Entanglement in correlated quantum systems: A quantum information perspective

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Quantum Information and Quantum Many-Body Systems

- Aim: Understand the physics of **quantum systems**
  composed of **many particles**

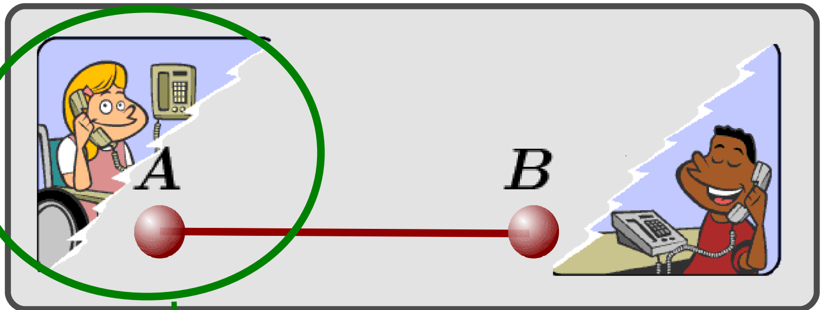
- In many cases, quantum correlations between particles
  are not very relevant (mean field theory)

- **Strong correlations** involved
  $\Rightarrow$ **entanglement** becomes important

- Entanglement Theory:
  - central part of quantum information theory
  - how can we **measure entanglement**?
  - **what can we do** with entanglement,
    and **what is impossible**?

Can we use quantum information techniques (in particular entanglement theory) to obtain a better understanding of quantum many-body systems?

Entanglement in Quantum Information



- two (and more) spins: **entanglement**

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}\Big[|0\rangle_A|0\rangle_B + |1\rangle_A|1\rangle_B\Big]$$

- **How much entanglement** is in some state

  e.g. $|\phi\rangle = \alpha|0\rangle_A|0\rangle_B + \beta|1\rangle_A|1\rangle_B$?

  $\leftrightarrow$ How much **perfect entanglement** $|\Psi^+\rangle$ does it contain?

- **reduced state** of Alice $\rho_A := \mathrm{tr}_B|\phi\rangle\langle\phi|$:

$$\rho_A = |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1|$$

- more entanglement $\leftrightarrow$ **more uncertainty** in ρ_A

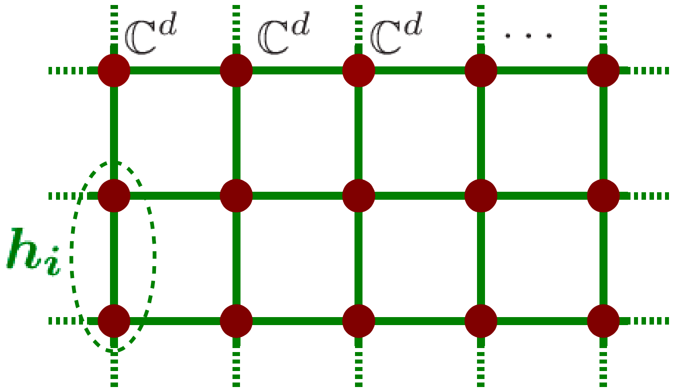
- measure of uncertainty (entanglement): **von Neumann entropy**

$$S(\rho_A) = -\mathrm{tr}[\rho_A \log_A]$$

  $\Rightarrow$ provides **quantitative measure** of entanglement

entropy = entanglement

Quantum many-body systems



- We consider systems composed of many (N)

  ***d*-level spins** $|0\rangle, |1\rangle, \dots, |d-1\rangle$

  with a **locality notion** ($\rightarrow$ lattice geometry)

- **Local Hamiltonian** $H = \sum_{i=1}^{M} h_i$

- H might be gapped: **energy gap** $\Delta(H) > 0$ betw. ground and excited states

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- Primary focus: **ground state** properties – $H|\Psi_0\rangle = E_0|\Psi_0\rangle$

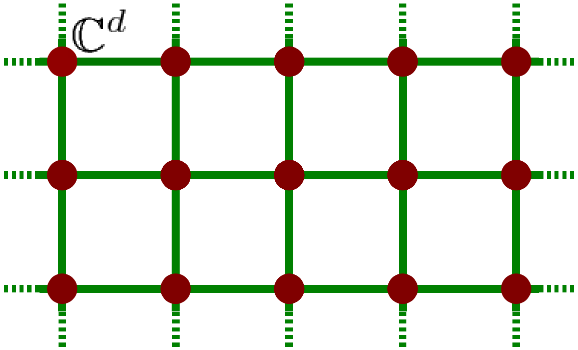
  … but we are also interested in **thermal states** $\rho = e^{-\beta H}$

  or the time evolution $|\Psi(t)\rangle = e^{iHt}|\Psi(t=0)\rangle$

- **Variational approach**:

  We seek for an **explicit form** of the **wavefunction** $|\Psi_0\rangle$

How hard is it to describe the ground state?

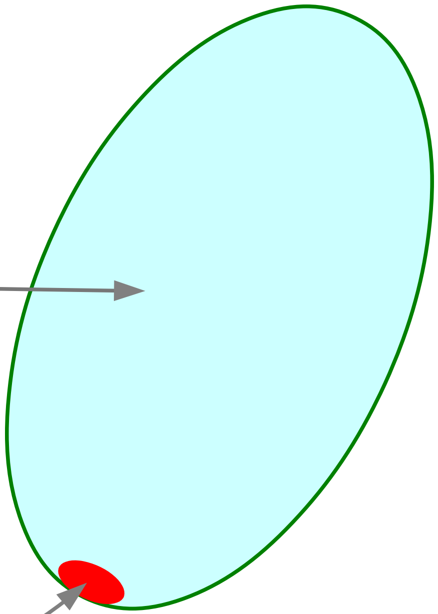


- N spins, $H = \sum_{i=1}^{M} h_i$
- can we **describe the ground state** $|\Psi_0\rangle$?

- Problem for large N:

$$|\Psi_0\rangle = \sum_{i_1,\ldots,i_N} c_{i_1\cdots i_N} |i_1,\ldots,i_N\rangle \ \in \ (\mathbb{C}^d)^{\otimes N} = \mathbb{C}^{(d^N)}$$

exponentially large
Hilbert space $\mathbb{C}^{(d^N)}$!



- But there is hope:

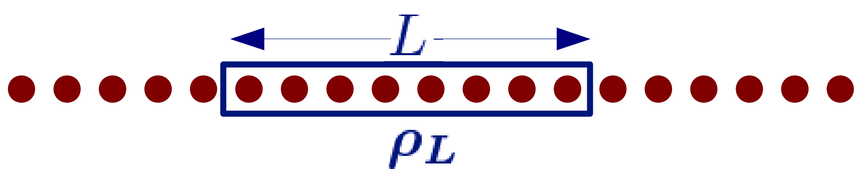
$\boldsymbol{H = \sum_{i=1}^{M} h_i}$ has only $\boldsymbol{M \propto N}$ **parameters**

$\rightarrow |\boldsymbol{\Psi_0}\rangle$ lives in **small region** of Hilbert space

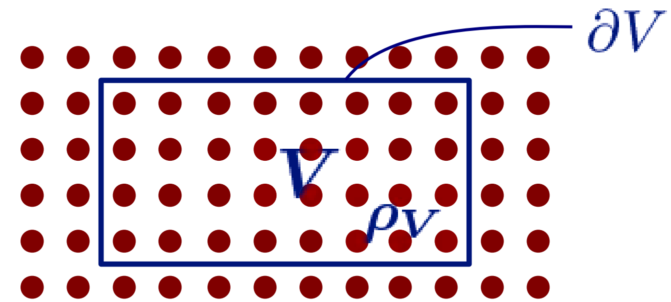
Can we find an **efficient description of ground states**
from which we can **efficiently compute quantities of interest**?

