Wave functions!

Hartree Fock.
- → MP2.
- → Coupled cluster
- → FCI, truncated CI.

MCSCF
- → CASP2, NEVPT2, MRLCC.
- → MRCI, MRCI+Q etc.
- → MRCC.

Hartree fock ⟹ single determinant obtained by minimizing the energy w.r.t. orbital rotations occupied/unoccupied.

CAS SCF ⟶ FCI in the active space. obtained by minimizing the energy w.r.t. orbital rotations between core/active/virtual

So we will start by looking at HF and the configuration interaction. Then we will combine the two to see how MCSCF is implemented.

Properties of determinants

$$|D\rangle = |\phi_1 \phi_2 \cdots \phi_n\rangle = \frac{1}{\sqrt{N}} \det[\underline{\Phi}]$$

$$\langle \phi_i | \phi_j \rangle = \delta_{ij} \quad \{\text{orthogonality}\}.$$

lets do an orbital transformation

$$\tilde{\underline{\Phi}} = \underbrace{\Phi X}_{\text{unitary transformation}}$$

$$\tilde{\phi}_i = \sum_j \phi_j X_{ji}$$

$$\det(\tilde{\underline{\Phi}}) = \det[\Phi X]$$

$$= \det[\Phi] \det[X]$$ → complex phase $\boxed{e^{i\theta}}$

or 1 if special orthogonal.

$|D_1\rangle = |\phi_1 \, \phi_2 \cdots \phi_n\rangle$. ϕ and α are completely differ

$|D_2\rangle = |\alpha_1 \, \alpha_2 \cdots \alpha_n\rangle$.

$$\langle D_1 | D_2 \rangle = \det \begin{bmatrix} \langle\alpha_1|\phi_1\rangle & \langle\alpha_1|\phi_2\rangle & \cdots \\ \langle\alpha_2|\phi_1\rangle & \vdots & \vdots \\ \vdots & \cdots & \langle\alpha_n|\phi_n\rangle \end{bmatrix}$$

<u>Energy optimization</u>

$|HF\rangle = e^{-\hat{\kappa}} |D\rangle$

→ some determinant with suboptimal orbitals.

$$E(\kappa) = \langle D | e^{-\hat{\kappa}^{+}} H e^{-\hat{\kappa}} | D \rangle.$$

$$= \langle D | \underline{e^{\hat{\kappa}} H e^{-\hat{\kappa}}} | D \rangle.$$

B.C.H. expansion.

core $i j k \ldots$

virt $a b c \ldots$

general, active $p q r \ldots$

$$E(\kappa) = \langle D | H + [\hat{\kappa}, H] + \frac{1}{2}[\hat{\kappa},[\hat{\kappa},H]] + \ldots | D \rangle.$$

$$\hat{\kappa} = \sum_{p>q} \kappa_{pq} (E_{pq} - E_{qp}) = \sum_{p>q} \kappa_{pq} E^{-}_{pq}.$$

$$\frac{\partial E}{\partial \kappa_{ij}} = \langle D|[E^-_{pq}, H]|D\rangle = 0$$

$$\langle D| E^-_{pq} H - H E^-_{pq} |D\rangle = 0 \qquad E_{ij}$$

i

j

if $p,q = ij$ {occupied}.

if $p,q = ab$ {unoccupied}.

$$\langle D| E^-_{pq} H - H E^-_{pq} |D\rangle = 0$$

At minimum.

$$\langle D|[E^-_{ai}, H]|D\rangle = 0$$

HF

$$\hookrightarrow \quad 2\langle D|[E_{ai}, H]|D\rangle = 0$$

$$2\langle D| E_{ai} H - H E_{ai}|D\rangle = -2\langle D|H E_{ai}|D\rangle = 0$$

$\therefore$ $\boxed{\langle D|H|D_i^a\rangle = 0}$ Brillion condition.

$$\langle D|[E^-_{pq}, H]|D\rangle = 0$$

$\Rightarrow$ $\boxed{\langle D|[E_{pq}, H]|D\rangle = 0}$ generalized Brillion Condition.

Hessian: $E^{2}_{pq,rs} = \frac{1}{2}\Big[\ \langle D|[E^-_{pq}, [E^-_{rs}, H]]|0\rangle$

$$\frac{1}{2} + \langle \Psi | [E_{rs}, [E_{pq}, H]] | \Psi \rangle \Big]$$

<u>Canonical Hartree Fock</u> :- [ROHF cannot be expressed as canonical HF].

