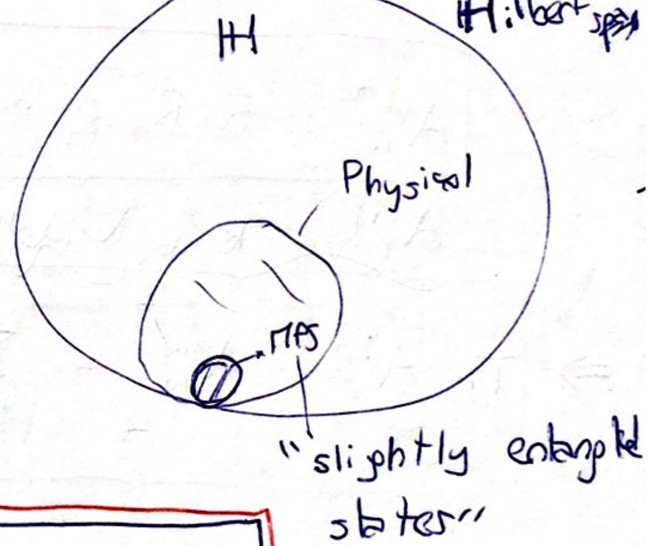
Lecture II : The physical corner of Hilbert space (I)

Matrix product states and tensor networks

Refs: - G. Vidal PRL (03)
- F. Verstraete, J.I. Cirac & V. Murg (0907.2796)
- R. Orus 1306.2164
- S.R. White, PRL 69, 2863-2866 (1992)

Matrix-product states (MPSs)



$\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2 \cdots \otimes \mathbb{H}_N$

$\mathrm{Dim}(\mathbb{H}_i) = d \qquad \forall i \in [N]$

$\Rightarrow \mathrm{Dim}(\mathbb{H}) = D = d^N$

$\Rightarrow$ Generic N-qudit state is $\boxed{|\psi\rangle = \sum_{i_1 \ldots i_N = 0}^{d-1} c_{\bar{i}} \, |\bar{i}\rangle}$ $\quad (\bar{i} = i_1 \ldots i_N)$

The state is univocally represented by the

N-index complex tensor $c_{\bar{i}}$ $\quad c_{i_1 i_2 \ldots i_N}$ (i_1, i_2, ..., i_N)

$\boxed{\#\ \text{Parameters} : \mathcal{O}(d^N) \text{ complex parameters}}$ $\quad (d^{2N} - 1$ real parameters$)$

very complex object!

Sub-class of physical states :

"MPS Ansatz"

MPS ⇒ Def:

$$\boxed{C_{\bar{i}} = \mathrm{Tr}\left[A_1^{(i_1)} A_2^{(i_2)} \dots A_N^{(i_N)}\right]}$$

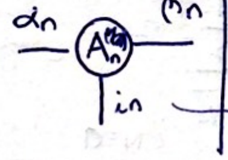
Breaking the wavefunction into small pieces:

$A_n^{(i_n)}$: R×R square matrix with elements $A^{(i_n)}_{n(\alpha_n,\beta_n)}$

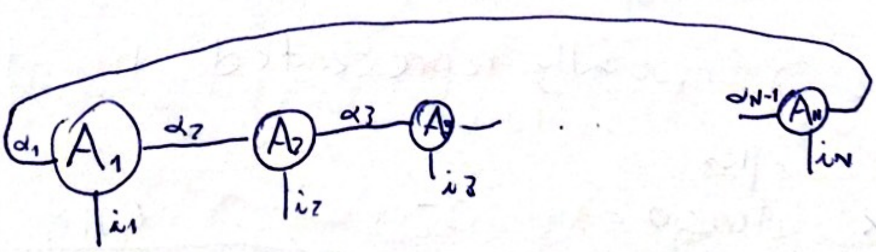
R = bond dimension

$$\Rightarrow \mathrm{Tr}\left[A_1^{(i_1)} \dots A_N^{(i_N)}\right] = \sum_{\alpha_1 \dots \alpha_{N-1}} A^{(i_1)}_{1(\alpha_1,\alpha_2)} A^{(i_2)}_{2(\alpha_2,\alpha_3)} \dots A^{(i_N)}_{N(\alpha_{N-1},\alpha_1)}$$