A physical guideline: The area law

- **Area law** for ground states of **gapped Hamiltonians**:

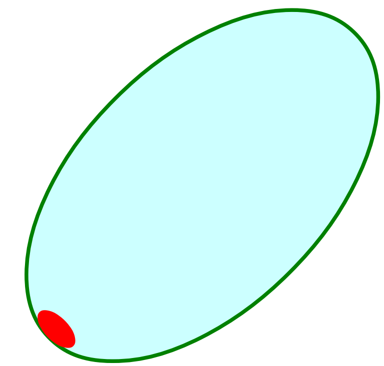


$S(\rho_L) \sim \text{const.}$



$S(\rho_V) \sim \partial V$

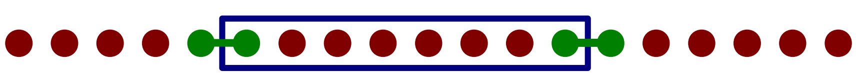
$\Rightarrow$ **entropy $S(\rho_L)$** of a region **scales as boundary**

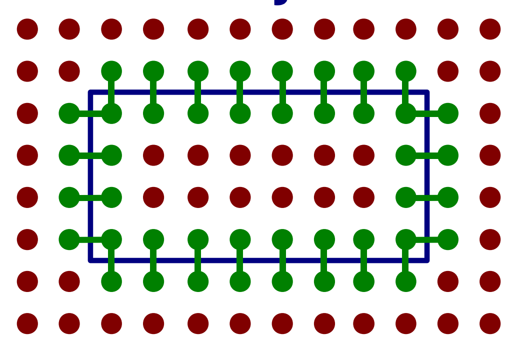


- Suprising: for random states, we expect $S(\rho_L) \sim \mathrm{Volume}$
- Even for **gapless systems:** $S(\rho_L) \sim \log L$ (1D)

- Quantum Information: entropy ≡ entanglement

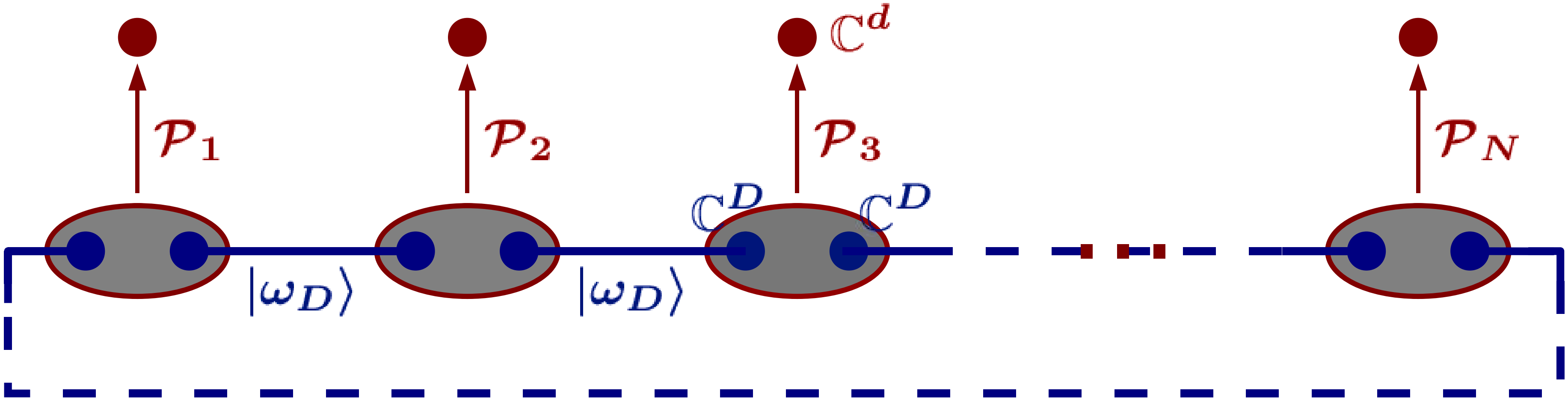
  $\Rightarrow$ **entanglement** located around the **boundary**





$\Rightarrow$ construct ansatz from **entanglement** between **adjacent sites**

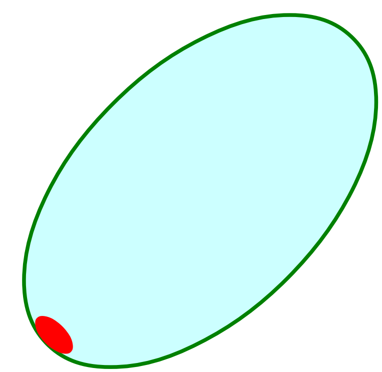
An ansatz for states with an area law



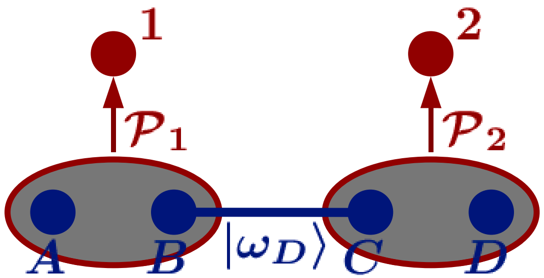
- each site composed of two **auxiliary particles** ("virtual particles") forming max. entangled **bonds** $|\omega_D\rangle := \sum_{i=1}^{D} |i,i\rangle$ (D: "bond dimension")
- apply **linear map** ("projector") $\mathcal{P}_k : \mathbb{C}^D \times \mathbb{C}^D \to \mathbb{C}^d$

$$\Rightarrow \quad |\psi\rangle = (\mathcal{P}_1 \otimes \cdots \otimes \mathcal{P}_N)|\omega_D\rangle^{\otimes N}$$

- satisfies **area law** by construction
- state characterized by $\mathcal{P}_1, \ldots, P_N \;\; \to \;\; NdD^2$ parameters
- family of states: enlarged by increasing D



Formulation in terms of Matrix Products



$$\mathcal{P}_s = \sum_{i,\alpha,\beta} A^{[s],i}_{\alpha\beta} |i\rangle\langle\alpha,\beta|$$

$A^{[s],i}$: $D \times D$ matrices

$$(\mathcal{P}_1 \otimes \mathcal{P}_2)|\omega_D\rangle = \Big[\sum_{i,\alpha,\beta} A^{[1],i}_{\alpha\beta}|i\rangle_1\langle\alpha,\beta|_{AB}\Big]\Big[\sum_{j,\gamma,\delta} A^{[2],j}_{\gamma\delta}|j\rangle_2\langle\gamma,\delta|_{CD}\Big]\Big[\sum_k |k,k\rangle_{BC}\Big]$$

$$= \sum_{i,j,\alpha,\delta}\Big[\sum_\beta A^{[1],i}_{\alpha\beta}A^{[2],j}_{\beta\delta}\Big]|i,j\rangle_{12}\langle\alpha,\delta|_{AD}$$

$\beta = \gamma$

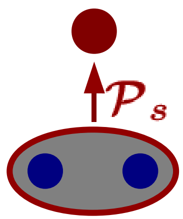
$$= \sum_{i,j,\alpha,\delta} (A^{[1],i}A^{2,j})_{\alpha\delta}|i,j\rangle_{12}\langle\alpha,\delta|_{AD}$$

- iterate this for the whole state $|\psi\rangle = (\mathcal{P}_1 \otimes \cdots \otimes \mathcal{P}_N)|\omega_D\rangle^{\otimes N}$:

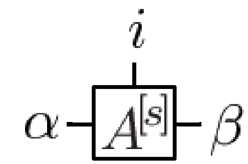
$$|\psi\rangle = \sum_{i_1,\ldots,i_N}[A^{[1],i_1}A^{[2],i_2}\ldots A^{N,i_N}]|i_1,\ldots,i_N\rangle$$ **Matrix Product State (MPS)**

(or $|\psi\rangle = \sum_{i_1,\ldots,i_N}\langle l|A^{[1],i_1}A^{[2],i_2}\ldots A^{[N],i_N}|r\rangle|i_1,\ldots,i_N\rangle$ for open boundaries)

Formulation in terms of Tensor Networks

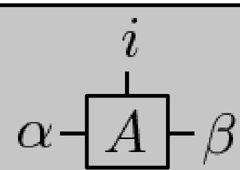


$$\mathcal{P}_s = \sum_{i,\alpha,\beta} A^{[s],i}_{\alpha,\beta} |i\rangle\langle\alpha,\beta| \qquad A^{[s],i}_{\alpha\beta} \equiv$$

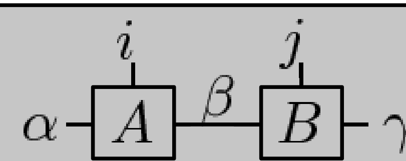


- **Tensor Network** notation:

