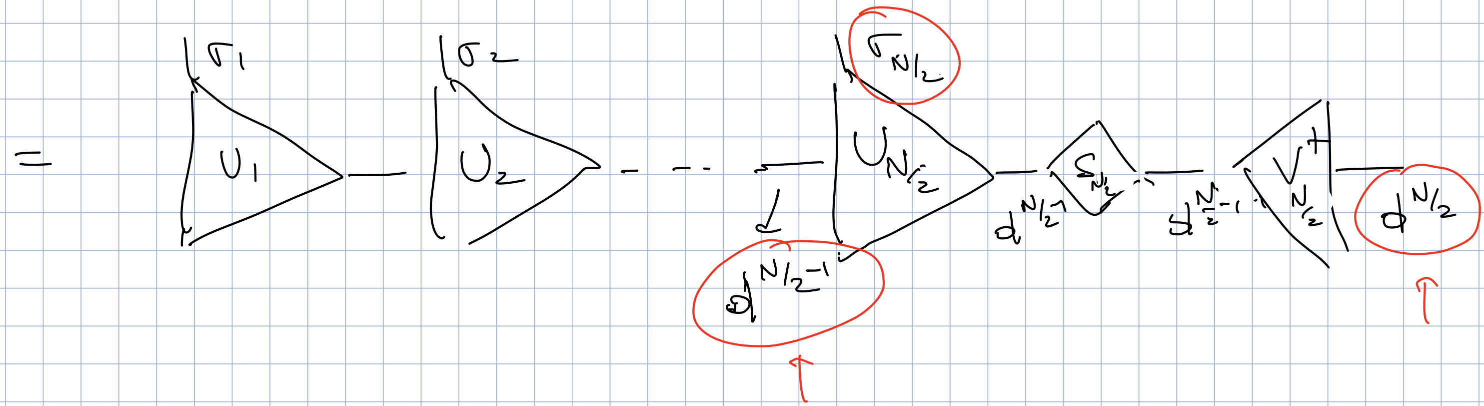
reshaping



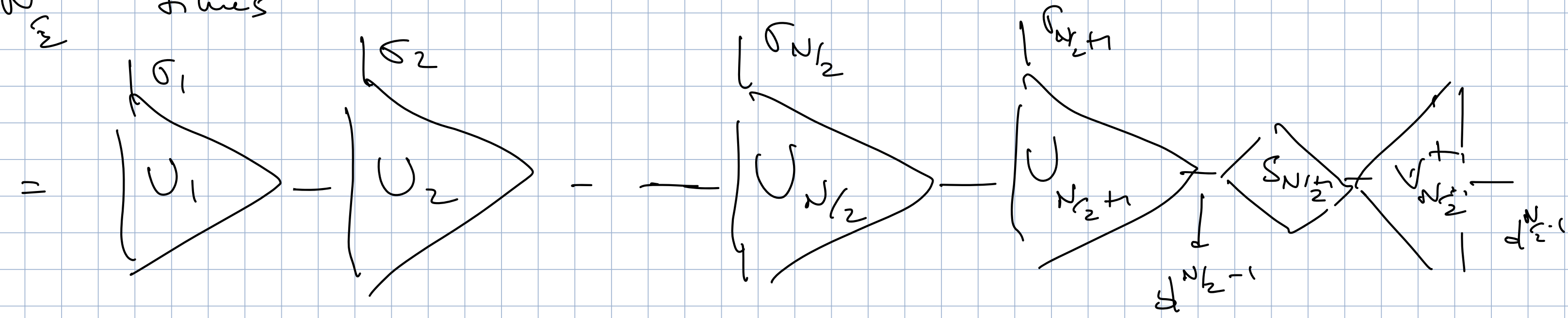
. . .

