IPAM/UCLA, Sat 24th Jan 2009

# Numerical Approaches to Quantum Many-Body Systems

QS2009 tutorials

lecture:

# Tensor Networks


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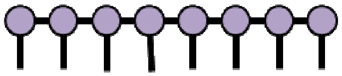
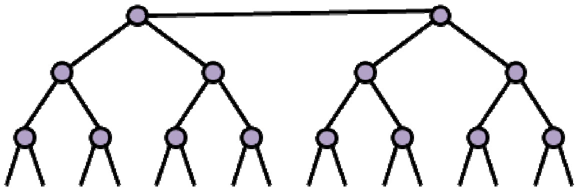
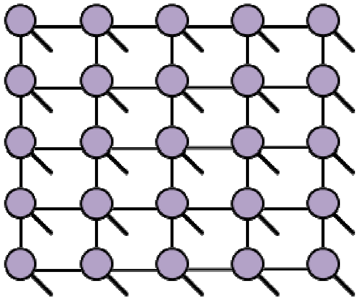
THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

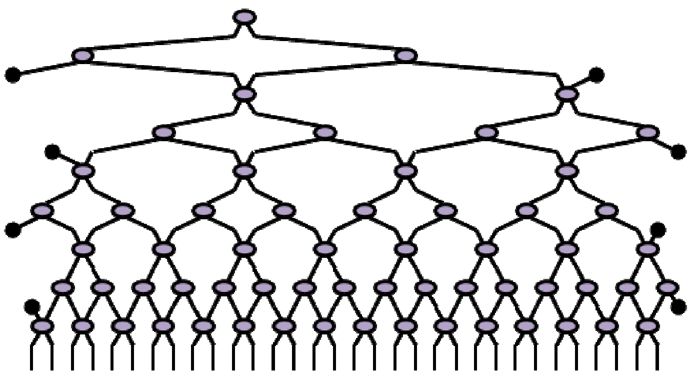
# Outline

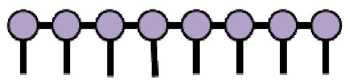


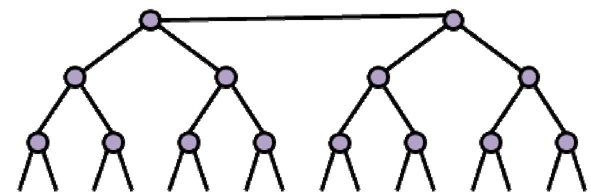


- Tensor Networks
- Computation of expected values
- Optimization of a tensor network
  (energy minimization, time evolution)





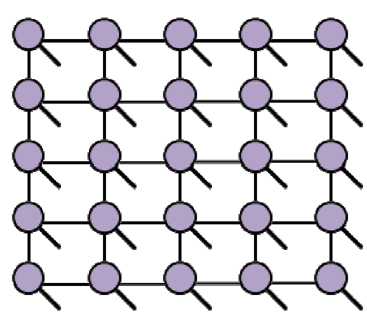


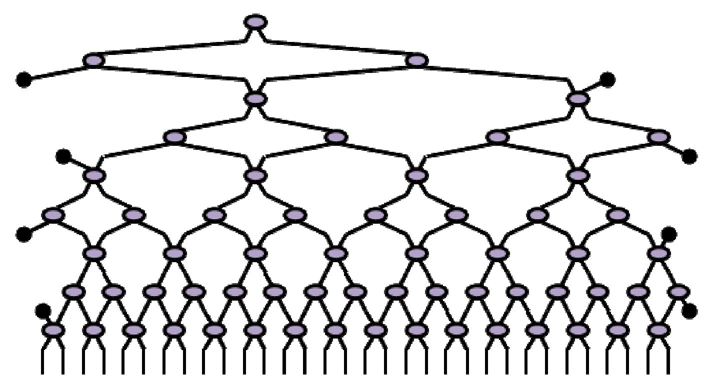


- Tensor Networks

- Computation of expected values

- Optimization of a tensor network
  (energy minimization, time evolution)



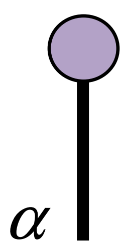


# Graphical representation of matrices/tensors

$$A = \begin{bmatrix} a_1 \\ a_2 \\ \mathrm{M} \\ a_m \end{bmatrix} \qquad B = \begin{pmatrix} b_{11} & \mathrm{K} & b_{1n} \\ \mathrm{M} & \mathrm{O} & \mathrm{M} \\ b_{m1} & \mathrm{L} & b_{mn} \end{pmatrix}$$