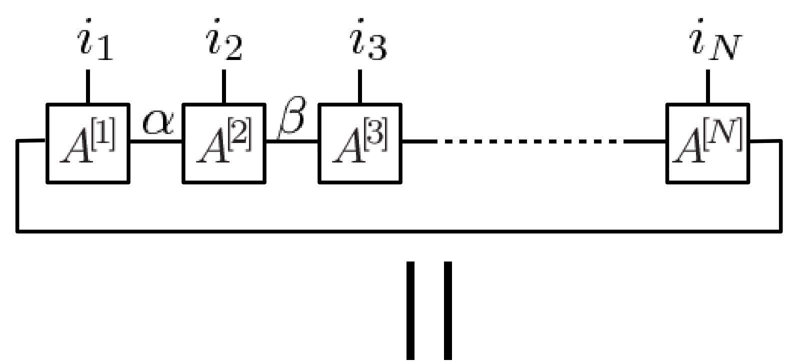
$$A^{i}_{\alpha\beta} \equiv$$



$$\sum_{\beta} A^{i}_{\alpha\beta} B^{j}_{\beta\gamma} \equiv$$

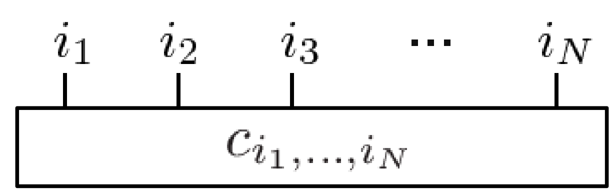


$$\mathbf{tr}[A^{[1],i_1} A^{[2],i_2} \ldots A^{[N],i_N}] =$$



- Matrix Product States can be written as

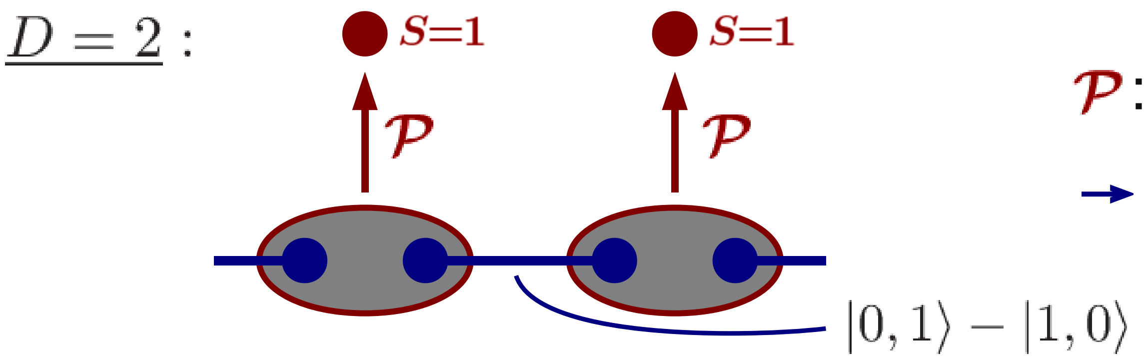
$$|\psi\rangle = \sum_{i_1,\ldots,i_N} c_{i_1,\ldots,i_N} |i_1,\ldots,i_N\rangle \qquad \text{with}$$



"Tensor Network States"

Examples

- The **AKLT state** [Affleck, Kennedy, Lieb & Tasaki, '87]



$\mathcal{P}$: projector onto $S=1$ subspace

→ **rotationally invariant** model

- **Exact ground state** of $H = \sum_i \left[\frac{1}{2}\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1} + \frac{1}{6}(\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1})^2 + \frac{1}{3}\right]$
- H has a **provable gap** (↔ Haldane conj. on integer-spin Heisenberg model)

$\Rightarrow$ MPS form a great **analytical toolbox** for correlated systems

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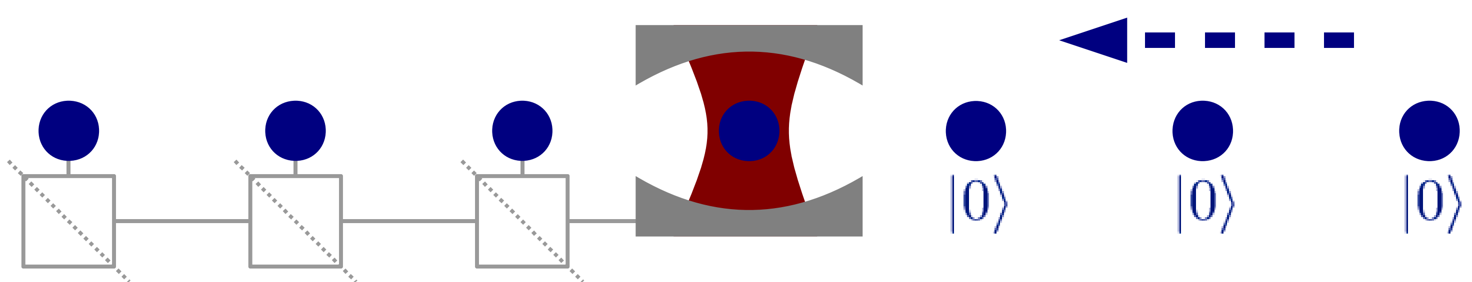
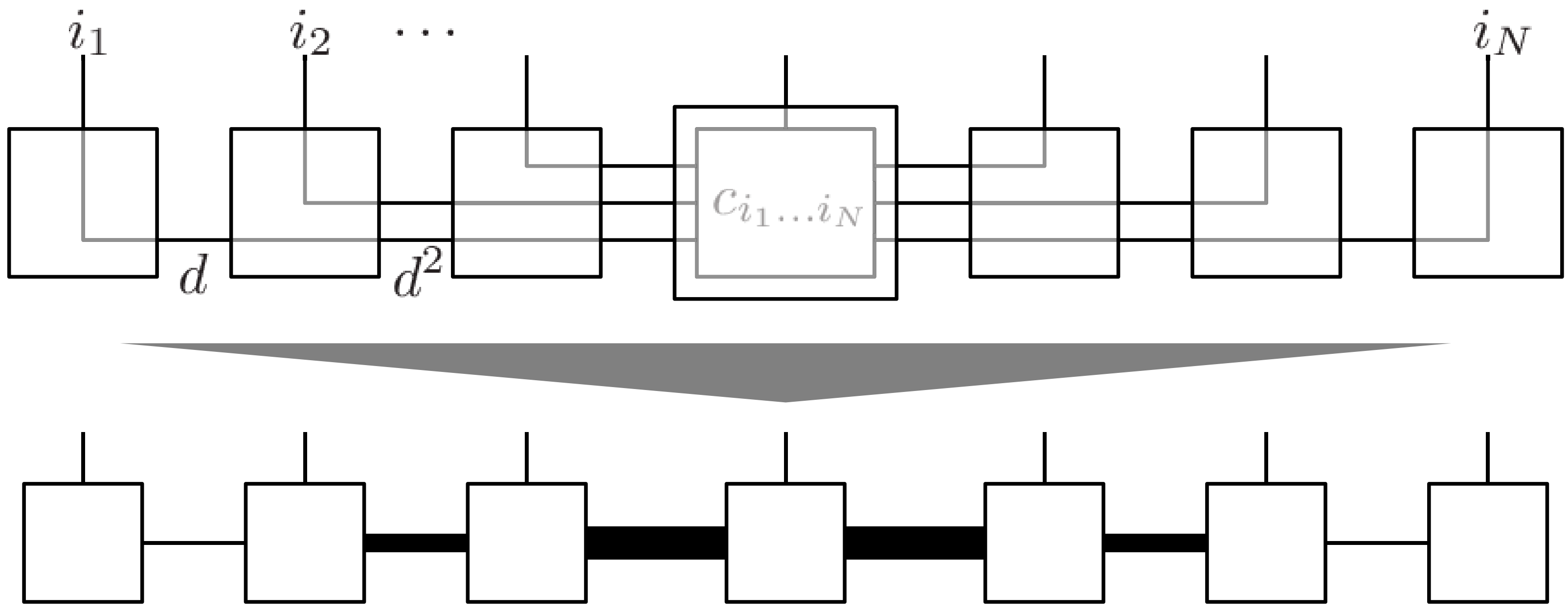
- MPS ↔ states which can be prepared with a **sequential scheme**, e.g. a beam of atoms going through a cavity:



When can we write state as MPS?

- Every state can be written as an MPS: $|\psi\rangle = \sum c_{i_1\ldots i_N}|i_1,\ldots,i_N\rangle$



- state with **entropic area law*** $S_\alpha(\rho_L) \leq S_{\max}$
  → efficient **MPS approximation** exists!

$$\||\Psi\rangle - |\mathrm{MPS}(D)\rangle\| \leq \text{const} \times \frac{N \;\; e^{c_\alpha S_{\max}}}{D^{c_\alpha}}$$

size N : linear scaling (poly if $S_{\max} \sim \log N$)

constant accuracy: $D \propto N^{1/c_\alpha}$

- Hastings '07: 1D gapped systems exhibit an area law!