→ virtual or bond indices

$A^{(i_n)}_{n(\alpha_n,\beta_n)} \leftrightarrow$ 

→ physical index

⇒ MPS : 

(with closed or periodic boundary conditions)

(open boundary conditions are also possible

$$c_{\bar{i}} = \underbrace{A_L A_1^{(i_1)}}_{A'^{(i_1)}_1} \dots \underbrace{A_N^{(i_N)} A_R}_{A'^{(i_N)}_N}$$

A_L → row vector, A_R → column vector)

Property (i): efficient classical despription:

~~N (R×R)~~ N × d R×R matrices:

⇒ Total number of complex parameters: $O(NdR^2)$

exponentiially less than general states

↓

(Efficiently classically simulatable DMRG)

present later, together with VII

(iii) - Every (injective) MPS is the unique ground state of a local, gapped frustration-free Hamiltonian (in 1D)

$\Rightarrow H = \sum_{n=1}^{N} H_n \Rightarrow H|\psi_{MPS}\rangle = 0$

- H_n acts non trivially on at most K (constant) sites
- short-ranged if K sites are contiguous
- gapped if $E_1 - E_0 = \Delta > 0 \ \forall N$
- frustration free if $\forall n \in [N], \ H_n|\psi_{MPS}\rangle = 0$

(ii) MPS are dense:

Any arbitrary state is an MPS if $R = O(d^N)$

- but ground state of 1D local gapped H can be approximated efficiently by constant-R MPS

White 92

- For critical 1D systems: $R = O\,\mathrm{Poly}(N)$

iv) Entanglement area law

- MPS satisfy 1D area law:

$$\boxed{S(\rho_{MPS_L}) = -\mathrm{Tr}\left[\rho_{MPS_L} \log(\rho_{MPS_L})\right] = O\left[\log(R)\right]}$$

(reduced over L sites)

constant in L!

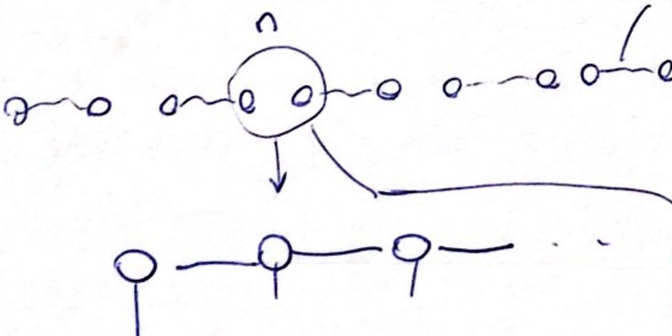
(In contrast, classical systems and most quantum ones display a volume-law)

No long-range entanglement!

More generally, in higher dimensions:

PEPSs: . MPS are particular cases (1D) of PEPS:

virtual bon $|\Phi_R\rangle = \frac{1}{\sqrt{R}} \sum_{k=0}^{R-1} |k\,k\rangle$ virtual qudits of d=R



local linear map

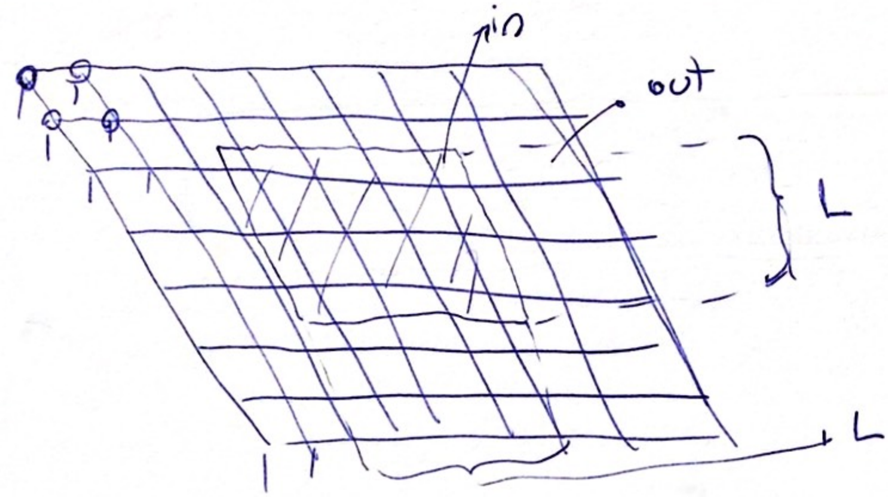
$$\boxed{\hat{A}_n = A^{(i_n)}_{n(\alpha_n,\beta_n)} |i_n\rangle\langle\alpha_n,\beta_n|}$$