$$E[\psi] = \sum_i \langle \phi_i | h | \phi_i \rangle + \frac{1}{2} \sum_{ij} \langle \phi_i \phi_j | \phi_i \phi_j \rangle - \langle \phi_i \phi_j | \phi_j \phi_i \rangle$$

$$\delta E = \sum_i \langle \delta\phi_i | h | \phi_i \rangle + \frac{1}{2} \sum_{ij} \langle \delta\phi_i \phi_j | \phi_i \phi_j \rangle - \langle \delta\phi_i \phi_j | \phi_j \phi_i \rangle$$

$$+ \text{c.c.}$$

$$= \sum_i \langle \delta \phi_i | F | \phi_i \rangle + \text{c.c.}$$

$$\underline{\underline{\hat{F}}} = \hat{h} + \hat{J} - \hat{K}$$ {fock operator}.

$$J = \sum_i \hat{J}_i$$

$$\hat{J}_i f(1) = \int \frac{\phi_i^*(2)\, \phi_i(2)}{r_{12}} \cdot f(1) \cdot dr_2 .$$

very strange. $\Longrightarrow$ $$\hat{K}_i f(1) = \int \frac{\phi_i^*(2) \cdot f(2)}{r_{12}} \phi_i(r_1) \, dr_2 .$$

$$F = \begin{array}{c|cc} & N & R-N \\ \hline N & \begin{bmatrix} ▨ & 0 \\ 0 & ▨ \end{bmatrix} & \\ R-N & & \end{array} \quad R \times R.$$

$f_{ia} = 0$ { optimization condition.

$\hat{F}\phi_i = \sum_k \lambda_{ki}\phi_k.$

eigenvectors { energy invariant to occ-occ transformations }.

$\tilde{\phi}_j = \sum \phi_i V_{ij}$

$\tilde{F}\tilde{\phi}_i = \varepsilon_i \tilde{\phi}_i$ ← ε_i are orbital energies

Show that $\varepsilon_i = \langle i|h|i\rangle + \sum_{j=1}^{N} \langle ij|ij\rangle - \langle ij|ji\rangle.$

$\varepsilon_a = \langle a|a\rangle + \sum$ " replace i with a.

$E \neq \sum_i \varepsilon_i - \frac{1}{2}\sum_i \langle \phi_i | J - K | \phi_i \rangle$

Koopman's Theorem :-

$IP_i = \langle HF | a_i^{+} H a_i | HF \rangle - E_{HF}.$

$= -f_{ii}$

Show this.

$EA = -\langle H | a_a H a_a^{+} | HF \rangle + E_{HF}$

$= -f_{aa}.$

Configuration Interaction :-

$$H|\Psi\rangle = E|\Psi\rangle .$$

$$H_{ij} = \langle D_i | H | D_j \rangle \qquad |\Psi\rangle = \sum_i C_i |D_i\rangle$$

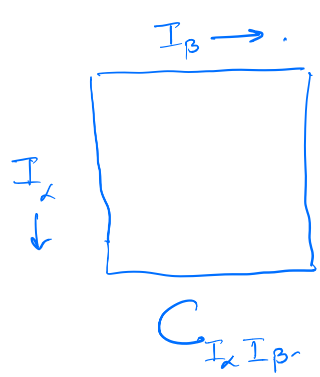
$\langle D_i | H | D_j \rangle \Longrightarrow$ slater condon rules

$$\hookrightarrow H = \sum_{pq} \langle p|h|q\rangle E_{pq} + \frac{1}{2}\sum_{\substack{pq\\rs}} \langle pr|qs\rangle \left(E_{pq}E_{rs} - \delta_{rq}E_{ps}\right)$$

$$= \sum_{pq} \underbrace{K_{pq}}_{h_{pq} + \sum_r \langle pr|rq\rangle} E_{pq} + \frac{1}{2}\sum_{\substack{pq\\rs}} g_{pqrs}\, E_{pq}E_{rs}$$

$$\Longrightarrow \text{Number of determinants} = \underbrace{\binom{K}{N_\alpha}}_{\{I_\alpha\}} \underbrace{\binom{K}{N_\beta}}_{\{I_\beta\}}$$

$$|\Psi\rangle = \sum_{I_\alpha I_\beta} C_{I_\alpha I_\beta} |I_\alpha\rangle |I_\beta\rangle$$



$$H = \sum_{pq} K_{pq} E_{pq} + \sum_{pqrs} g_{pqrs} E_{pq} E_{rs}$$

$$\sigma_{I_\alpha I_\beta} = \frac{1}{2} \sum_{\substack{pqrs \\ K_\alpha K_\beta \\ J_\alpha J_\beta}} g_{pqrs} \langle I_\alpha I_\beta | E_{pq} | K_\beta K_\alpha \rangle \langle K_\alpha K_\beta | E_{rs} | J_\alpha J_\beta \rangle C_{J_\alpha J_\beta}$$