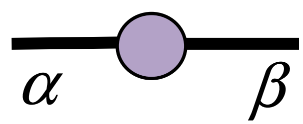
- vector

$$a_\alpha$$



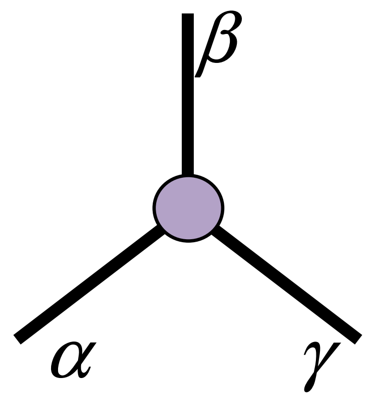

- matrix

$$b_{\alpha\beta}$$



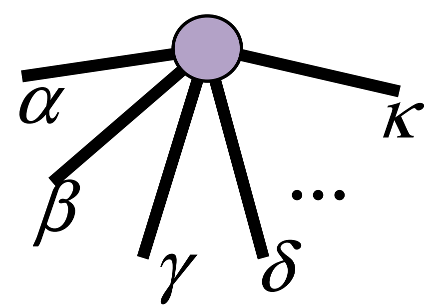

- rank 3 tensor

$$c_{\alpha\beta\gamma}$$




- rank p tensor

$$c_{\alpha\beta\gamma\mathrm{K}\,\kappa}$$

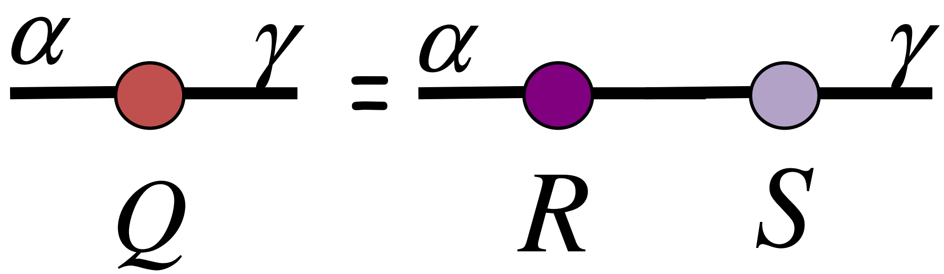


# Graphical representation of matrices/tensors

- product of tensors

$$Q = RS$$

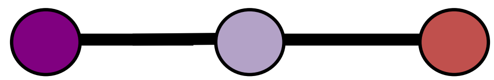
$$q_{\alpha\gamma} = \sum_{\beta} r_{\alpha\beta} s_{\beta\gamma}$$



# Graphical representation of matrices/tensors

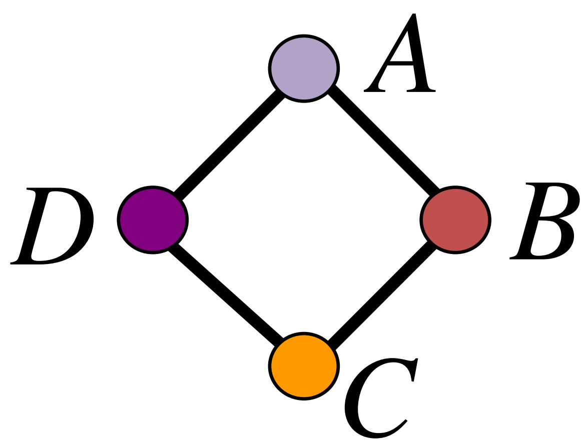
- other examples:

