Quantum Information and Quantum Many-body Systems

– Lecture 2 –

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Matrix Product States

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

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

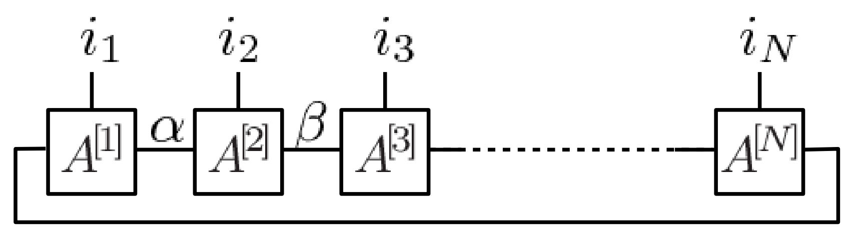
$s = 1, \ldots, N$: site index

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

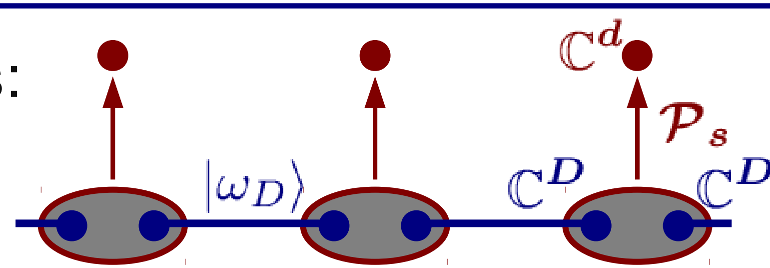
$\alpha, \beta = 0, \ldots, D-1$: left/right virtual system (indices)

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

- Tensor Network notation:



- construction with bonds:



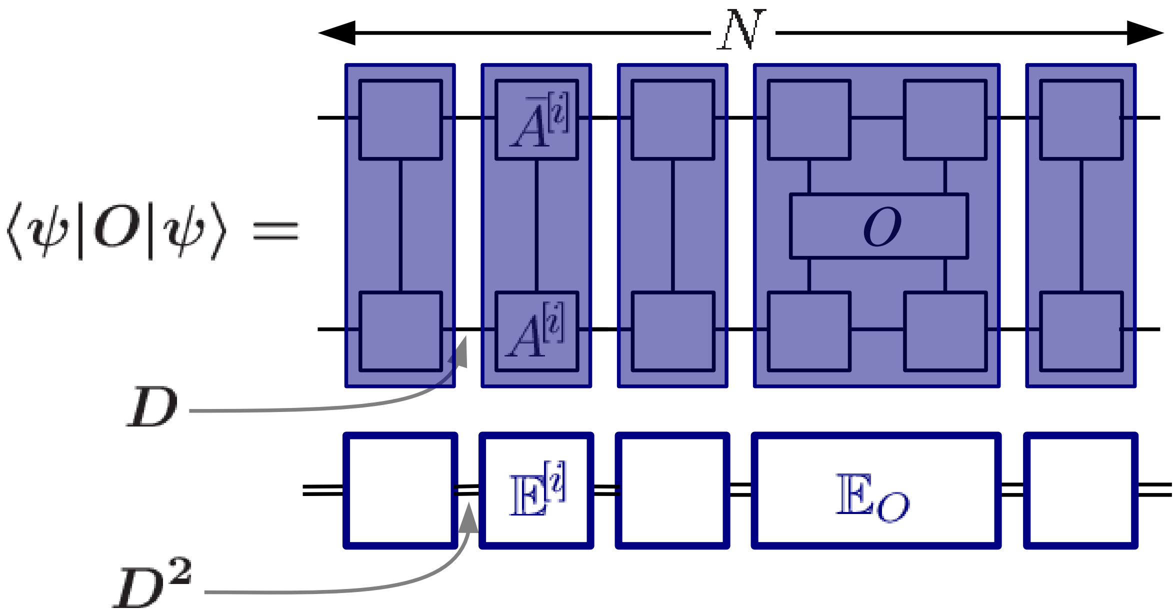
$|\omega_D\rangle = \sum_{i=0}^{D-1} |i, i\rangle$