Exercise: show that $\boxed{|\psi_{MPS}\rangle = \hat{A}_1 \dots \hat{A}_n \; |\Phi_R\rangle^{\otimes N}}$

Since $\hat{A}_n$ are local they cannot create entanglement

$\Rightarrow S_{MPS} = O(\log(R))$

Area law of a 2D square lattice PEPS:



L x L square

$$\Rightarrow |\psi\rangle = \sum_{\bar{i}, \bar{\alpha}} A^{(i_{11})}_{11}(\bar{\alpha}_{11}) \, A^{(i_{12})}_{12}(\bar{\alpha}_{12}) \cdots A^{(i_{NN})}_{NN}(\bar{\alpha}_{NN}) \, |\bar{i}\rangle$$

$$= \sum_{\bar{\alpha}} \left(\sum_{\bar{i}_{in}} A^{(\bar{i}_{in})}_{\bar{\alpha}_{in+border}} |\bar{i}_{in}\rangle \right) \left(\sum_{\bar{i}_{out}} A^{(\bar{i}_{out})}_{\bar{\alpha}_{out+border}} |\bar{i}_{out}\rangle \right)$$

short hand notation

~~$|\psi_{in}(\bar{\alpha}_{in})\rangle$~~ ~~$|\psi_{out}(\bar{\alpha}_{out})\rangle$~~

But $\bar{\alpha}_{in}$ and $\bar{\alpha}_{out}$ share $4L$ virtual indices $\Rightarrow$

$$\Rightarrow \boxed{|\psi\rangle = \sum_{\bar{\alpha}_{border}} \underbrace{\left(\sum_{\bar{\alpha}_{in}, \bar{i}_{in}} A^{\bar{i}_{in}}_{\bar{\alpha}_{in}, \bar{\alpha}_{border}} |\bar{i}_{in}\rangle \right)}_{|\psi_{in}(\bar{\alpha}_{border})\rangle} \underbrace{\left(\sum_{\bar{\alpha}_{out}} A^{(\bar{i}_{out})}_{\bar{\alpha}_{out}, \bar{\alpha}_{border}} |\bar{i}_{out}\rangle \right)}_{|\psi_{out}(\bar{\alpha}_{border})\rangle}}$$

sub normalized

$$\Rightarrow \boxed{\rho_{in} = \sum_{\bar{\alpha}_b, \bar{\alpha}_b'} X_{\bar{\alpha}_b, \bar{\alpha}_b'} \, |\psi_{in}(\bar{\alpha}_b)\rangle\langle\psi_{in}(\bar{\alpha}_b')|}$$

with $X(\bar{\alpha}_b, \bar{\alpha}_b') := \langle \psi_{out}(\bar{\alpha}_b') | \psi_{out}(\bar{\alpha}_b) \rangle$

- $|\psi\rangle$ contains at most $\log(R^{4L})$ bits of entanglement accross the border

- Rank of ρ_{in} at most R^{4L} !