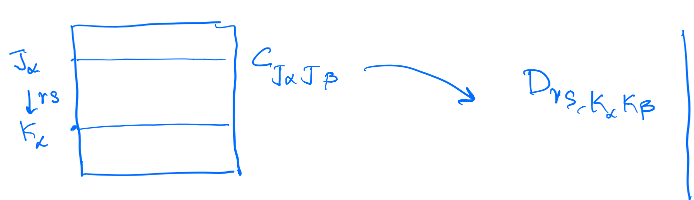
$$D_{rs, K_\alpha K_\beta} = \sum_{J_\alpha J_\beta} \langle K_\alpha K_\beta | E_{rs} | J_\alpha J_\beta \rangle C_{J_\alpha J_\beta}$$

$$G_{pq, K_\alpha K_\beta} = \frac{1}{2} \sum_{rs} g_{pqrs} D_{rs, K_\alpha K_\beta}$$

$$\sigma_{I_\alpha I_\beta} = \sum_{\substack{pq, \\ K_\alpha K_\beta}} \langle I_\alpha I_\beta | E_{pq} | K_\alpha K_\beta \rangle G_{pq, K_\alpha K_\beta}$$

$$D_{rs, K_\alpha K_\beta} = \sum_{J_\alpha} \langle K_\alpha | E^\alpha_{rs} | J_\alpha \rangle C_{J_\alpha J_\beta} + \sum_{J_\beta} \langle K_\beta | \underline{\underline{E^\beta_{rs}}} | J_\beta \rangle C_{J_\alpha J_\beta}$$

E^β_{rs}



$$|\psi\rangle = e^{-\hat{\kappa}} \sum_i c_i |D_i\rangle \qquad \text{[MCSCF parametrization]}$$

$$E(\hat{\kappa}, c) = \frac{\langle \psi(c)| e^{\hat{\kappa}} H e^{-\kappa} |\psi(c)\rangle}{\langle \psi(c)| e^{\kappa} e^{-\kappa} |\psi(c)\rangle} = \frac{\langle \psi(c)| e^{\kappa} H e^{-\kappa} |\psi(c)\rangle}{\langle \psi(c)|\psi(c)\rangle}$$

$$\frac{\partial E}{\partial c_i} = \sum_j 2 H_{ij} c_j - 2 E c_i$$

$$\frac{\partial E}{\partial \kappa_{pq}} = \langle 0| [E^-_{pq}, H] |0\rangle.$$

$$\frac{\partial E}{\partial \kappa_{pq} \partial \kappa_{rs}} = \frac{1}{2}\left[\langle [E^-_{pq}, [E^-_{rs}, H]] \rangle + \langle [E^-_{rs}, [E^-_{pq}, H]] \rangle \right]$$

↳ You just need the 2-RDM.

Density matrix renormalization group in the age of Matrix Product States [Ulrich Schollwöck]

<u>SVD</u>:

$$M_{n\times m} = U_{n\times n} S_{n\times n} V^{\dagger}_{n\times m}.$$

$\boxed{n<m}$

$$U = \begin{bmatrix} | & | & | & | \end{bmatrix}$$

$\boxed{U^{\dagger} U = \mathbb{I} \text{ and } U U^{\dagger} = \mathbb{I}}$

↳ orthogonal matrix

$$S = \begin{bmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_n \end{bmatrix}$$

↳ singular matrix

non-zero eigenvalues = rank (r).

$$V^{\dagger} \Rightarrow \begin{bmatrix} \text{———} \\ \text{———} \\ \text{———} \end{bmatrix}$$

$\boxed{V^{\dagger} V = \mathbb{I}}$

↳ orthogonal rows.

if you want to approximate M (rank r) by a matrix M' ($r' < r$) then it is given by.

$$M' = U\, S'\, V^{+} \qquad S^{+} = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 \cdot \sigma_{r'} & & \\ & & 0 & \\ & & & 0 \end{bmatrix}$$

$\downarrow$

$$U' = \underset{n \times r}{\begin{bmatrix} | & | & | \end{bmatrix}} \underset{r \times r}{\begin{bmatrix} & \\ & \end{bmatrix}} \underset{r \times m}{\begin{bmatrix} — \\ — \\ — \end{bmatrix}}$$

only $U'^{+} U' = I$ and $\boxed{U U^{+} \neq I}$

---

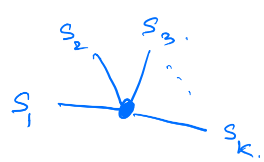
take an arbitrary state in the fock space.

$$|\psi\rangle = \sum C_{s_1 s_2 \ldots s_k} |s_1 s_2 \ldots s_k\rangle$$

$s_1 = 0, 1$ in this case we often use spin orbitals.

$s_1 = 0, \alpha, \beta, \uparrow\downarrow$.

but we can use general ~~symbol~~ "d" ~~for~~ # states in an orbital.



C.

k-dimensional tensor.