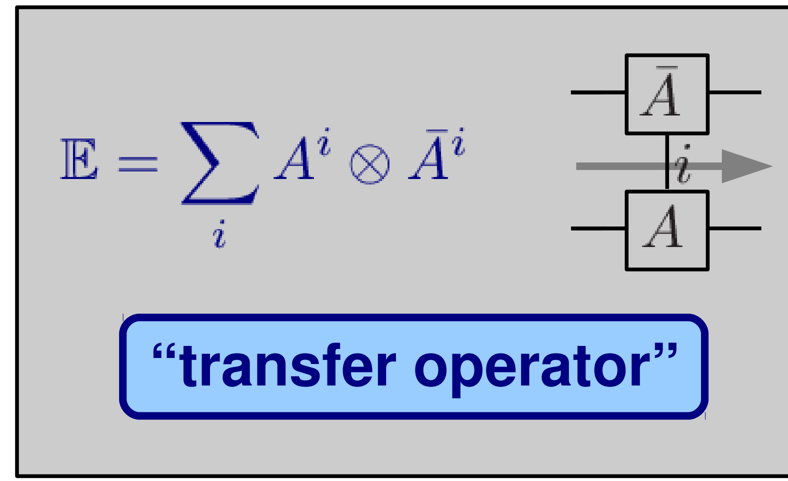
$\mathcal{P}_s = \sum_{i\alpha\beta} A^{[s],i}_{\alpha\beta} |i\rangle\langle\alpha, \beta|$

- **good approximation** for states with an **area law**, in particular **ground states** of **local Hamiltonians**, with $D = \mathrm{poly}(N)$
- D serves as a "tuning parameter" to **enlarge the class** of states
- for large enough D , any state can be written as an MPS

Computing with MPS

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





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

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

  $\rightarrow$ computation time $\propto N \cdot D^6 = \mathrm{poly}(N)$

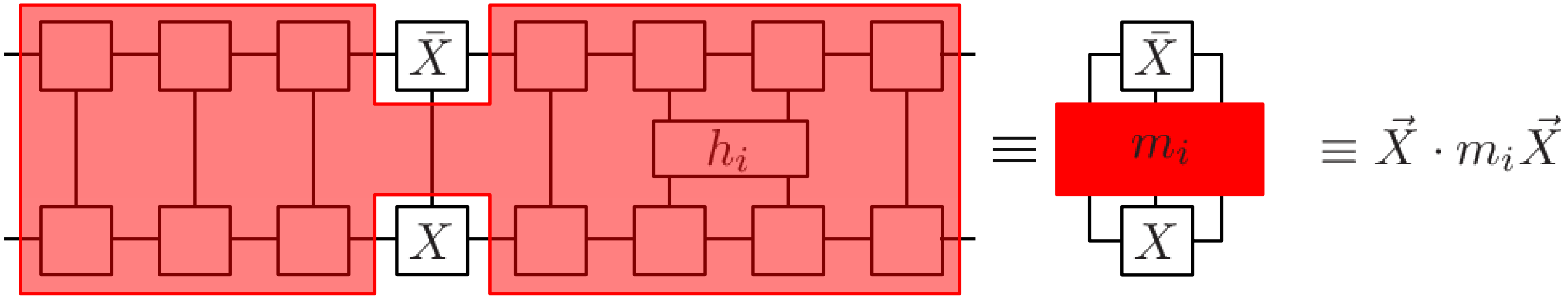
- OBC scaling: D^4 [and if done properly, even D^5 (PBC) and D^3 (OBC)]

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**



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

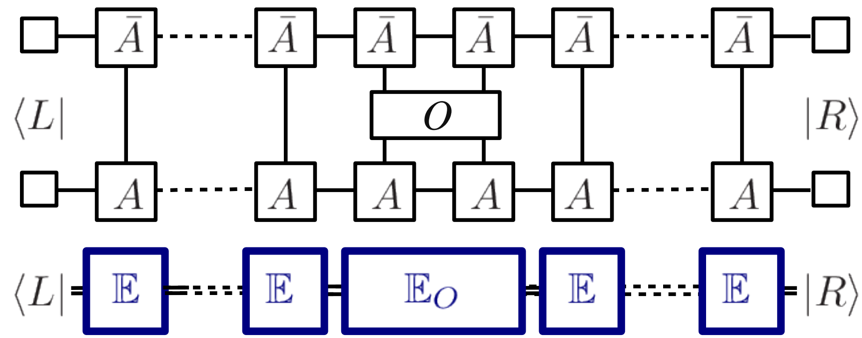
- generalized eigenvalue problem $M\vec{X} = \lambda N\vec{X}$ $\rightarrow$ efficiently solvable!

