Outline:

(1) Entanglement and Matrix Product States

- Quantifying entanglement: Reduced density matrices, SVD, entropy
- Ground states of local Hamiltonian: Area law
- MPS representation
- Example: AKLT
- Diagramatic representation of tensors
- Canonical form
- Symmetries

(2) Symmetry protected topological phases

- Symmetry fractionalization
- Cohomology for on-site symmetries
- Anti unitary symmetries
- Fermionic phases

(3) Numerical simulations and detection of topological phases

- Generalized transfer matrix $\rightsquigarrow$ Projective representations
- String order
- MPS as variational wave function: DMRG / TEBD

(1) Entanglement and Matrix Product States

Outline: Area law
Efficient representation: MPS
Canonical form
Symmetries

Entanglement (bipartite)

A B

o o o | o o o

$$|\psi\rangle \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$$

$$\rho_A = \mathrm{Tr}_B\, |\psi\rangle\langle\psi| , \quad \rho_B = \mathrm{Tr}_A\, |\psi\rangle\langle\psi|$$

(von-Neumann) entanglement entropy $S = -\mathrm{Tr}_A\, \rho_A \cdot \log \rho_A = -\mathrm{Tr}_B\, \rho_B \log \rho_B$

Entangled state has mixed ρ_A, ρ_B (i.e., $S \neq 0$)

Schmidt decomposition:

Schmidt values Schmidt states

$$|\psi\rangle = \sum_{\alpha=1}^{\min(N_A, N_B)} \lambda_\alpha\, |\phi_\alpha\rangle_A\, |\phi_\alpha\rangle_B , \quad \lambda_1 \geq \lambda_2 \geq \cdots \geq 0$$

$$\langle \phi_\alpha | \phi_{\alpha'} \rangle = \delta_{\alpha\alpha'} \qquad \text{(unique up to dg)}$$

$$\rho_A = \sum_\alpha \lambda_\alpha^2\, |\phi_\alpha\rangle_A\, {}_A\langle\phi_\alpha| , \quad \rho_B = \sum_\alpha \lambda_\alpha^2\, |\phi_\alpha\rangle_B\, {}_B\langle\phi_\alpha|$$

and thus $S = -\sum \lambda_\alpha^2 \cdot \log \lambda_\alpha^2$. (normalization: $\sum_\alpha \lambda_\alpha^2 = 1$)

Entanglement spectrum $\{-2\cdot\ln\lambda\}$ (eigenvalues of e^{-S})

Examples: * Product state $\rightsquigarrow \lambda_1 = 1, \lambda_{\alpha>1} = 0$ and $S = 0$

o o o | o o o

* Maximally entangled state $\rightsquigarrow \lambda_1 = \dots = \lambda_N = 1/\sqrt{N}$ and $S = \log N$

$\sum_{\alpha=1}^{N} \frac{1}{\sqrt{N}} |\alpha\rangle|\alpha\rangle$ o o o | o o o

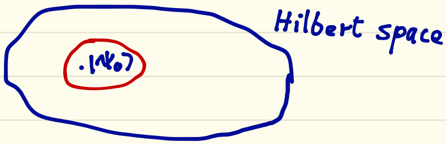
* Random state : Entanglement close to S_{max} [Page]

$\left[S = \frac{L}{2} \log d - \frac{1}{2} \right]$

Area law

Ground states of (gapped) local Hamiltonians fulfill the area law $S = L^{D-1}$ [proof exists for 1D, Hastings]

1D $\underbrace{\text{o o o | o o o}}_{L}$ $S(L) = \text{const.}$ $(L > \xi)$



(gapless $S \sim \log L$)

Ground states are "close" to product states $\rightsquigarrow$ efficient representation

Matrix product states

General many-body state

$$|\psi\rangle = \sum \psi_{i_1 \dots i_L} |i_1\rangle|i_2\rangle \cdots |i_L\rangle, \quad i_n = 1 \dots d$$

$\psi_{i_1 \dots i_L}$ is a rank L tensor $\rightsquigarrow$ need to store d^L $\mathbb{C}$ numbers!