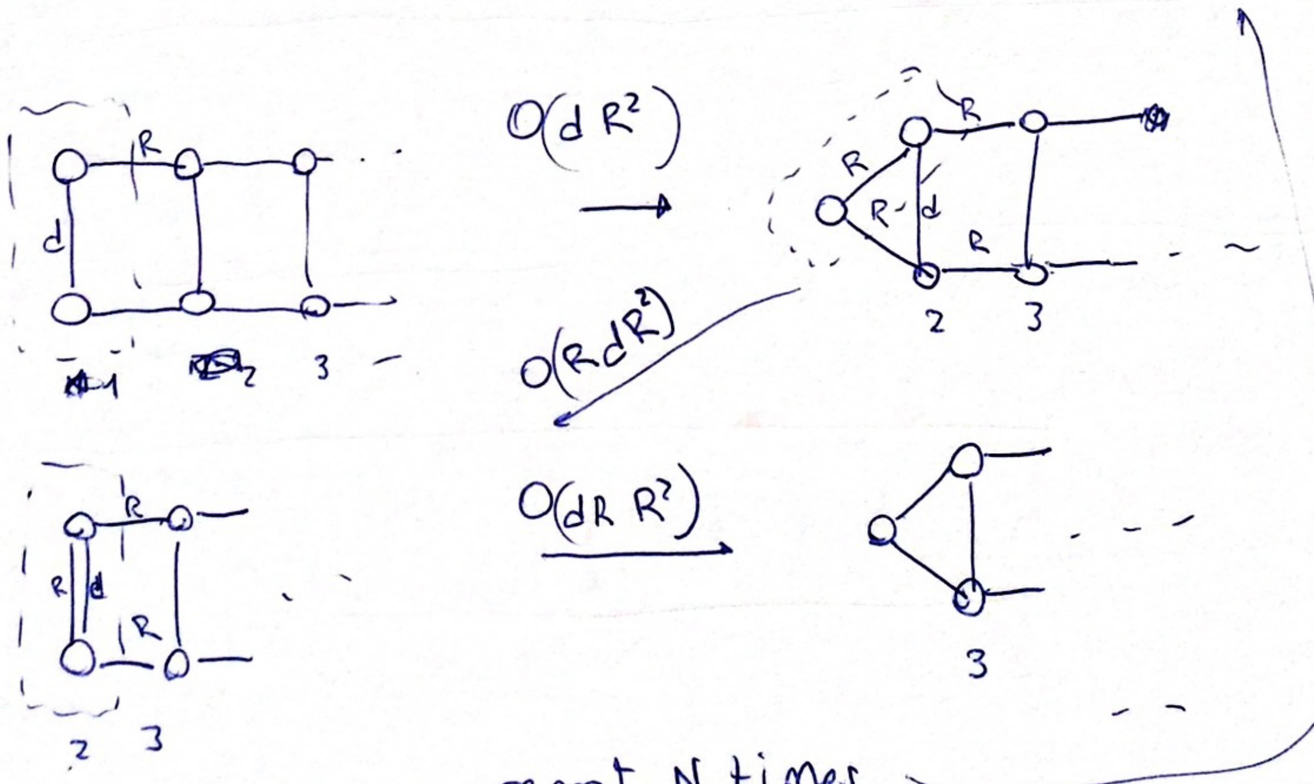
$$\Rightarrow \boxed{S(\rho_{in}) \le O\left[4L \log(R)\right]}$$

(Each "broken bond" contributes with log(R)")

4L: area of the border!

V) Efficient exact calculation of local observable expectation values and state overlaps

- Time complexity of the contraction between two MPSs : $\boxed{O(N d R^3)}$

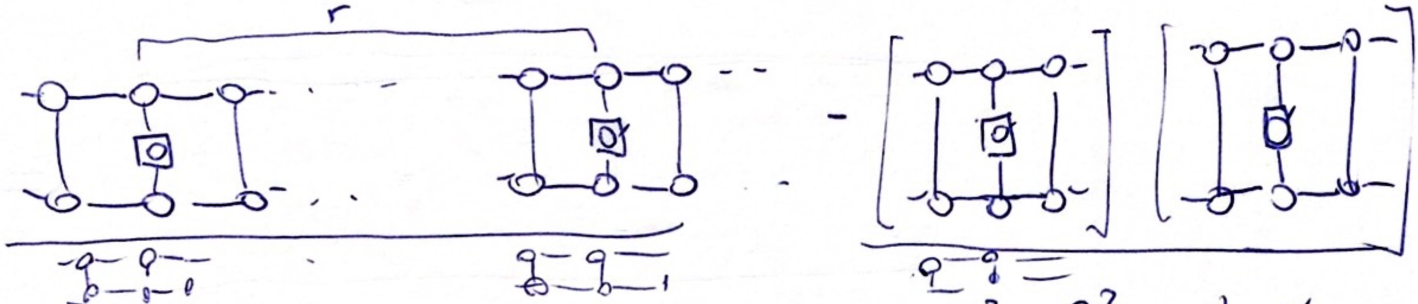


repeat N times

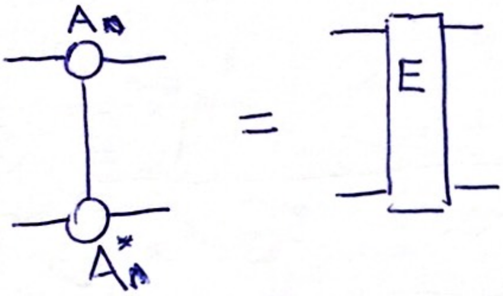
N

VI) Finite correlation length (exponential decay of correlations)