A short wrap-up on MPS

- Matrix Product States: ansatz for 1D system of N d-level systems $(\mathbb{C}^d)^{\otimes N}$

$A^{[s],i}_{\alpha\beta}$

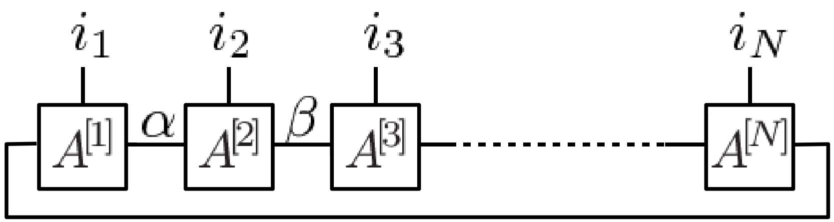
$s = 1, \ldots, N$: site index

$i = 0, \ldots, d-1$: physical system (physical index)

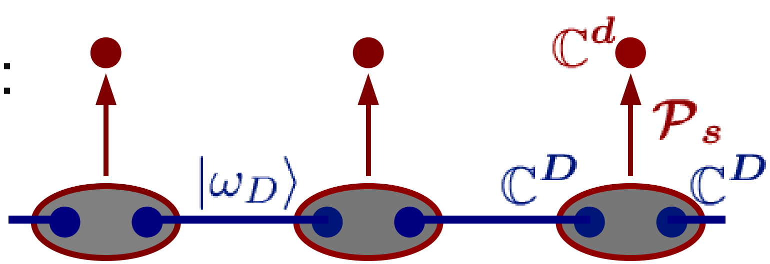
$\alpha, \beta = 0, \ldots, D-1$: left/right virtual system ("bond")

- Matrix Product notation: $|\psi\rangle = \sum_{i_1,\ldots,i_N} \mathbf{tr}[A^{[1],i_1} A^{[2],i_2} \ldots A^{N,i_N}] |i_1, \ldots, i_N\rangle$

- Tensor Network notation:



- construction with bonds:



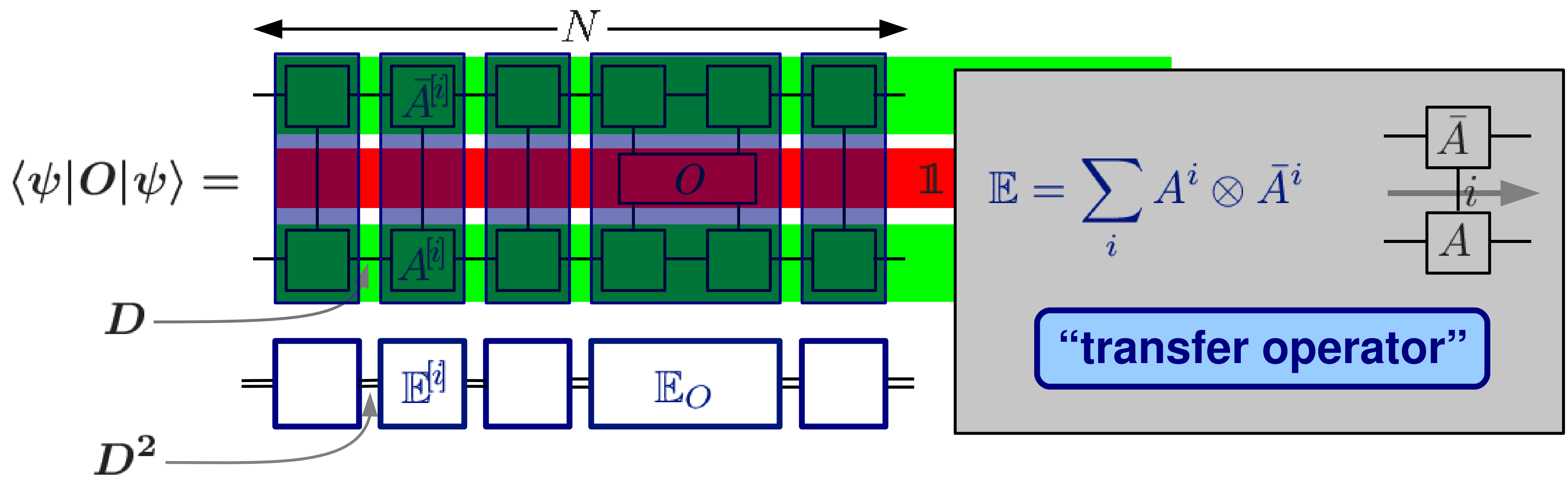
$|\omega_D\rangle = \sum_{i=0}^{D-1} |i, i\rangle$

$\mathcal{P}_s = \sum_{i\alpha\beta} A^{[s],i}_{\alpha\beta} |i\rangle\langle\alpha, \beta|$

- **good approximation** for **ground states** of 1D systems
- **bond dimension** D serves as a tuning parameter to **enlarge class** of states

Computing with MPS

- Given an MPS $|\psi\rangle$, can we compute exp. values $\langle\psi|O|\psi\rangle$ for local O ?



$$\langle\psi|O|\psi\rangle = \mathbf{tr}[\mathbb{E}^{[1]}\mathbb{E}^{[2]}\cdots\mathbb{E}^{[k-1]}\,\mathbb{E}_O\,\mathbb{E}^{[k+2]}\cdots\mathbb{E}^{[N]}]$$

- computing $\langle\psi|O|\psi\rangle$ = multiplication of $D^2{\times}D^2$ matrices

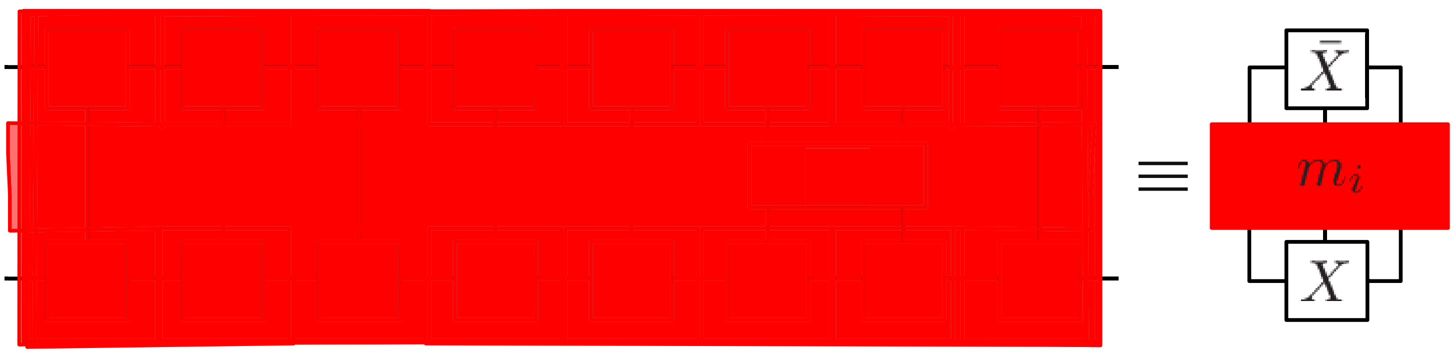
  $\rightarrow$ computation time $\propto N \cdot D^6 = \mathrm{poly}(N)$
- OBC scaling: D^4 [and if done properly, even D^5 (PBC) and D^3 (OBC)]
- works also for **correlation functions**, string order parameters, etc.

Numerical simulations with MPS

- MPS as **variational ansatz**: find MPS $|\psi\rangle \equiv |\psi[A^{[1]},\dots,A^{[N]}]\rangle$ (fixed D)

  which minimizes $E(|\psi\rangle) = \dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \sum_i \dfrac{\langle\psi|h_i|\psi\rangle}{\langle\psi|\psi\rangle}$

- Optimize **one tensor $A^{[s]} =: X$ at a time**



$\equiv \vec{X}\cdot m_i \vec{X}$

$\rightarrow$ minimize $\boldsymbol{E(X)} = \dfrac{\langle\psi[X]|H|\psi[X]\rangle}{\langle\psi[X]|\psi[X]\rangle} = \dfrac{\vec{X}\cdot M\vec{X}}{\vec{X}\cdot N\vec{X}}$ over X

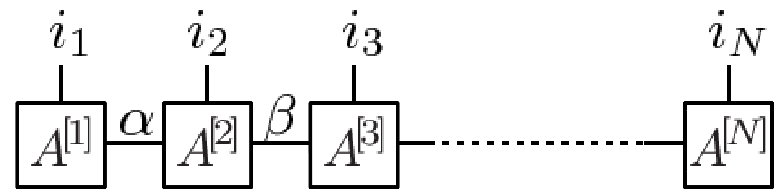
- generalized eigenvalue problem $M\vec{X} = \lambda N\vec{X}$ $\rightarrow$ efficiently solvable!