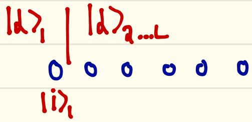
Product state : $\Psi_{i_1 \cdots i_L} = \phi^{[1],i_1} \cdots \phi^{[L]i_L}$, $\phi^{[n]i_n} \in \mathbb{C}$

Matrix-product state : $\Psi_{i_1 \ldots i_L} = A^{[1]i_1} \cdots A^{[L],i_L}$, $A^{[n]i_n}$ are matrices
(MPS)

- Every state can be expressed exactly as MPS.
- State "close" to product state have small bond dimension χ

Write a general state $|\Psi\rangle$ as MPS

Successive Schmidt decompositions :



$$|\Psi\rangle = \sum_{i_1}\sum_{\alpha} A^{[1]i_1}_{\alpha} |i_1\rangle_1 |\alpha\rangle_{2\ldots L} \quad , \quad A^{[1]i_1}_{\alpha} = \left[{}_1\langle i_1|\, {}_{2\ldots L}\langle \alpha|\right] |\Psi\rangle$$

$$= \sum_{i_1 i_2, \alpha, \beta} A^{[1]i_1}_{\alpha} A^{[2]i_2}_{\alpha\beta} |i_1\rangle_1 |i_2\rangle_2 |\beta\rangle_{3\ldots L} \, , \quad A^{[2]i_2}_{\alpha\beta} = \left[{}_1\langle \alpha|\, {}_2\langle i_2|\right] |\beta\rangle_{3\ldots L}$$

... (until finished)

Schmidt states with small λ_α can be discarded $\rightsquigarrow$ compression!

<u>Examples</u>

GHZ : $|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\downarrow\downarrow\rangle\right)$ has MPS has $\chi = 2$

MPS representation $A^{\uparrow} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $A^{\downarrow} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

AKLT : $S=1$ spin chain with $H = \sum P^{S=2}_{j,j+1} = \sum \vec{S}_j \vec{S}_{j+1} + \frac{1}{3}(S_j S_{j+1})^2 + \frac{2}{3}$

$|\psi_0\rangle$: 

$S=1$ $\quad$ $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

 : $|+\rangle = |\uparrow\uparrow\rangle$, $|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, $|-\rangle = |\downarrow\downarrow\rangle$

The MPS representation is then

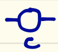
$$A^+ = \sqrt{\tfrac{2}{3}}\,\sigma^+ \quad , \quad A^0 = -\tfrac{1}{\sqrt{3}}\,\sigma^z \quad , \quad A^- = -\sqrt{\tfrac{2}{3}}\,\sigma^- \quad .$$

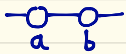
MPS as variational wavefunction (DMRG) : Optimize the energy within the space of MPS with bond dim. χ

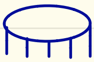
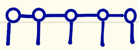
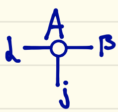
<u>Tensor network notation</u>

Useful diagramatic representation of tensornetworks :

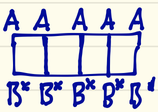
Scalar $a \hat{=}$  , vector $a_i \hat{=}$  , matrix $a_{ij} \hat{=}$ 

tensor operations : $c_{ik} = \sum_j a_{ij} b_{jk}$ $\rightsquigarrow$ 

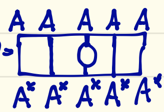
= 

Matrix product :  $\approx$  , 

Overlap :

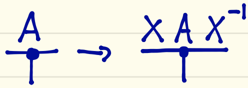
$\langle\psi|\phi\rangle =$ 

Expectation value :

$\langle\psi|O|\psi\rangle =$ 

Canonical form of MPS

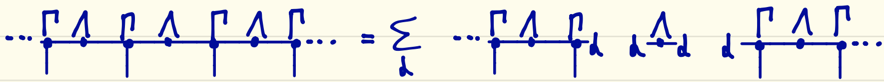
From now on: $A^{[n]i_n} = A^{i_n}$ and $L \to \infty$ / Pure states

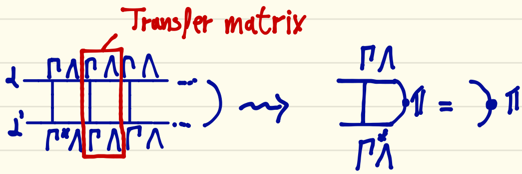
MPS are not uniquely defined: 