$$x^{\dagger} A y$$

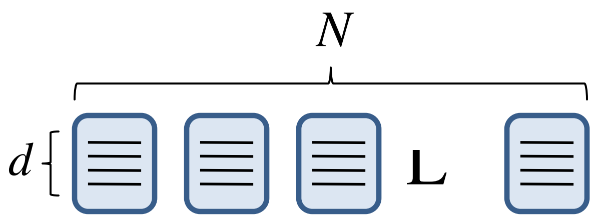


$$\sum_{\alpha\beta\gamma} c_{\alpha\beta\gamma} c^{*}_{\alpha\beta\gamma}$$


$$trABCD$$

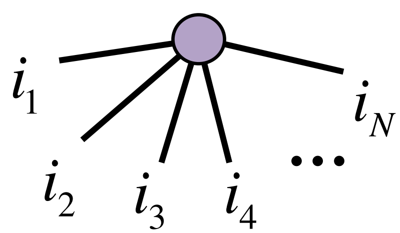


# Tensor Networks




$$H_1 \otimes H_2 \otimes \ldots \otimes H_N$$

$$\left|\Psi_{GS}\right\rangle = \sum_{i_1=1}^{d}\sum_{i_2=1}^{d} \mathrm{L} \sum_{i_N=1}^{d} c_{i_1 i_2 \ldots i_N} \left|i_1\right\rangle \left|i_2\right\rangle \ldots \left|i_N\right\rangle$$