- Two-body correlator: $\boxed{C_r = \langle O_i \, O'_{i+r} \rangle - \langle O_i \rangle \langle O'_{i+r} \rangle}$



- Consider the transfer matrix: $E_{\mathbb{1}}$ $R^2 \times R^2$ matrix



$$\boxed{E_{\mathbb{1}} = \sum_{\mu=1}^{R^2} \lambda_\mu \, |\lambda_\mu^R)(\lambda_\mu^L|}$$

right eigenvector

left eigenvector

(spectral decomposition)

$\lambda_1 > \lambda_2 \geq \lambda_3 \geq \lambda_4 \dots$

$$\Rightarrow E_{\mathbb{1}}^{\ell} = \sum_\mu \lambda_\mu^{\ell} |\lambda_\mu^R)(\lambda_\mu^L| = \lambda_1^{\ell} \sum_{\mu=1}^{R^2} \left(\frac{\lambda_\mu}{\lambda_1}\right)^{\ell} |\lambda_\mu^R)(\lambda_\mu^L|$$

for $\ell \gg 1$

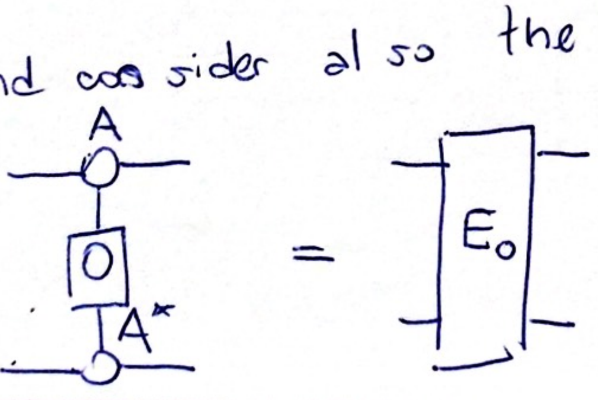
$$\simeq \boxed{\lambda_1^{\ell} |\lambda_1^R)(\lambda_1^L| + \lambda_2^{\ell} \sum_{\mu=2}^{\omega+1} |\lambda_\mu^R)(\lambda_\mu^L|}$$

λ_1 non-degenerate

ω : degeneracy of λ_2

- And consider also the matrix:

$R^2 \times R^2$ matrix



$$\Rightarrow \langle O_i \, O'_{i+r} \rangle \approx \frac{E_1^{\,l_L} \, E_O \, E_1^{\,r} \, E_{O'} \, E_1^{\,l_R}}{E_1^{\,l_L + l + l_R + 2}}$$

$$= \underbrace{\frac{(\lambda_1^L | E_O | \lambda_1^R)(\lambda_1^L | E_{O'} | \lambda_1^R)}{\lambda_1^2}}_{\langle O_i \rangle \langle O'_{i+l} \rangle} - \frac{\left(\frac{\lambda_2}{\lambda_1}\right)^{r-1} \sum_{\mu=2}^{w+1} (\lambda_1^L | E_O | \lambda_\mu^R)(\lambda_\mu^L | E_{O'} | \lambda_1^R)}{\lambda_1^2}$$

$$\Rightarrow \boxed{C_r \approx \left(\frac{\lambda_2}{\lambda_1}\right)^{r-1} \sum_{\mu=2}^{w+1} \frac{(\lambda_1^L | E_O | \lambda_\mu^R)(\lambda_\mu^L | E_{O'} | \lambda_1^R)}{\lambda_1^2} \approx e^{-r/\xi} \, O(w)}$$

with $\boxed{\xi = -\frac{1}{\ln \left| \lambda_2 / \lambda_1 \right|}}$ (finite correlation length)