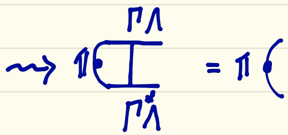
represents same state

Bonds are directly related to the Schmidt decomposition
and $A = \Gamma \cdot \Lambda$ $(\Lambda_{\alpha\alpha} = \lambda_\alpha)$ [Vidal]

$$|\Psi\rangle = \sum_\alpha |\alpha\rangle_L \, \lambda_\alpha \, |\alpha\rangle_R$$



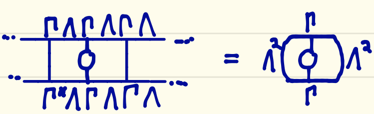
$\delta_{\alpha\alpha'} = {}_R\langle \phi_\alpha | \phi_{\alpha'} \rangle_R =$ 

[similar for the right] 

$\Leftrightarrow$ Transfermatrices have left/right eigenvalue 1 with eigenvector $\mathbb{1}$

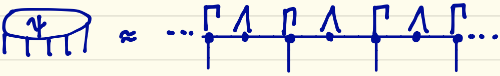
Uniquely defines the MPS up to a U(1) phase and dg in λ_α.

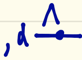
- Convenient to evaluate expectation values:

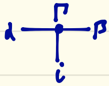
$\langle \Psi | O_1 | \Psi \rangle =$ 

(2) Symmetry protected topological phases

$$|\psi\rangle = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha\rangle_L |\alpha\rangle_R$$



 $= \lambda_\alpha \delta_{\alpha\beta}$

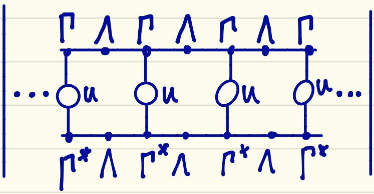
 $= \Gamma^i_{\alpha\beta}$

Symmetries of MPS

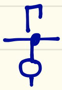
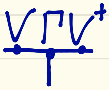
Assume $|\psi\rangle$ invariant under an onsite symmetry g:

$$\left[\otimes_j u_j(g)\right]|\psi\rangle = \alpha|\psi\rangle, \quad |\alpha| = 1. \quad \text{(e.g., } \mathbb{Z}_2 \text{ sym. in Ising param.)}$$

"mixed transfermatrix"

 $= 1 \Leftrightarrow$  has a largest eigenvalue of modulus 1.

[Perez Garcia] showed that this is equivalent to

 $= e^{i\theta}$  $, [V, \Lambda] = 0$

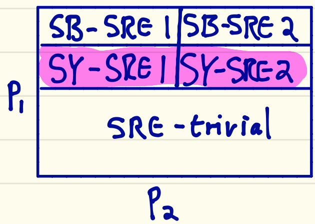
$$\sum_j u_{ij} \Gamma^j = e^{i\theta} V \Gamma^i V$$

The same can be derived for TR $\Gamma \to \Gamma^*$ and inversion $\Gamma \to \Gamma^T$

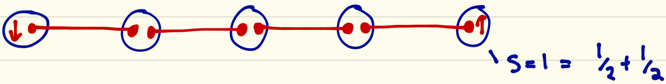
Brief review of Quantum Phases

Gapped quantum phases in 1D:

- No LRE / simple / complete



Example: S=1 AKLT Hamiltonian



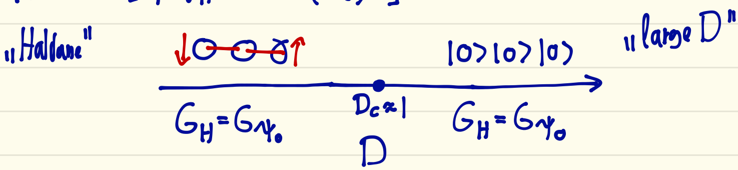
$\bullet\!\!-\!\!\bullet = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

- Bulk has full symmetry $[G_H = G_\psi]$
- $S=\frac{1}{2}$ edge spins

Example

S=1 chain with single ion anisotropy

$$H = \sum \left[\vec{S}_i \vec{S}_{i+1} + D\cdot (S_i^z)^2\right]$$



Symmetries: Translation, $\mathbb{Z}_2 \times U(1) \supseteq \mathbb{Z}_2 \times \mathbb{Z}_2$, TR, Inversion

"hidden $\mathbb{Z}_2\times\mathbb{Z}_2$ sym. breaking" $\left[U_K = \prod_{j<k} \exp\left(i\pi S_j^z S_k^x\right)\right]$

How to distinguish the phases?