$\xRightarrow{\text{view}}$ s_1 —•— $d^{(k-1)}$

$\Big\Downarrow$ SVD.

$$C = \sum_{a_1} U_{s_1, a_1} S_{a_1, a_1} (V^{+})_{a_1, s_2 \ldots s_k}.$$

$$= \sum_{a_1} U_{s_1, a_1} C_{(a_1 s_2), \ldots s_k}$$

$$C = \sum_{\substack{a_1 \\ a_2}} U_{s_1 a_1} U_{(a_1 \sigma_2) a_2} C_{a_2 s_3 \cdots s_L}$$

$$= \sum_{a_1 \cdots a_n} U^{s_1}_{a_1} U^{s_2}_{a_1 a_2} U^{s_3}_{a_2 a_3} \cdots U^{s_k}_{a_{k-1}}$$

$$= A^{s_1} A^{s_2} \cdots A^{s_k}$$ {matrix product States}

$$\sum_{a_{l-1} s_L} U_{(a_{l-1} s_L), a_l} U_{(a_{l-1} s_L), a_{l'}} = S_{a_l, a_{l'}}$$

$$= \sum_{s_L a_{l-1}} A^{s_L +}_{a_l, a_{l-1}} A^{s_l}_{a_{l-1}, a_{l'}} = \boxed{\sum_{s_l} A^{s_l +} A^{s_l} = \mathbb{I}}$$

Left Canonical form

$$C_{s_1 s_2 \cdots s_k} = \sum_{a_{k-1}} \underbrace{U_{s_1 s_2 \cdots a_{k-1}} S_{a_{k-1} a_{k-1}}}_{} (V^+)_{a_{k-1}, s_k}$$

$$= \sum_{a_{k-1}} C_{s_1 s_2 \cdots (s_{k-1} a_{k-1})} B^{s_k}_{a_{k-1}} = \sum_{\substack{a_{k-2} \\ a_{k-1}}} C_{s_1 s_2 \cdots a_{k-2}} B^{s_k}_{a_{k-2} a_{k-1}}$$

$$= \sum_{a_{k-1}} C_{s_1 \cdots s_{k-2} s_{k-1} a_{k-1}} B^{s_k}_{a_{k-1}}$$

$$= \sum_{\substack{a_{k-2} \\ a_{k-1}}} C_{s_1 \cdots s_{k-2} a_{k-2}} \boxed{B^{s_{k-1}}_{a_{k-2} a_{k-1}}} B^{s_k}_{a_{k-1}}.$$

$$\sum_{a_{\ell-1}, s_\ell} B^{s_\ell}_{a_{\ell-1} a_\ell} B^{s_\ell}_{a'_{\ell-1} a_\ell} = \sum_{s_\ell} B^{s_\ell} B^{s_\ell +} = \mathbb{I}.$$

<u>Right canonical form.</u>

<u>Mixed Canonical form:</u>

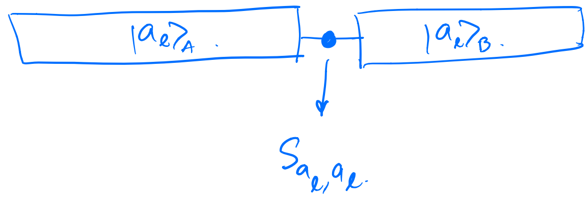
$$C_{s_1 s_2 \cdots s_\ell} = \sum \left(A^{s_1} \cdots A^{s_\ell}\right)_{a_\ell} S_{a_\ell, a_\ell} (V^+)_{a_\ell, s_{\ell+1} \cdots s_k}.$$

$$= \sum_{a_\ell} \left(A^{s_1} \cdots A^{s_\ell}\right)_{a_\ell} S_{a_\ell, a_\ell} \left(B^{s_{\ell+1}} \cdots B^{s_{k-1}} B^{s_k}\right)_{a_\ell}$$

$$= \sum_{a_\ell} \left(A^{s_1} \cdots A^{s_\ell}\right)_{a_\ell} S_{a_\ell, a_\ell} \left(B^{s_{\ell+1}} \cdots B^{s_k}\right)_{\underline{\underline{a_\ell}}}.$$

$$= \sum |a_\ell\rangle_A \, S_{a_\ell a_\ell} \, |a_\ell\rangle_B.$$

a_ℓ.



$$|a_\ell\rangle_A = \sum_{s_1 \cdots s_\ell} \left(A^{s_1} \cdots A^{s_\ell}\right)_{1, a_\ell} |s_1 \cdots s_\ell\rangle$$

$$|a_\ell\rangle_B = \sum_{s_{\ell+1} \cdots s_K} \left(B^{s_{\ell+1}} \cdots B^{s_K}\right)_{a_\ell, 1} |s_{\ell+1} \cdots s_K\rangle$$

$$\langle a_\ell' | a_\ell\rangle_A = \sum_{s_1 \cdots s_\ell} \left(A^{s_\ell \dagger} \cdots A^{s_1 \dagger}\right)\left(A^{s_1} \cdots A^{s_\ell}\right).$$