All slightly entangled states are an MPS (of small R) ⑧

Schmidt decomposition:

Theorem: $|\psi\rangle \in \mathbb{H}_A \otimes \mathbb{H}_B$, arbitrary fin.: $\mathrm{Dim}(\mathbb{H}_A) = D_A < \infty$, $\mathrm{Dim}(\mathbb{H}_B) = D_B < \infty$

$\Rightarrow \exists$ orthonormal bases $\{|\Phi_A^{(\alpha)}\rangle\}_\alpha$ and $\{|\Phi_B^{(\alpha)}\rangle\}_\alpha$ of $\mathbb{H}_A$ and $\mathbb{H}_B$ s.t.

$$\boxed{|\psi\rangle = \sum_{\alpha=1}^{R} \lambda^{(\alpha)} |\Phi_A^{(\alpha)}\rangle \otimes |\Phi_B^{(\alpha)}\rangle}$$

, with $\lambda_\alpha \geq 0$, $R \leq \min(D_A, D_B)$

Schmidt coeffs.

Schmidt rank

(Proof hint: singular value decomposition)

~~Now: $|\psi\rangle \in \mathbb{H}_1 \otimes \mathbb{H}_2 \ldots \otimes \mathbb{H}_N = \mathbb{H}$ (N qudits)~~

Schmidt rank a valid measure of entanglement

$$\Rightarrow \boxed{S(\rho_A) = S(\rho_B) \leq \log_2 (R)}$$

(maximally entangled state)

Now, $|\psi\rangle \in \mathbb{H}_1 \otimes \mathbb{H}_2 \cdots \mathbb{H}_N = \mathbb{H}$ (N qudits)

$$\Rightarrow \boxed{R_{max} = \cancel{2^{N}}\; 2^{N/2}}$$

Assumption : $\boxed{R_{max} = \mathrm{Poly}(N)}$ (~~exponentially~~ slightly entangled)

$$\Rightarrow |\psi\rangle = \underbrace{\sum_{\bar{i}} c_{\bar{i}} |\bar{i}\rangle}_{\text{SD for } 1:2\ldots N} = \sum_{\alpha_1} \overset{\text{Schmidt coeffs.}}{\lambda_{1(\alpha_1)}} |\Phi_1(\alpha_1)\rangle |\Phi_{2..N}(\alpha_1)\rangle$$

Schmidt vectors

$|\Phi_1(\alpha_1)\rangle = \sum_{i_1} \Gamma^{(i_1)}_{1(\alpha_1)} |i_1\rangle$ expansion in comp. basis

$\Gamma^{(i_1)}_{1(\alpha_1)}$: arbitrary coefficien.

$$= \sum_{i_1, \alpha_1} \Gamma^{(i_1)}_{1(\alpha_1)} \lambda_{1(\alpha_1)} |i_1\rangle |\Phi_{2..N}(\alpha_1)\rangle$$

$$|\Phi_{2..N}(\alpha_1)\rangle = \sum_{i_2} \underbrace{|i_2\rangle}_{\text{comp. basis}} \underbrace{|\tau^{(i_2)}_{3\ldots N}(\alpha_1)\rangle}_{\text{subnormalized arbitrary states}}$$

- Now, expand $|\tau^{(i_2)}_{3\ldots N}(\alpha_1)\rangle$ in the Schmidt basis of $12:3\ldots N$ $\Rightarrow$ At most R non zero terms in the expansion

$$\Rightarrow \boxed{|\tau^{(i_2)}_{3\ldots N}(\alpha_1)\rangle = \sum_{\alpha_2} \underbrace{\Gamma^{(i_2)}_{2(\alpha_1,\alpha_2)}}_{\text{arbitrary coeff}} \underbrace{\lambda_{2(\alpha_2)}}_{\text{corresponding Schmidt coeffs}} |\Phi_{3\ldots N}(\alpha_2)\rangle}$$

Trivial example:

$$|\phi\rangle = |00\rangle + |01\rangle + |10\rangle + |11\rangle \overset{SD}{=} 1\,|++\rangle + 0\,|--\rangle$$