SPT order in 1D

1D SPT stabilized by different symmetries: on-site, TR, inversion, ...

Focus on on-site symmetries, e.g. spin flip symmetries:

$$\left[\bigotimes_j U_j(g)\right]|\psi\rangle = \alpha|\psi\rangle, \quad |\alpha| = 1$$

Representations of a group can be linear or projective.

Projective representations

Operators $u(g)$ form a projective representation (PR) if

$$u(g) \cdot u(h) = e^{i\phi_{gh}} \cdot u(g \cdot h),$$

$\{e^{i\phi_{gh}}\}$ is the factor set (fulfils consistency cond.: Associativity).

[2-cochain $G \times G \to U(1)$]

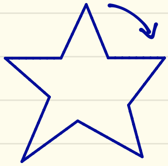
If $\forall gh: \phi_{gh} = 0$, the representation is linear.

Allowing to change the phases $u'(g) = e^{i\alpha} \cdot u(g)$, which PR can be transformed into each other?

$$\phi'_{gh} = \phi_{gh} + \alpha_{gh} - \alpha_g - \alpha_h$$

Equivalent PR belong to the same cohomology class $H^2(G, U(1))$

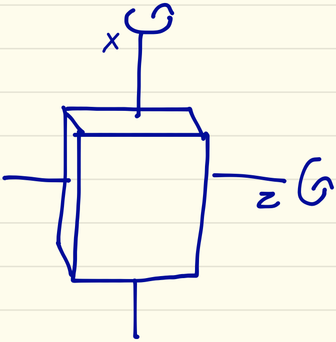
Example $\mathbb{Z}_N : \{1, R, R^2, \dots, R^{N-1}\}$



$R^N = \mathbb{1} \Rightarrow U^N = e^{i\phi}\mathbb{1}$

Redefinition $\tilde{U}_R = e^{-i\phi/N} U_R$ removes the phase : All pr. rep. equivalent

Example: $\mathbb{Z}_2 \times \mathbb{Z}_2 : \{1, R_x, R_z, R_x R_z\}$



$U_x^2 = U_z^2 = 1$

$R_x R_z = R_z R_x \Rightarrow U_x U_z = e^{i\phi_{xz}} U_z U_x$

Phase $\phi_{xz} = 0, \pi$ cannot be removed : 2 classes

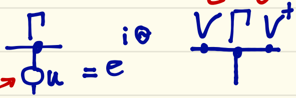
[Integer / half integer representation]

Classification of 1D SPT

$|\Psi\rangle$ symmetric under $\otimes_j U_j(g)$ with $U_j(g)$ being a linear on-site representation of g:

χ dimensional

Projective representation



, $[V, \Lambda] = 0$

linear representation of $g \in G$

The projective representation together with the phase $e^{i\theta}$ classify different SPT.

Example: $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry in $S=1$ spin chain

Sufficient to look at two generators, e.g. R_x, R_z.

On-site representation in terms of $S=1$ operators:

$$u_x = e^{i\pi S_x}, \quad u_z = e^{i\pi S_z} \quad \text{(linear representations)}$$

Thus the MPS transforms as

$$\boxed{\sum_k [u_x]_{jk} \Gamma_k = e^{i\Theta_x} V_x \Gamma_k V_x^+}$$

$R_{x/z}^2 = 1 \Rightarrow \Theta_{x/z} = 0, \pi$

V_x, V_z can be linear or projective representions of $\mathbb{Z}_2 \times \mathbb{Z}_2$, i.e., $V_x \cdot V_z = \pm V_z V_x$.