- DMRG algorithm: Repeatedly sweep through lattice & optimize

  [Density Matrix Renormalization Group – White, '92]
- converges very quickly
- does (typically) not get stuck in local minima [but hard instances exist!]
- approximation error for local observables: typ. $\sim \exp[-D]$

Wrap-up: Matrix Product States & simulations

- **Matrix Product States (MPS)**:
  efficient description of ground states
  of (gapped) 1D systems

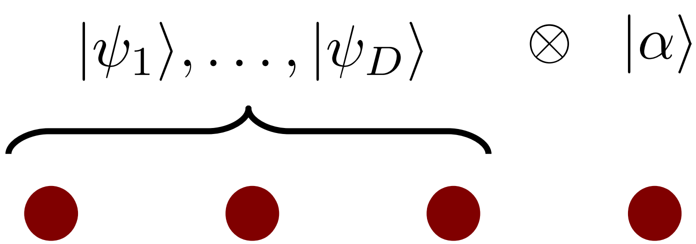


- expectation values of **local observables**, correlation functions etc.
  can be **computed efficiently**

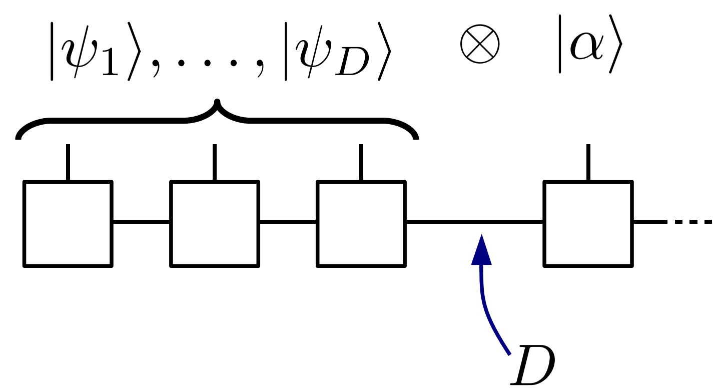
- can be used to build **variational method: DMRG**

- relation to **Wilson RG (NRG)**:

<u>NRG</u>: keep D states with lowest energy for given block

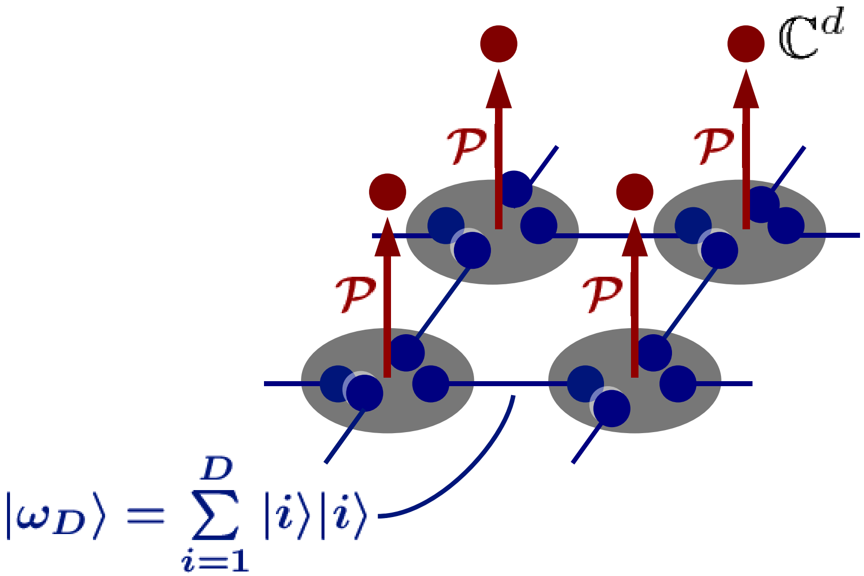


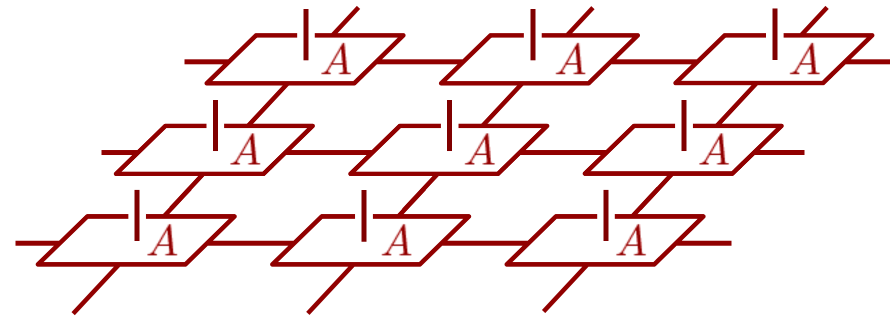
<u>DMRG</u>: keep D states most important for ground state entanglement



Projected Entangled Pair States

- Natural generalization of MPS to two dimensions:



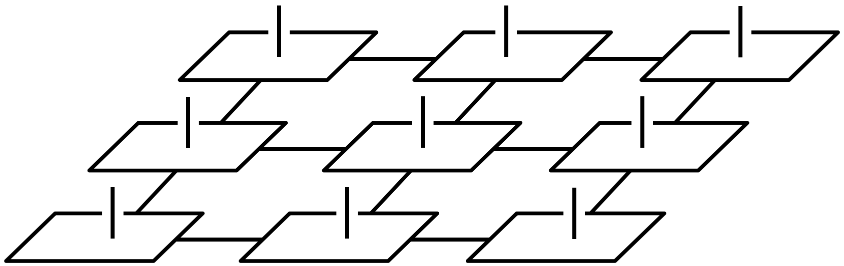


Projected Entangled Pair States (PEPS)

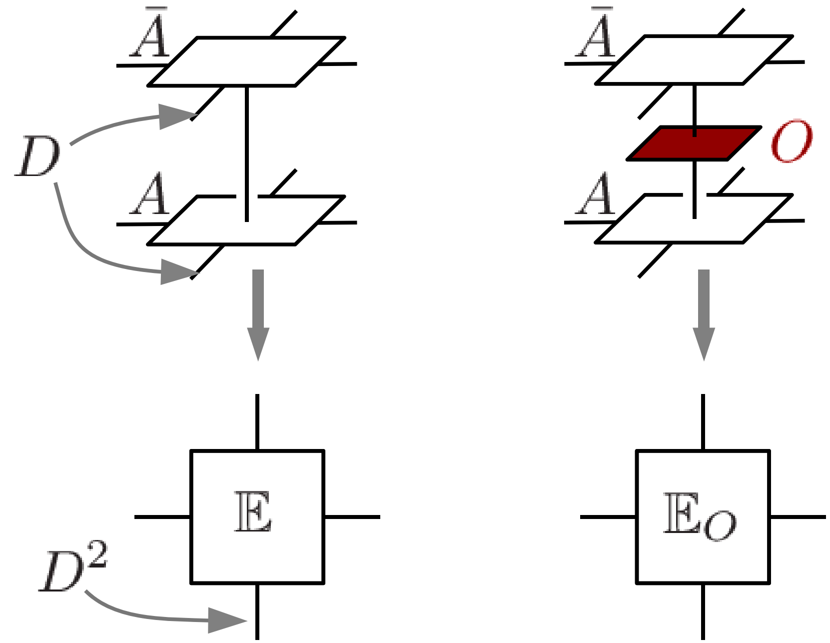
- **approximate ground/thermal states** of local Hamiltonians well
- PEPS form a **complete family** with accuracy parameter D.
- PEPS appear as **exact ground states** of local Hamiltonians
  $\rightarrow$ can be used to construct **exactly solvable models**

Computing expectation values for PEPS

- Can we compute expectation values (energy, correlation functions)?