$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \qquad |-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

$$\Rightarrow |\phi\rangle = |0\rangle\left(\frac{|+\rangle + |-\rangle}{\sqrt{2}}\right) + |0\rangle\left(\frac{|+\rangle - |-\rangle}{\sqrt{2}}\right) + |1\rangle\left(\frac{|+\rangle + |-\rangle}{\sqrt{2}}\right) + |1\rangle\left(\frac{|+\rangle - |-\rangle}{\sqrt{2}}\right)$$

But, because of SD $\Rightarrow |\phi\rangle = |0\rangle \frac{1}{2\sqrt{2}}\left(|+\rangle + 0|-\rangle\right) + |0\rangle \frac{1}{2\sqrt{2}}\left(|+\rangle + 0|-\rangle\right)$

$$+ |1\rangle \frac{1}{2\sqrt{2}}\left(|+\rangle + 0|-\rangle\right) + |1\rangle \frac{1}{2\sqrt{2}}\left(|+\rangle + 0|-\rangle\right)$$

$$\Rightarrow |\psi\rangle = \sum_{\substack{i_1\alpha_1 \\ i_2\alpha_2}} \Gamma^{(i_1)}_{1(\alpha_1)}\, \lambda_1(\alpha_1)\, \Gamma^{(i_2)}_{2(\alpha_1,\alpha_2)}\, \lambda_2(\alpha_2)\, |i_1 i_2\rangle\, |\Phi_{3\ldots N}(\alpha_2)\rangle$$

Iterating the procedure N times:

$$\boxed{|\psi\rangle = \sum_{\bar{i},\bar{\alpha}} \overbrace{\Gamma^{(i_1)}_{1(\alpha_1)}\, \lambda_1(\alpha_1)\, \underbrace{\Gamma^{(i_2)}_{2(\alpha_1,\alpha_2)}\, \lambda_2(\alpha_2)}_{A^{(i_2)}_{2(\alpha_1,\alpha_2)}} \cdots \Gamma^{(i_N)}_{N(\alpha_{N-1})}\, \lambda_N(\alpha_{N-1})}^{c_{\bar{i}}}\, |\bar{i}\rangle}$$

"Canonical form of an MPS"

Readily gives the SD in the $1\ldots L : L+1 \ldots N$ bipartition

unique, MPSs invariant under gauge transformation

$$A_n\, A_{n+1} \rightarrow (A_n\, T)\,(T^{-1} A_{n+1})$$

$$\boxed{|\psi\rangle = \sum_{\alpha_L} \lambda_{L(\alpha_L)} |\Phi_{1\ldots L}(\alpha_L)\rangle |\Phi_{L+1\ldots N}(\alpha_L)\rangle .}$$

where
$$|\Phi_{1\ldots L}(\alpha_L)\rangle = \sum_{\alpha_1 \ldots \alpha_{L-1}} \Gamma^{(i_1)}_{1(\alpha_1)} \lambda_{1(\alpha_1)} \cdots \Gamma^{(i_L)}_{L(\alpha_{L-1},\alpha_L)} |i_1 \ldots$$

$$|\Phi_{L+1\ldots N}(\alpha_L)\rangle = \sum_{\alpha_{L+1} \ldots \alpha_{N-1}} \Gamma^{(i_{L+1})}_{L+1(\alpha_L,\alpha_{L+1})} \cdots \lambda_{N-1(\alpha_{N-1})} \Gamma^{(i_N)}_{N(\alpha_{N-1})} |i_{L+1} \ldots i_N\rangle$$

"SD in the $1 \ldots L : L+1 \ldots N$ bipartition"

Exercise : show it (by induction over L)

classical simulation of slightly entangled computations

theorem (Vidal 03) : Any pure-state computation where $R \leq \mathrm{Poly}(N)$ can be classically simulated (by updating the MPS description after each gate) with $\mathrm{Poly}(N)$ memory and time

$\Rightarrow$ Entanglement is necessary for quantum computational supremacy !

VII) - Hasting's (0705.2024): An area law for 1D quantum systems

. H is gapped + 1D + local (short-ranged) + unique ground state

$\Rightarrow$ ground state satisfies area law

$\Rightarrow$ MPS

- Brandão & Horodecki : 1206.2947

1D + $\underbrace{\text{finite correlation length}}_{\Updownarrow}$ $\Rightarrow$ area law $\Rightarrow$ MPS

exponential decay of correlations.