- DMRG algorithm: Repeatedly sweep through lattice & optimize

  [Density Matrix Renormalization group – White, '94]
- converges very quickly
- does (typically) not get stuck in local minima [but hard instances exist!]
- approximation error for local observables: typ. $\sim \exp[-D]$

Expectation values in infinite systems

- What about **infinite systems**?
- Translational Invariance (TI): $A^{[s]} \equiv A$

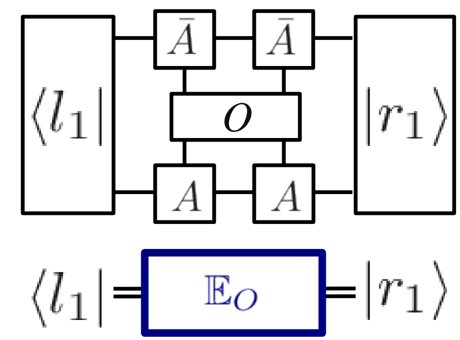


$$\frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle} = \lim_{N\to\infty} \frac{\langle L|\mathbb{E}^N \; \mathbb{E}_O \; \mathbb{E}^N|R\rangle}{\langle L|\mathbb{E}^N \; \mathbb{E}^2 \; \mathbb{E}^N|R\rangle}$$

- eigendecomposition (for simplicity, assume $|\lambda_1| > |\lambda_2| \geq \ldots$ & no Jordan blocks)

$$\mathbb{E} = \sum_k \lambda_k |r_k\rangle\langle l_k| \;\Rightarrow\; \mathbb{E}^N = \sum_k \lambda_k^N |r_k\rangle\langle l_k| \to \lambda_1^N |r_1\rangle\langle l_1|$$

$$\boldsymbol{\frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\langle l_1|\mathbb{E}_O|r_1\rangle}{\langle l_1|\mathbb{E}^2|r_1\rangle}}$$



- largest eigenvalue degenerate, $|\lambda_1| = |\lambda_2|$ etc.:
  dependency on boundary conditions $\langle L|$ and $|R\rangle$

- Allows to build **numerical methods** for infinite systems

Correlation functions

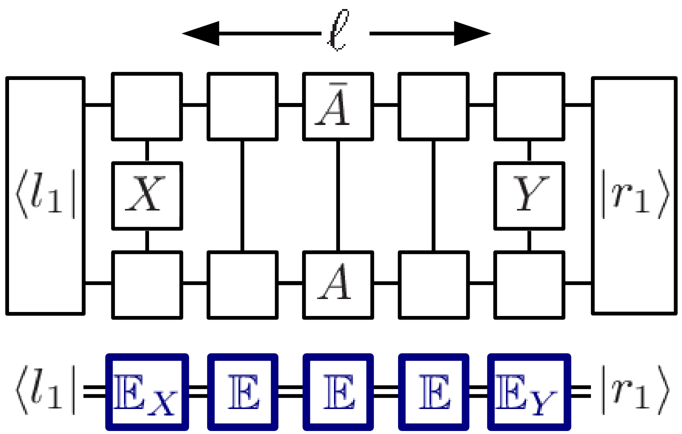
- How do correlation functions in (infinte, TI) MPS behave?

$$\langle X_i Y_j \rangle := \frac{\langle \psi | X_i Y_j | \psi \rangle}{\langle \psi | \psi \rangle}$$

and

$$C(X_i, Y_j) = \langle X_i Y_j \rangle - \langle X_i \rangle \langle Y_j \rangle$$

"connected correlation function"



$$\langle X_0 Y_{\ell+1} \rangle = \frac{\langle l_1 | \mathbb{E}_X \, \mathbb{E}^\ell \, \mathbb{E}_Y | r_1 \rangle}{\langle l_1 | \mathbb{E}^{\ell+2} | r_1 \rangle}$$

$$\mathbb{E}^\ell = \sum_k \lambda_k^\ell |r_k\rangle\langle l_k|$$

$$\propto \sum_k \left(\frac{\lambda_k}{\lambda_1} \right)^\ell \frac{\langle l_1 | \mathbb{E}_X | r_k \rangle \langle l_k | E_Y | r_1 \rangle}{\lambda_1^2}$$

- $|\lambda_k| = |\lambda_1|$: distance-independent **long-range correlations** (e.g.: GHZ state)
- $|\lambda_k| < |\lambda_1|$: **exponentially decaying correlations** $\sim e^{-\ell/\xi}$ $(\xi = -\log|\frac{\lambda_k}{\lambda_1}|)$
- there cannot be algebraically decaying correlations $\sim \ell^{-\beta}$

absolute value of **spectrum of** $\mathbb{E}$ →

- degenerate: long-range correlations
- ratio of largest & 2nd eigenvalue, λ and λ'
  $\leftrightarrow$ correlation length $\xi = -\log|\lambda'/\lambda|$
- no algebraic (=critical) decay of correlations