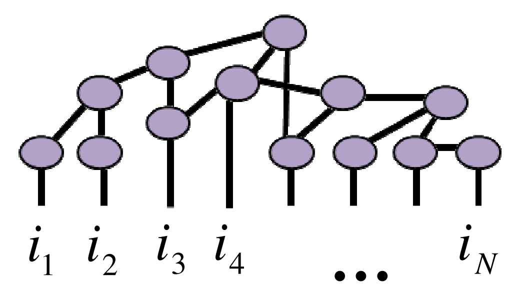



$d^N$ coefficients

Monte Carlo sampling

$O(N\beta)$ samples

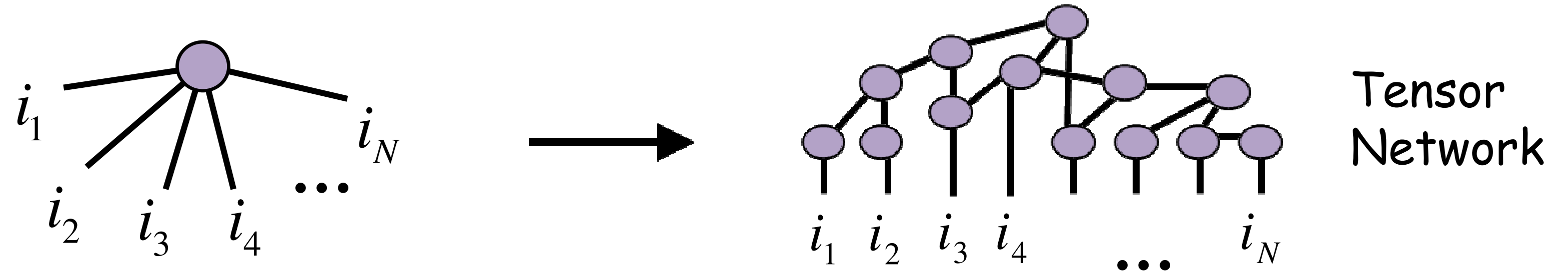
Tensor Network




$O(N)$ coefficients

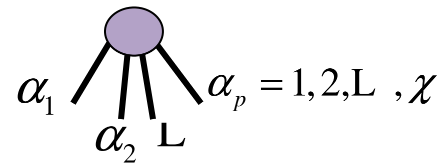
# Tensor Networks

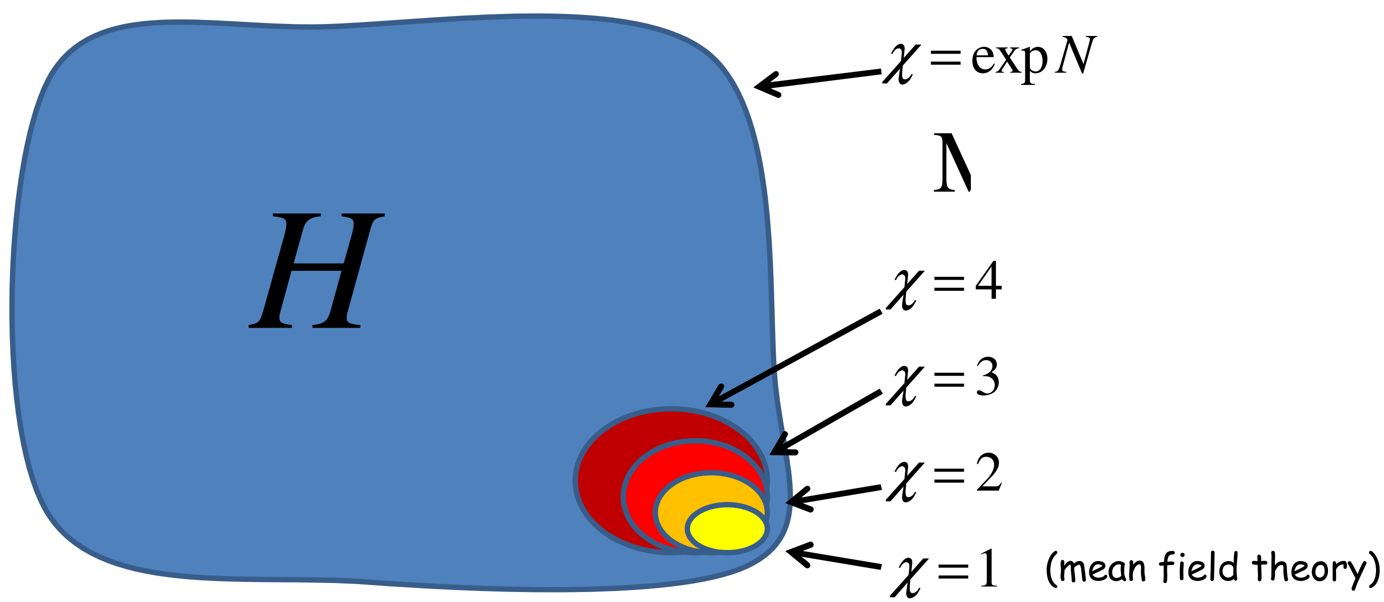
$$|\Psi_{GS}\rangle = \sum_{i_1=1}^{d}\sum_{i_2=1}^{d}\cdots\sum_{i_N=1}^{d} c_{i_1 i_2 \ldots i_N} |i_1\rangle|i_2\rangle\ldots|i_N\rangle$$




$d^N$ coefficients

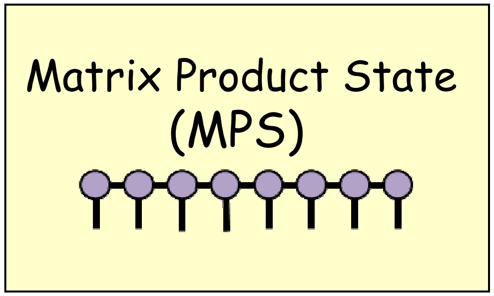
$O(N\chi^p)$ coefficients



# Tensor Networks

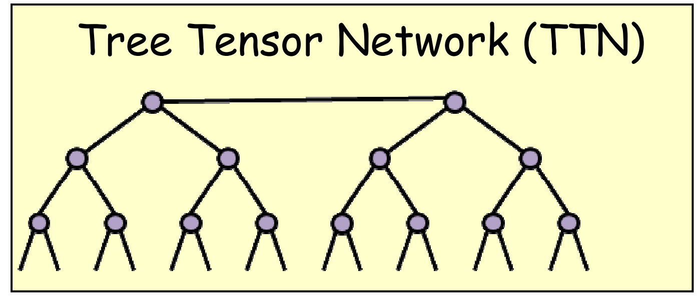
examples of tensor network representations:



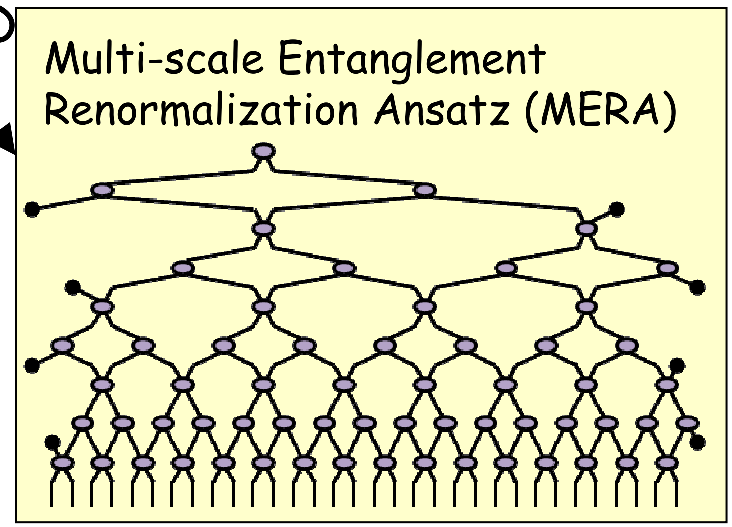

1D

Wilson (NRG) 1975
Fannes, Nachtergaele, Werner 1992
White 1992 (DMRG)
Oestlund, Rommer 1995
time evolution in 1D - 2003
...