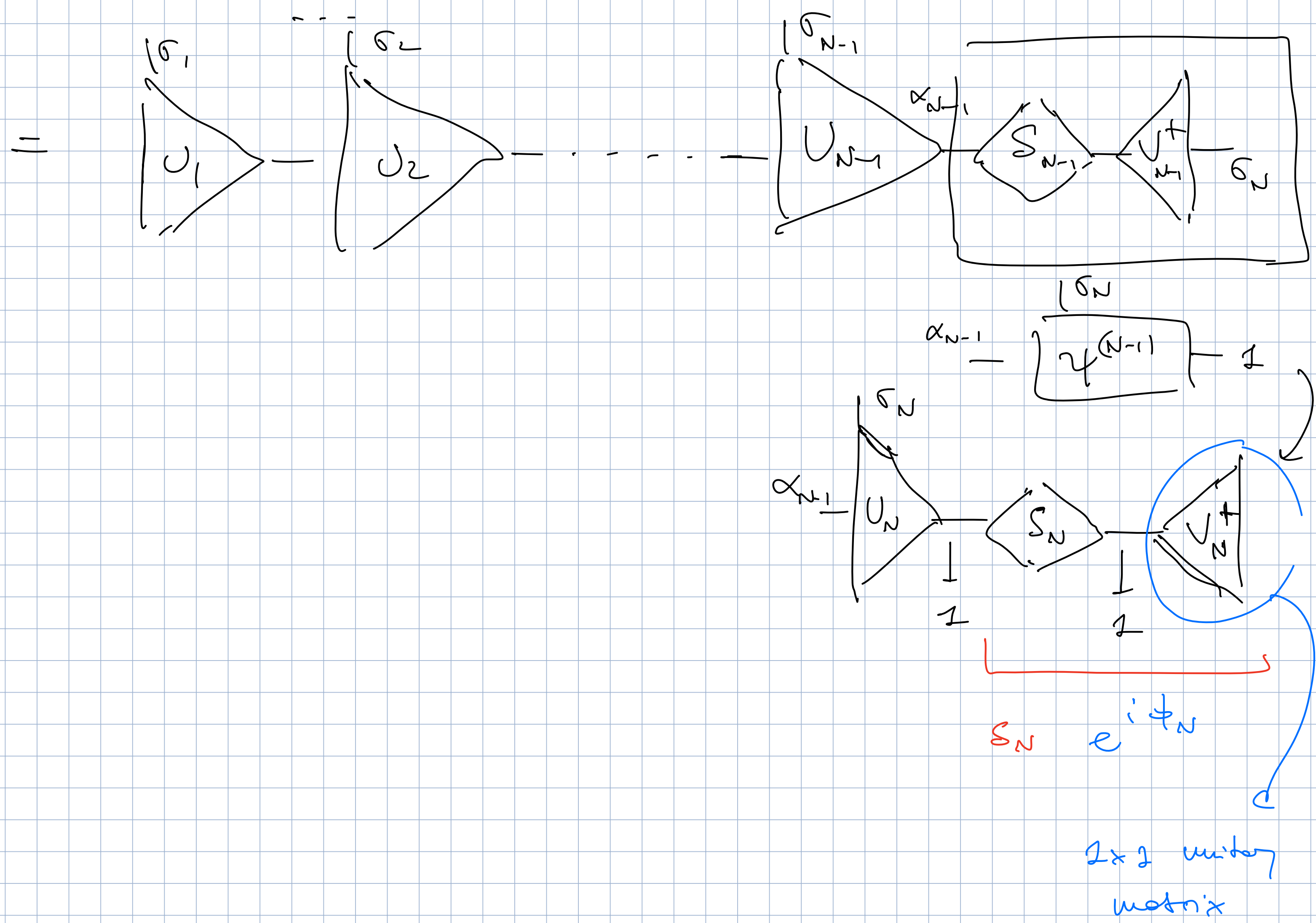
$n = N/2 - 1$ times




=
σ1
σ2
σN/2
U1
U2
UN/2
SN/2
V+N/2
d^(N/2-1)
d^(N/2)

N/2 times


=
σ1
σ2
σN/2
σN/2+1
U1
U2
UN/2
UN/2+1
d^(N/2-1)


=
σ1
σ2
σN-1
αN-1
U1
U2
UN-1
SN-1
V+N-1
σN
ψ(N-1)
1
UN
SN
V+N
sN
e^(iφN)
2x2 unitary matrix

Result: left-canonical matrix-product form