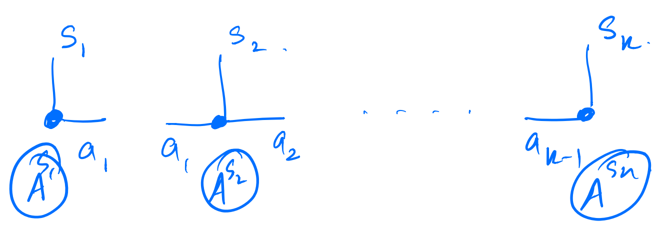
$$= \delta_{a_\ell', a_\ell}$$

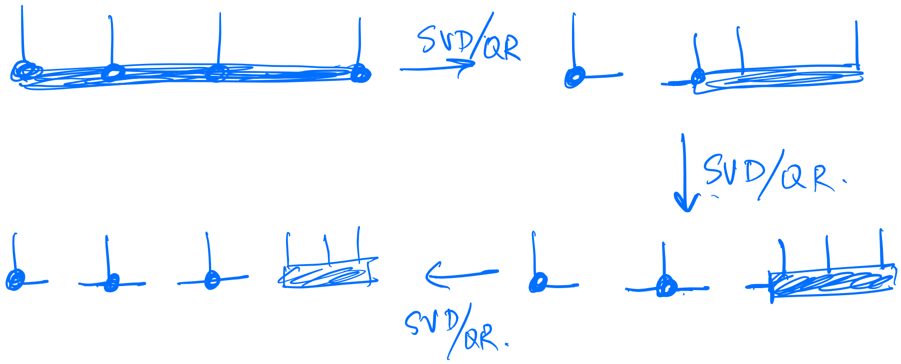
$$\langle a_\ell' | a_\ell\rangle_B = \delta_{a_\ell', a_\ell}. \;\|$$

<u>lets</u> look at the graphical notation

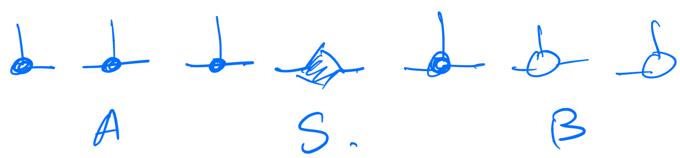
$$|\psi\rangle = \sum_{s_1 \cdots s_K} A^{s_1} A^{s_2} \cdots A^{s_K} |s_1 \cdots s_K\rangle.$$

$$A^{s_1}_{a_1} \quad A^{s_2}_{a_1 a_2} \cdots \quad A^{s_K}_{a_{K-1}}$$





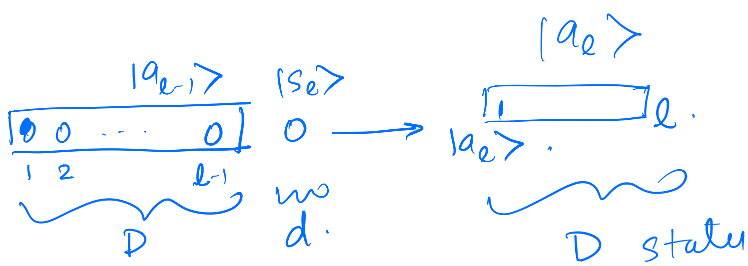
Mixed Canonical!



So far we have not performed any truncation, but we can do that now; the matrix

$A^{s_\ell}_{a_{\ell-1} a_\ell}$ — the bond dimension of $a_\ell \leq \boxed{M}$ — the size of the row/columns of all matrices

the truncation of the bond-dimension to M is related to the concept of decimation



$$|a_\ell\rangle = \sum_{a_{\ell-1} s_\ell} \langle a_{\ell-1} s_\ell | a_\ell \rangle \; |a_{\ell-1}\rangle |s_\ell\rangle$$

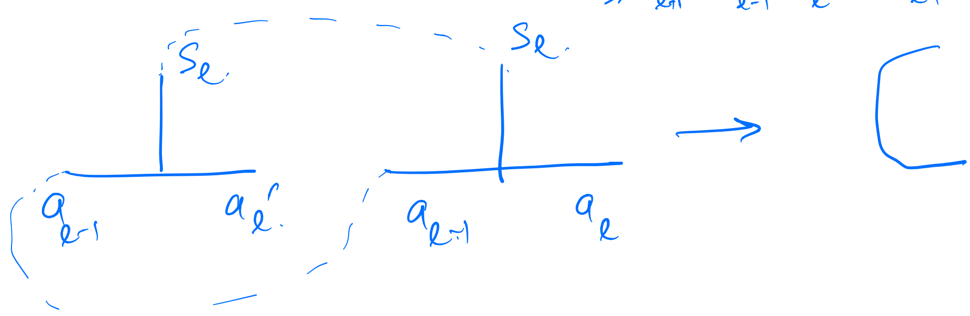
$$= \sum_{a_{\ell-1} s_\ell} A^{s_\ell}_{a_{\ell-1} a_\ell} \; \underline{|a_{\ell-1}\rangle} \, |s_\ell\rangle$$