- Use **transfer operators** $\mathbb{E}\,,\ \mathbb{E}_O$:



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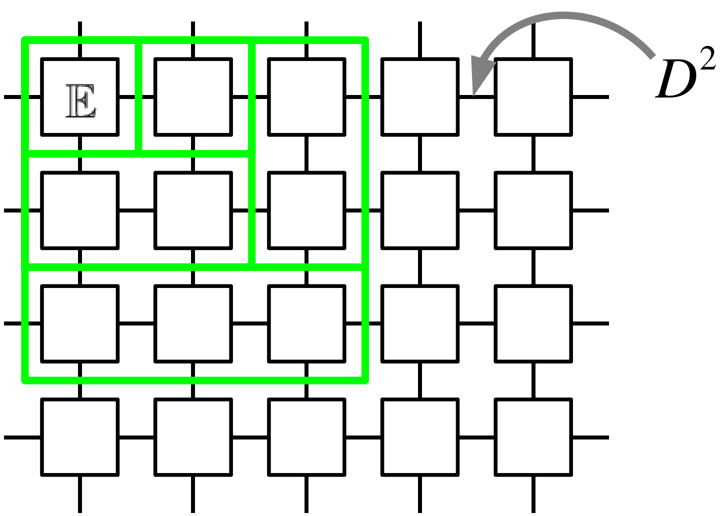

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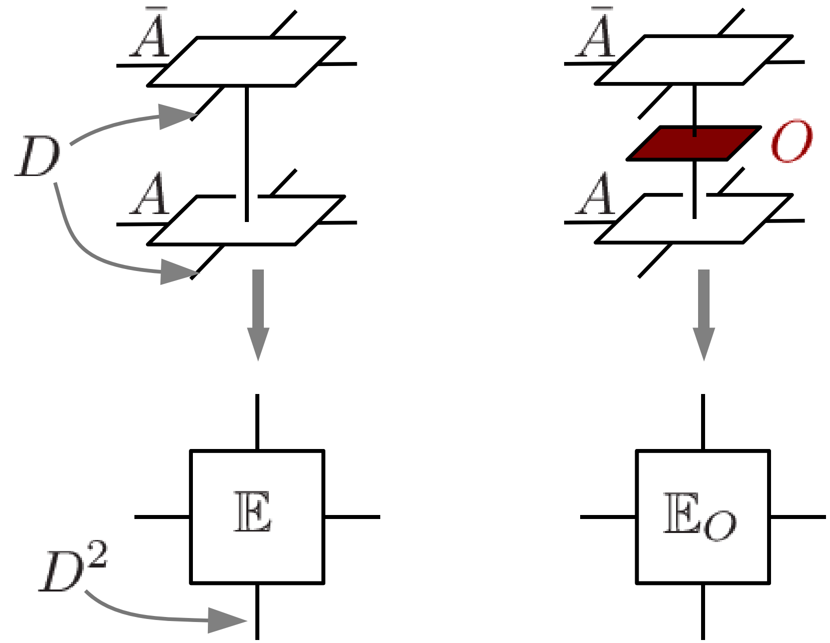
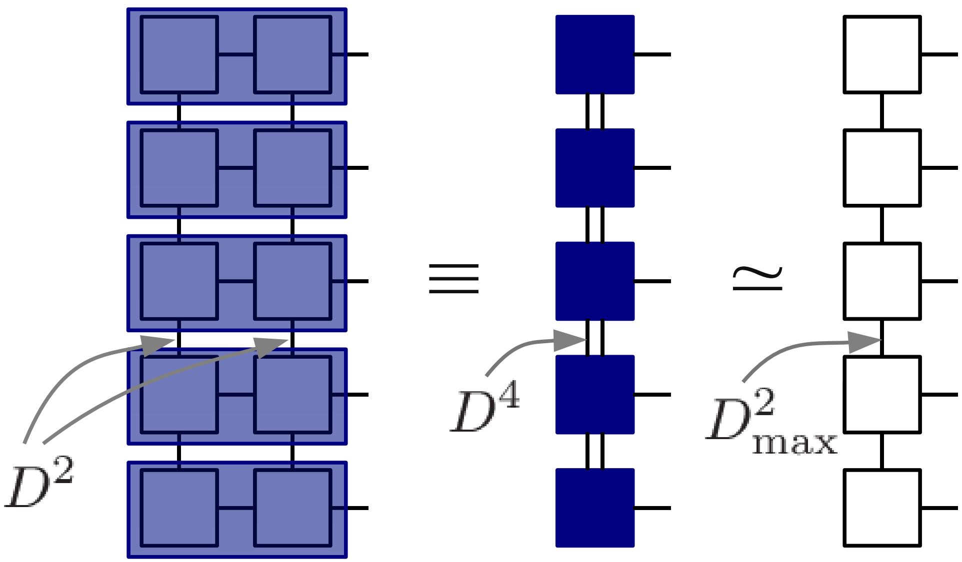


- Need to keep track of all **indices at the boundary**
  $\rightarrow$ contraction requires to store **exponentially large tensor**
- Contracting PEPS **computationally hard** (**#P**, the "counting version" of **NP**)
- Numerical calculations require **approximation methods**!

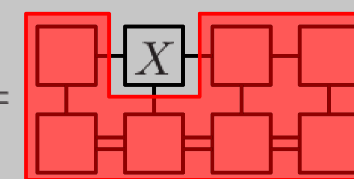
Approximate contraction of PEPS

- Solution: proceed column-wise and truncate the bond dimension



- $D^4 \to D^2_{\max}$: either **truncation** or find **best MPS approximation**

best MPS approximation:

$\langle \Psi_{D^4} | \Psi_{\alpha D^2} \rangle =$ 

linear in X , iterate as in DMRG

- Allows for **approximate contraction** of PEPS
- **Error** in approximation is **known** (and, in practice, very small)!
- Can be used to build **variational algorithms** for 2D systems
- Computational resources scale like D^8

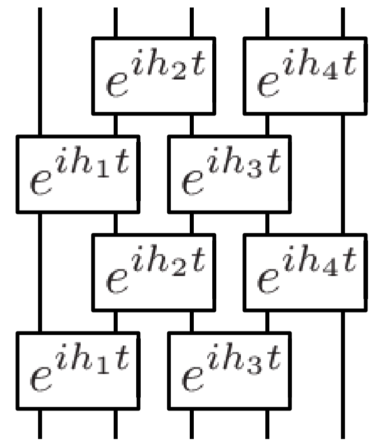
Simulation of time evolution with MPS

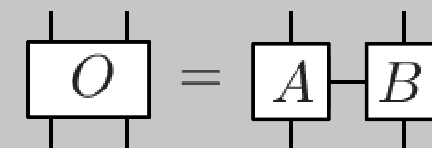
- Can we use MPS for simulating **time evolution**?

$$|\psi(t)\rangle = e^{iHt}|\psi(0)\rangle$$, with initial state $|\psi(0)\rangle$ MPS, and $H = \sum h_i$

- Trotter expansion:

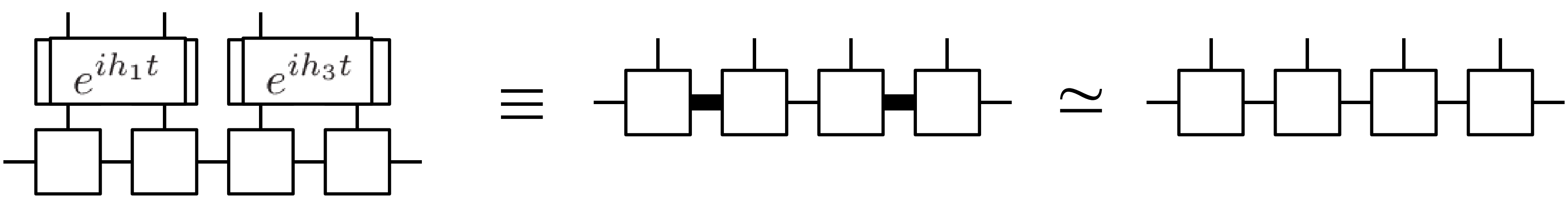
$$e^{iHt} = \left[e^{iH\delta t}\right]^N$$
$$\approx \left(\exp[i \sum_{\text{even}} h_i \delta t] \exp[i \sum_{\text{odd}} h_i \delta t]\right)^N$$