AKLT: $\Gamma^{-1} = \sqrt{\frac{2}{3}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \Gamma^0 = -\frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \Gamma^{+1} = -\sqrt{\frac{2}{3}} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

$$u_z = \begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix} \rightsquigarrow V_z = \sigma_z$$

$$\left[\text{e.g., } \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}\right]$$

$$u_x = \begin{pmatrix} & & -1 \\ & -1 & \\ -1 & & \end{pmatrix} \rightsquigarrow V_x = \sigma_x$$

$$\rightsquigarrow V_x V_z = \underline{\underline{-}} V_z V_x$$

$|0\rangle|0\rangle$: $V_x = V_z = \mathbb{1}$

$$\rightsquigarrow V_x V_z = \underline{\underline{+}} V_z V_x$$

- AKLT phase has degeneracies in the ES since Λ commutes with V_x, V_z and $V_x V_z = -V_z V_x$.

$$\left[\Lambda |\phi_n\rangle = \Lambda_n |\phi_n\rangle ,\ \Lambda \underbrace{V_x |\phi_n\rangle}_{|\phi_n'\rangle} = \Lambda_n \cdot V_x |\phi_n\rangle \text{ and } \langle\phi_n'|\phi_n\rangle = 0 \right]$$

- AKLT can be generalized to higher spin S

  even S : fractionalization into integer spin $\Rightarrow$ „trivial"
  odd S : fractionalization into half-integer spin $\Rightarrow$ SPTP

Inversion symmetry

SPT can be protected by inversion symmetry

$$\underset{-3}{\circ} \quad \underset{-2}{\circ} \quad \underset{-1}{\circ} \;\Big|\; \underset{0}{\circ} \quad \underset{1}{\circ} \quad \underset{2}{\circ} \qquad : \quad i = -i-1$$

MPS transforms as $\Gamma \to \Gamma^T$: $\Gamma^T = \pm V \Gamma V^\dagger$ and $V = \pm V^T$

Time reversal symmetry

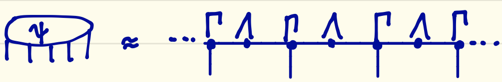
MPS trasforms as $\Gamma \to \Gamma^*$: $\Gamma^* = \pm V \cdot \Gamma V^\dagger$ and $V = \pm V^T$

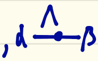
(3) Numerical simulations and detection of topological phases

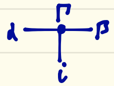
Outline: - Generalized transfer matrix ⇝ Projective representations
⇝ String order
- MPS as variational wave function (DMRG / TEBD)
- Towards 2D: TPS

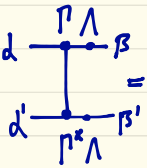
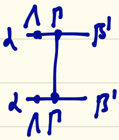
<u>MPS:</u>

$$|\psi\rangle = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha\rangle_L |\alpha\rangle_R$$



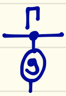
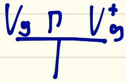
,  $= \lambda_\alpha \delta_{\alpha\beta}$

 $= \Gamma^i_{\alpha\beta}$

 $= T^R_{\alpha\alpha',\beta\beta'}$,  $= T^L_{\alpha\alpha',\beta\beta'}$

T^R, T^L have left/right dominant ev. $\mathbb{1} \hat{=} \delta_{\alpha\alpha'}$.

State $|\psi\rangle$ is symmetric under $\left[\bigotimes_j U_j(g)\right] |\psi\rangle = \alpha |\psi\rangle$, $|\alpha| = 1$

 $= e^{i\theta}$  , $[V_g, \Lambda] = 0$ (Perez-Garcia '07)

⇝ V_g are projective representation of the symmetry!

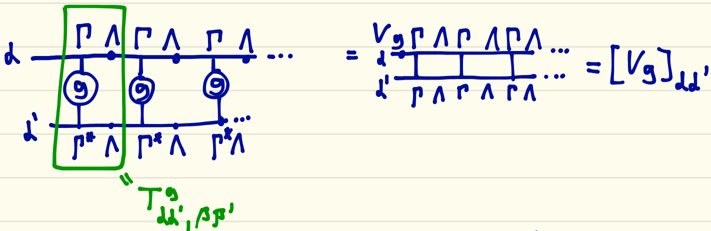
$\boxed{\mathbb{Z}_2\times\mathbb{Z}_2 : \quad V_x V_z = \pm V_z V_x}$

$\boxed{\text{Inversion } (\Gamma_j \to \Gamma_j^T) : \quad V_I V_I^* = \pm 1}$

$\boxed{\text{TR } (\Gamma_j \to \sum e^{-i\pi[S^y]_{jk}} \cdot \Gamma_k^*) : \quad V_{TR} V_{TR}^* = \pm 1}$

How to detect the phases in numerical simulations?