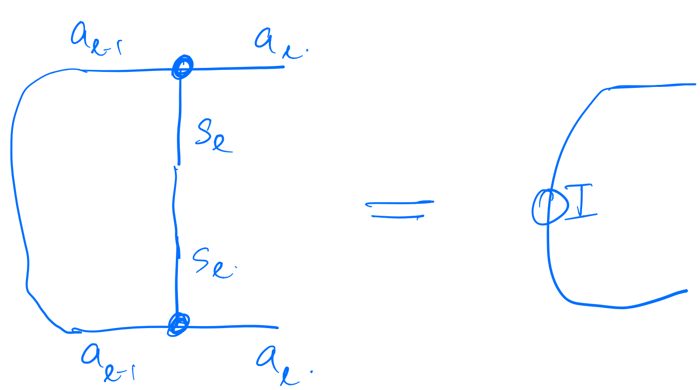
$$= \sum_{\substack{a_{\ell-2} \\ s_{\ell-1} s_\ell}} A^{s_{\ell-1}}_{a_{\ell-2} a_{\ell-1}} A^{s_\ell}_{a_{\ell-1} a_\ell} \; |a_{\ell-2}\rangle |s_{\ell-1}\rangle |s_\ell\rangle$$

$$= \sum \underbrace{A^{s_1} A^{s_2} \cdots A^{s_\ell}}_{\text{decimation matrices}} |s_1\rangle |s_2\rangle \cdots |s_\ell\rangle$$

<u>matrix contraction:</u>

$$\sum_{s_\ell} A^{s_\ell^\dagger} A^{s_\ell} = I \qquad \sum_{s_\ell a_{\ell-1}} A^{s_\ell}_{a_{\ell-1} a'_\ell} A^{s_\ell}_{a_{\ell-1} a_\ell}$$





Entanglement Entropy :-

A B.

$$|\psi\rangle = \sum_{\alpha} S_\alpha \, |\alpha\rangle_A |\alpha\rangle_B .$$

$$\boxed{\langle\psi|\psi\rangle = 1 = \sum_\alpha S_\alpha^2 .}$$

Decimation $\Longrightarrow$ discard the smallest singular values.

$$\rho_A = \mathrm{Tr}_B \left[|\psi\rangle\langle\psi| \right] = \underline{\sum S_\alpha^2 \, |\alpha\rangle_A \langle\alpha|_A} .$$

Shannon - Entropy

$$S(\rho_A) = -\mathrm{Tr}\left[\rho_A \ln \rho_A\right] = -\sum_\alpha S_\alpha^2 \ln(S_\alpha^2)$$

a) $\frac{1}{2}\left[|\uparrow\downarrow\rangle + |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\downarrow\uparrow\rangle\right]$

$= (|\uparrow\rangle + |\downarrow\rangle) \otimes (|\uparrow\rangle + |\downarrow\rangle)$ product states

b) $\frac{1}{\sqrt{2}}\left[|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right]$

singular value $(0, 1)$

$$|\psi\rangle = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \Longrightarrow S = -0 \ln 0 - 1 \ln 1 = 0 .$$

$$|\psi\rangle = \begin{array}{cc} & \begin{array}{cc} \uparrow & \downarrow \end{array} \\ \begin{array}{c} \uparrow \\ \downarrow \end{array} & \begin{bmatrix} 1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} \end{bmatrix} \end{array} \Longrightarrow S = 0.7 .$$

Entanglement Entropy :- how entangled states are.

$$|\psi\rangle = |\psi_A\rangle |\psi_B\rangle .$$

$$\boxed{S = 0}$$

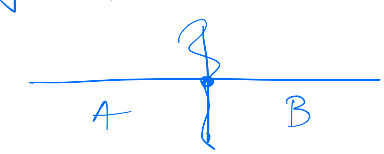
make a measurement on A $\rightarrow$ does not interfere with measurement on B.