$$O = \sum_i A_i \otimes B_i$$

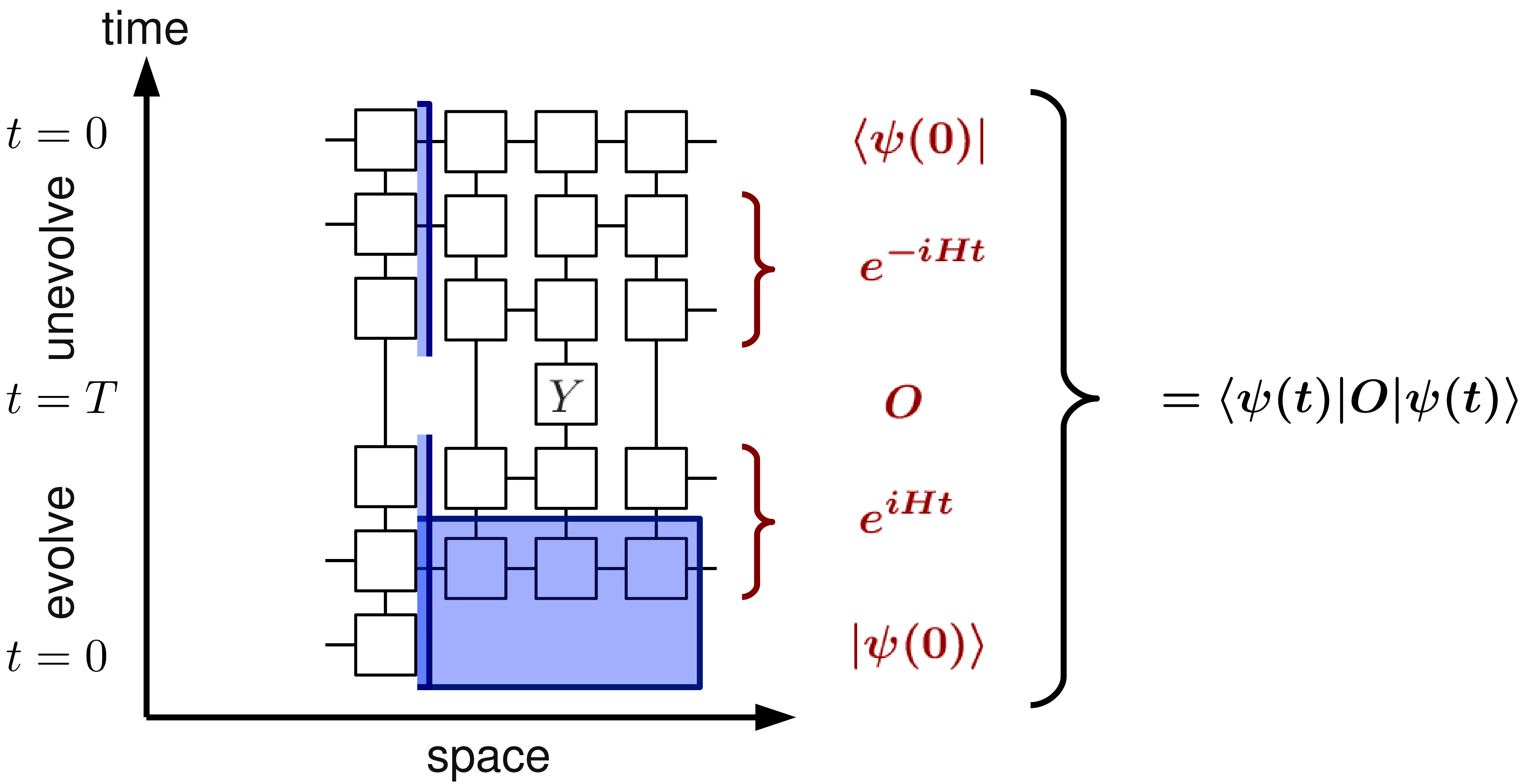
- Iterate: **Evolve** $|\psi(t)\rangle$ **for** δt and **approximate by MPS** with original D :



- Also useful for ground states (imag. time evol. $e^{-\beta H}|\chi\rangle \to |\Psi_0\rangle$ for $\beta \to 0$)

Entropy growth & alternative contraction

- State $|\psi(t)\rangle$ at all times **described by an MPS**
- Problem: **Entropy** in time evol. typically **grows linearly** (and $D \sim \exp[S]$!).
- solution: **contract in space direction**, not in time direction!

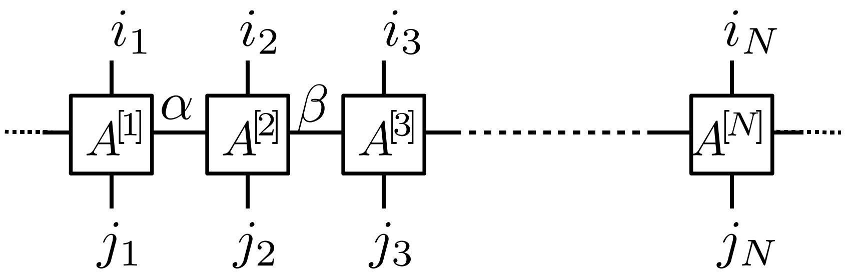


Thermal states, excited states

- Simulation of **thermal states** with MPS:

$$\rho = \sum c^{j_1,\ldots,j_N}_{i_1,\ldots,i_N} |i_1,\ldots,i_N\rangle\langle j_1,\ldots,j_N|$$

with $c^{j_1,\ldots,j_N}_{i_1,\ldots,i_N} =$



"Matrix Product Density Operator" (MPDO)

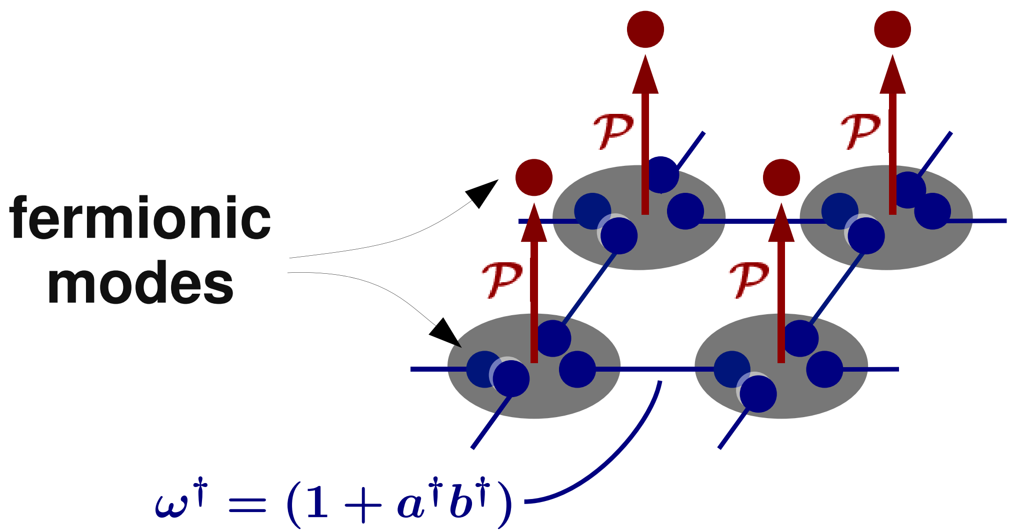
- Write $\boldsymbol{\rho = e^{-\beta H/2}\mathbb{1}e^{-\beta H/2}}$ and proceed like for time evolution!

- Simulation of **excited states** with MPS:
  - find ground state $|\Psi_0\rangle$
  - minimize $\langle\Psi_1|H|\Psi_1\rangle$ subj. to $\langle\Psi_0|\Psi\rangle_1 = 0$ (linear constraint)

Simulating fermionic systems

- can we use similar ideas to simulate **fermionic systems**?
- 1D: fermionic systems $\leftrightarrow$ spin systems (Jordan-Wigner transformation)

- 2D: construct **fermionic PEPS (fPEPS)**:



$$\mathcal{P} = \sum A^i_{\alpha\beta\gamma\delta} (\hat{p}^\dagger)^i (\hat{a})^\alpha (\hat{b})^\beta (\hat{c})^\gamma (\hat{d})^\delta$$

$\mathcal{P}$ maps virtual fermionic modes $\hat{\alpha}, \hat{\beta}, \hat{\gamma}, \hat{\delta}$ to physical mode $\hat{p}$

$\mathcal{P}$ has fixed parity

fPEPS: $|\Psi\rangle = \langle \Omega_{\mathrm{virt}} | (\mathcal{P} \otimes \mathcal{P} \otimes \cdots)(\omega^\dagger \otimes \omega^\dagger \otimes \cdots) | \Omega_{\mathrm{virt}}, \Omega_{\mathrm{phys}} \rangle$

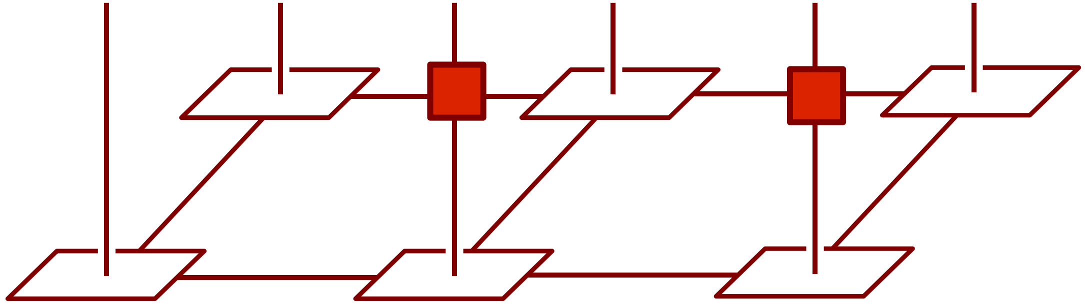
Computing with fermionic tensor networks

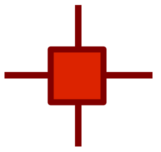
- Calculations with fermionic tensor networks:

  Need to keep track of **anticommutation relations**!