<u>MPS Framework</u>: Dominant eigenvector of generalized transfer matrix



$\Rightarrow U_g$ is eigenvector of T^g with eigenvalue α, $|\alpha| = 1$

Construct <u>„non-local order parameter"</u> (String order)

Inversion: $\mathcal{O}_I(x) = \langle \psi_0 | I_x | \psi_0 \rangle$

$=$ 

$= \pm \mathrm{Tr}\, \varrho^2$

MPS based algorithms

Given a Hamiltonian H, how to obtain the ground state MPS? Time evolution?
$\rightsquigarrow$ DMRG / TEBD

Time evolving block decimation (TEBD)

Real and imaginary time evolution of MPS

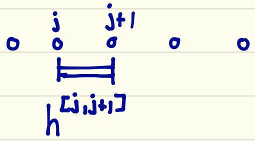
Time evolution in real time:

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

Time evolution in imaginary time yields GS:

$$|\psi_0\rangle = \lim_{\tau\to\infty} \frac{e^{-H\tau}\,|\psi_i\rangle}{\| e^{-H\tau}\,|\psi_i\rangle\|}$$

Assume the Hamiltonian has the form $H = \sum_j h^{[j,j+1]}$



Decompose the Hamiltonian $H = F + G$

$$F = \sum_{\text{even } j} h^{[j+1]} \quad , \quad G = \sum_{\text{odd } j} h^{[j,j+1]}$$

$$[F^j, F^k] = [G^j, G^k] = 0$$
$$[G, F] \neq 0$$

Baker-Campbell-Harsdorff $\left[\, e^{\varepsilon A} \cdot e^{\varepsilon B} = e^{\varepsilon(A+B) + \frac{\varepsilon^2}{2}[A,B] + \cdots} \,\right]$

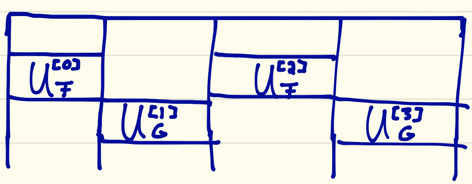
Decompose time evolution $\exp(-iHt) = \left[\exp(-iH \underbrace{t/N}_{=\delta t})\right]^N$

$$e^{-i\delta t(F+G)} = \underbrace{e^{-i\delta t F}}_{U_F} \cdot \underbrace{e^{-i\delta t G}}_{U_G} + O(\delta t^2)$$

Two chains of two-site gates

$$U_F = \prod_{\text{even } j} e^{-iF^{[i]}\delta t} \quad , \quad U_G = \prod_{\text{even } j} e^{-iG^{[i]}\delta t}$$

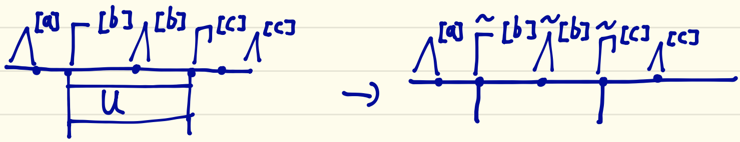
Back to MPS :



$|\psi(0)\rangle$

$|\psi(\delta t)\rangle$

Need an algorithm to project back to MPS form

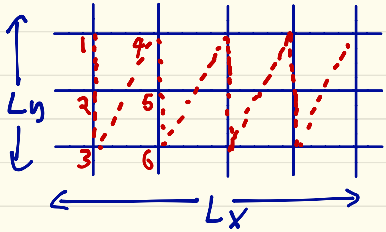


TEBD algorithm

[Slides]

MPS in 2D

MPS are have a 1D structure ⇝ Snake in 2D



While Hamiltonian local in 2D, it becomes long ranged in 1D repr. ⇝ Area law violated

Bond dimension $\chi \sim \exp(L_y)$

$\underbrace{\mathcal{O}(L_x \cdot e^{L_x})}_{\text{MPS}}$ vs $\underbrace{\mathcal{O}(e^{L_x L_y})}_{\text{ED}}$ ⇝ more efficient than ED!