$S \neq 0$

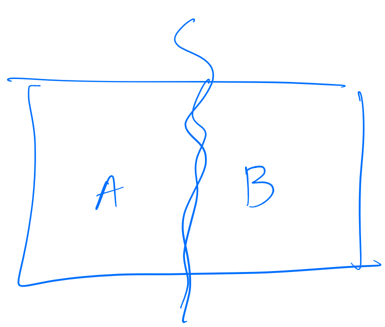
low entanglement $|\psi\rangle = \sum_i |\psi_A^i\rangle_B \, |\psi_i\rangle_B$

for 1-D systems S_a^2 decay exponentially fast.

$$e^{-c \ln^2 a}$$



for 2-D system



$$e^{-\ln^2 a / W}$$

Area law Entanglement

max Entropy of MPS $\boxed{\ln_2 D}$

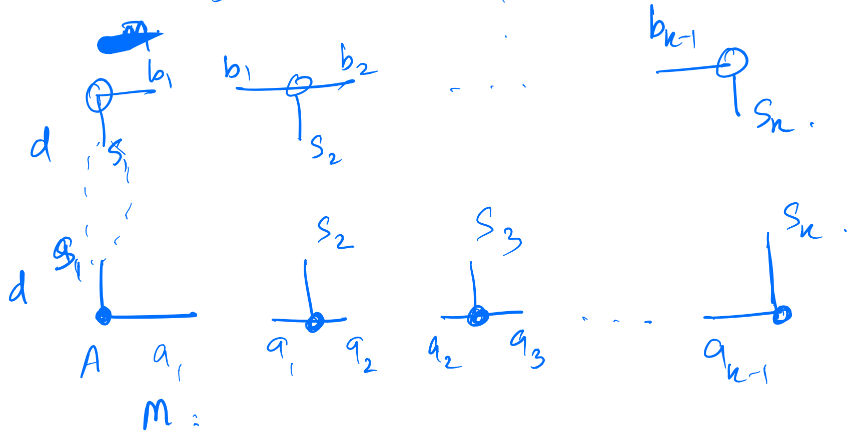
$$\Longrightarrow \quad \boxed{\begin{array}{l} S = \text{constant} \\ S \propto W \end{array}}$$

$\langle \psi_2 | \psi_1 \rangle$ Overlap of two MPS :-

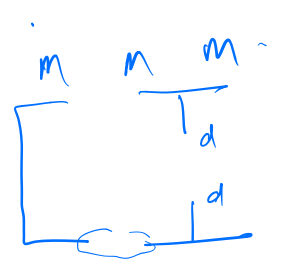
$$\left[\sum_{\substack{\{b_i\} \\ \{s_i'\}}} B_{b_1}^{s_1' *} B_{b_1 b_2}^{s_2' *} \cdots B_{b_{n-1}}^{s_n' *} \langle s_1' \cdots s_n' | \right] \left[\sum_{\substack{\{a_i\} \\ \{s_i\}}} A_{a_1}^{s_1} A_{a_1 a_2}^{s_2} \cdots A_{a_{n-1}}^{s_n} | s_1 \cdots s_n \rangle \right]$$

$$\sum_{\substack{\{b_i\} \\ \{a_i\} \\ \{s_i\}}} \left(B_{b_1}^{s_1} B_{b_1 b_2}^{s_2} \cdots B_{b_{n-1}}^{s_n} \right) \left(A_{a_1}^{s_1} A_{a_1 a_2}^{s_2} \cdots A_{a_{n-1}}^{s_n} \right)$$

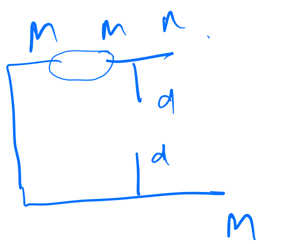
$$= \sum_{\substack{\{a_i\} \\ \{b_i\}}} (AB[s_1])_{b_1 a_1} (AB[s_2])_{b_1 a_1 b_2 a_2} \cdots (BA[s_n])_{b_{n-1} a_{n-1}}$$



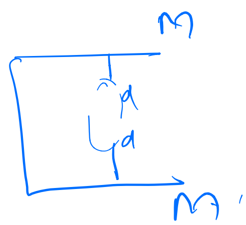
dD^2



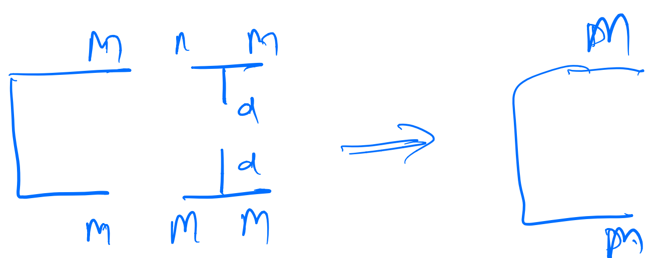
dD^3



$d^2 D^3$.