- Is **efficient computation** still possible? $\Rightarrow$ **Yes!**

- E.g., introduce fermionic swap tensors:



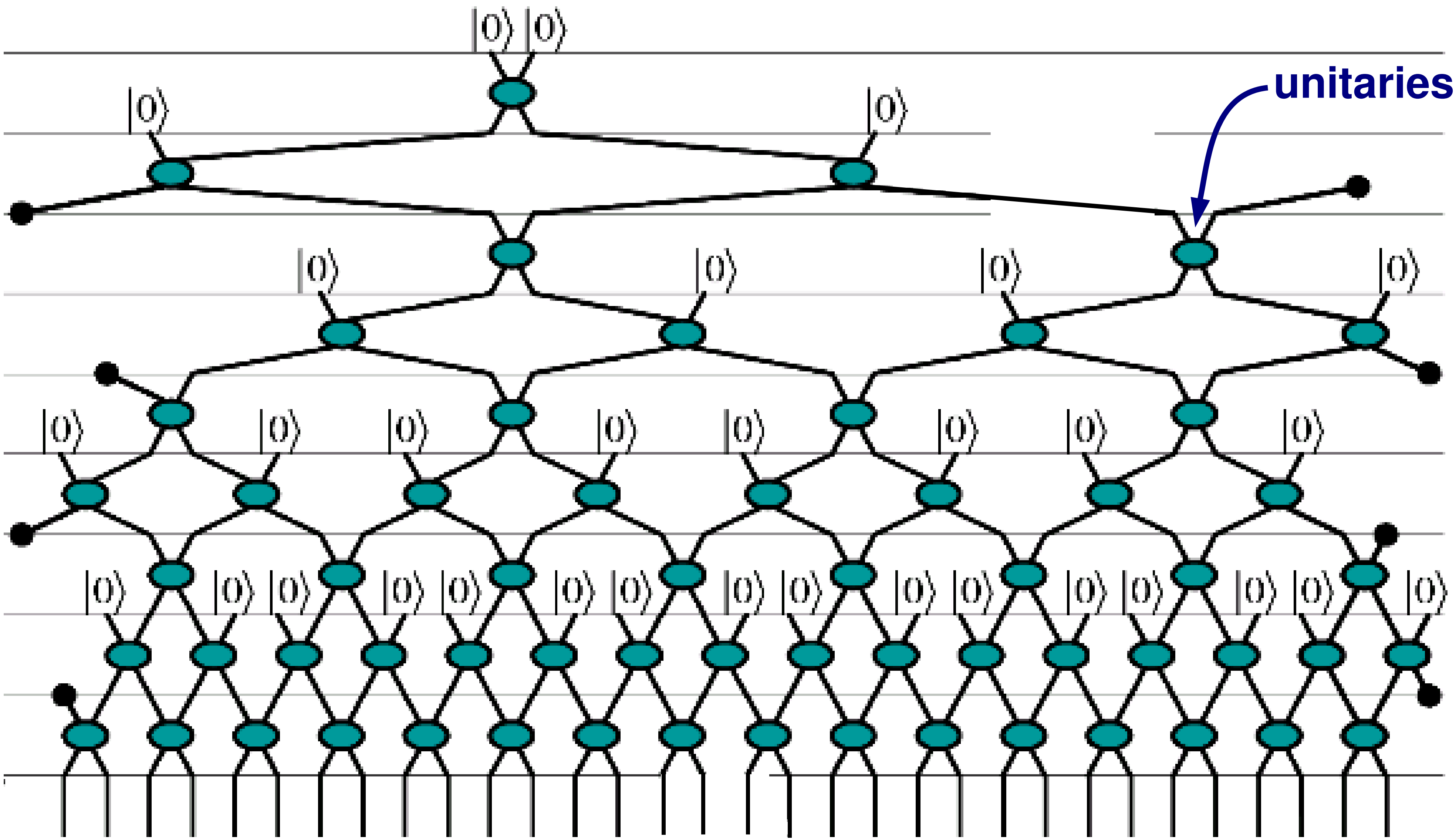


"fermionic swap":
crossing & (-1) if
both modes occupied

- Contract PEPS as before, but keep track of any swap occuring.

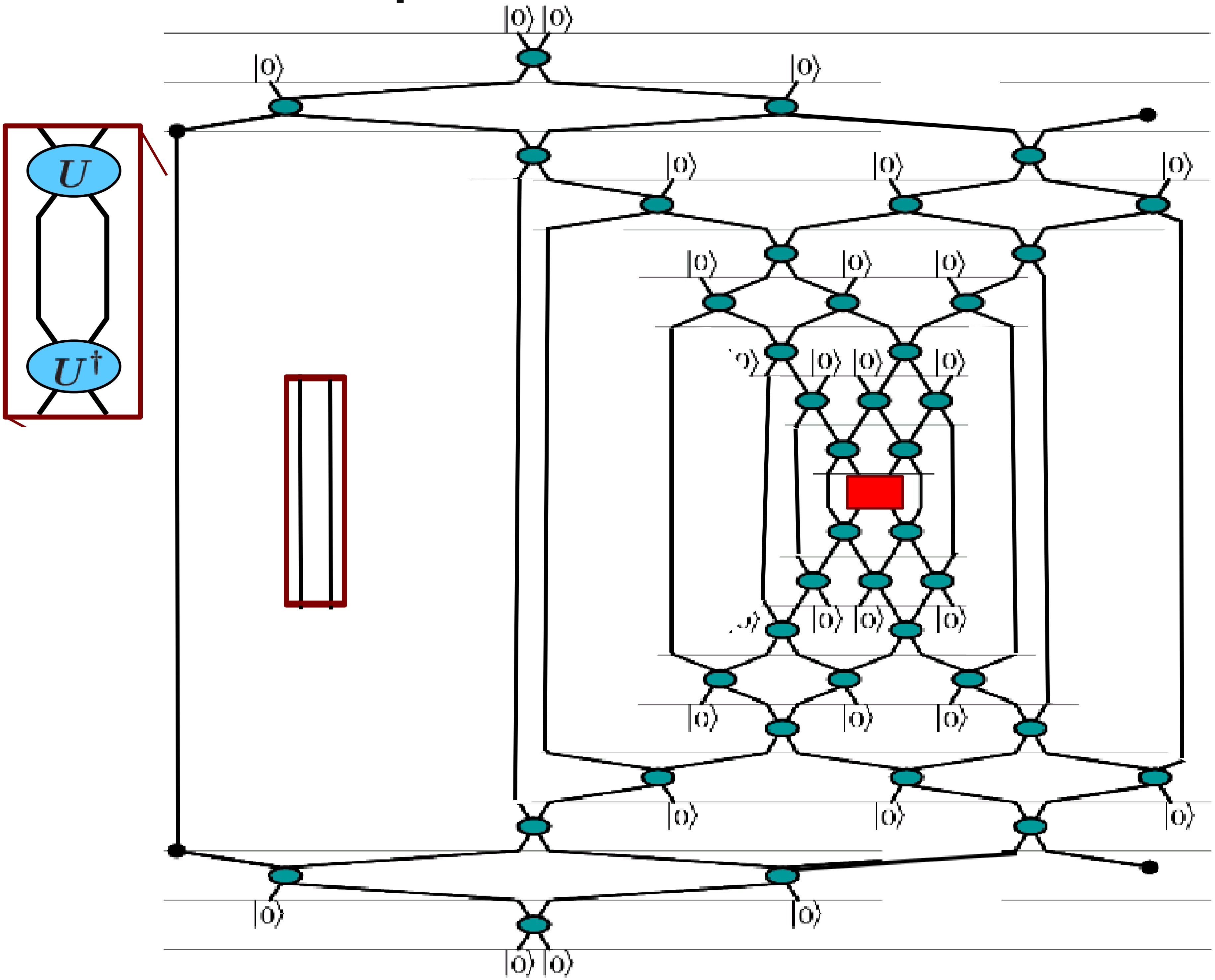
Unitary networks: MERA

- can we also model **scale-invariant critical systems** using tensor networks?



Multi-scale entanglement renormalization ansatz (MERA)

Expectation values for MERA



Conclusions

- **Matrix Product States (MPS)** and **Projected Entangled Pair States (PEPS)** approximate **ground states** of **local Hamiltonians** well
- MPS form the basis for an **efficient variational algorithm** (DMRG)
- beyond 1D (PEPS): variational method with **controlled approximations**
- extensions to **time evolution, thermal states, excitations, infinite systems**
- **fermionic statistics** can be naturally incorporated
- **MERA (Multi-scale entanglement renormalization ansatz)**:
  Tensor network ansatz for scale-invariant systems