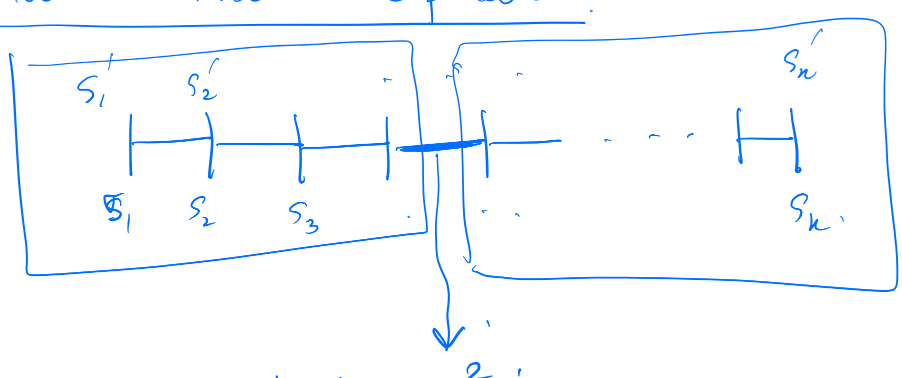
$d D^2$.



$$\left[d m^3 + d^2 m^3 + d m^2\right] = O(d^2 m^3)$$

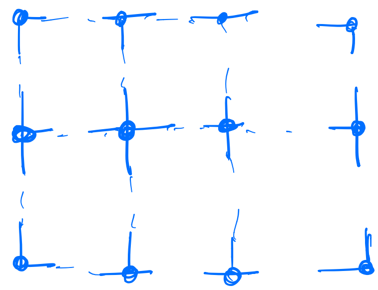
$$O\left[K d^2 m^3\right]$$

Matrix Product Operators -

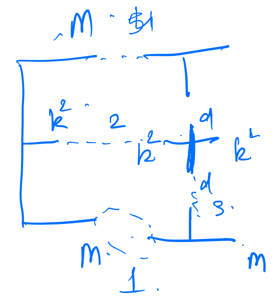


bond .. k^2.

dimension

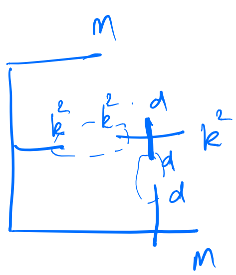
$E =$ 

after some sweeps

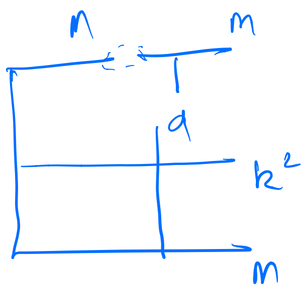


$$d k^2 m^3 + m^2 k^4 d^2 + m^2 d^2 k^2$$

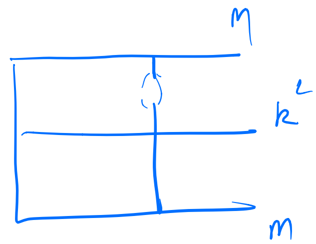
$$m^3 d^2 k^2$$



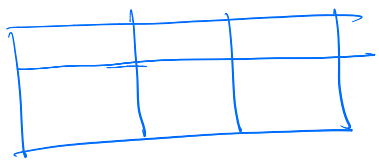
$$k^4 d^2 m^2$$



$$m^3 d^2 k^2$$

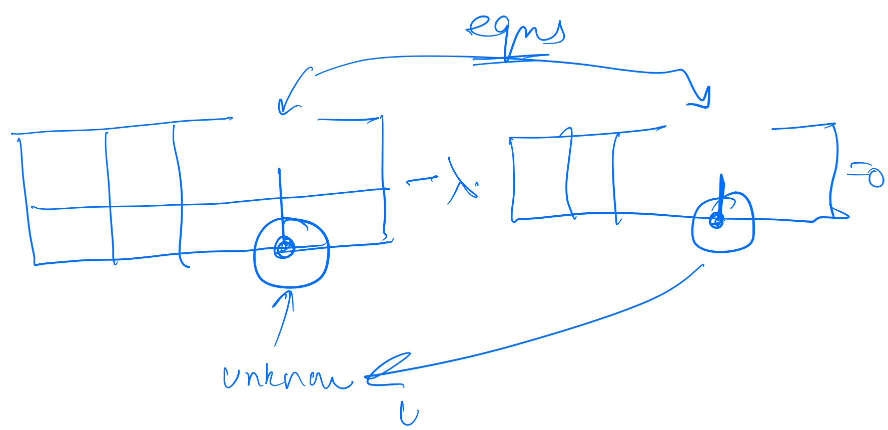


$m^2 k^2 d$



$$L = \langle\psi|H|\psi\rangle - \lambda\left[\langle\psi|\psi\rangle - 1\right]$$

$$\frac{\partial L}{\partial M^s}.$$



Briefly talk about the 2-site algorithm.

$\boxed{\text{Fill in the blanks}}$