1D/2D

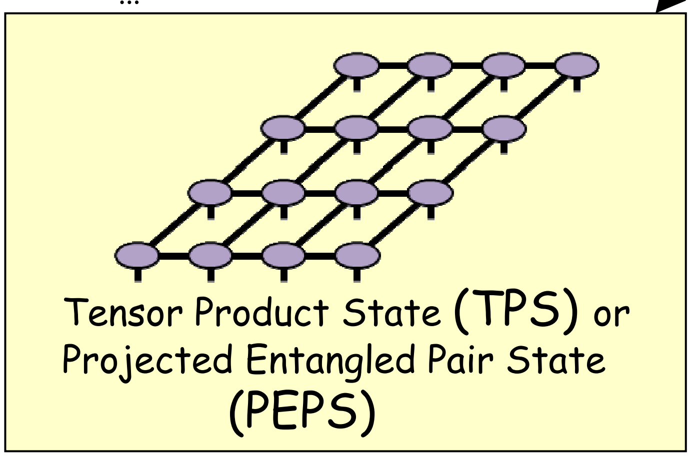



1D/2D




(next lecture!)

2D

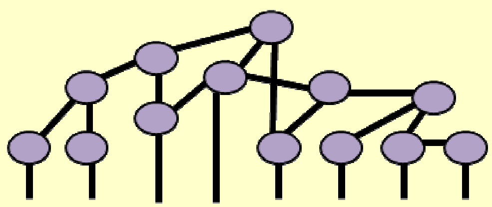



Nishino 2000
Verstraete, Cirac 2004
...

# What do we want to be able to do with a tensor network?

• efficient specification of the state

$$|\Psi\rangle = \sum_{i_1 i_2 \dots i_N} c_{i_1 i_2 \dots i_N} |i_1\rangle |i_2\rangle \dots |i_N\rangle$$



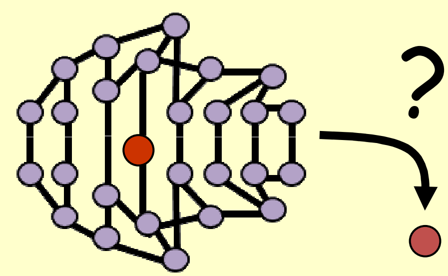
• efficient computation of expected values

$$\langle \Psi | \sigma^{[4]} | \Psi \rangle$$

$|\Psi\rangle$

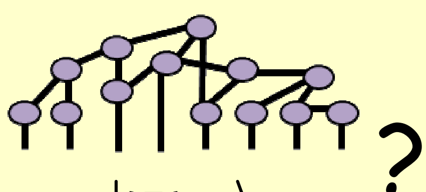
$\sigma^{[4]}$

$\langle \Psi |$



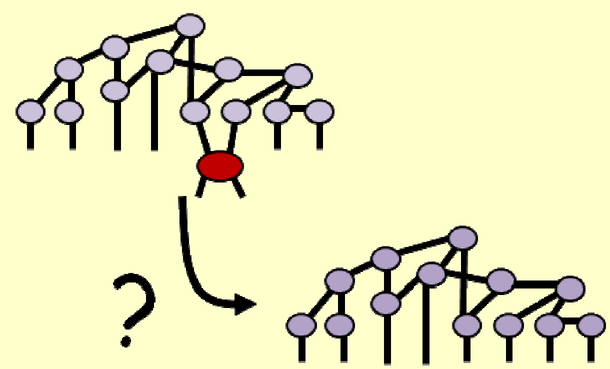
• efficient computation of states of interest:

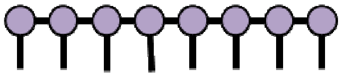
e.g. ground state

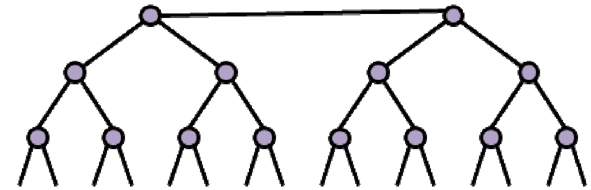


$|\Psi_{GS}\rangle$

• efficient simulation of time evolution



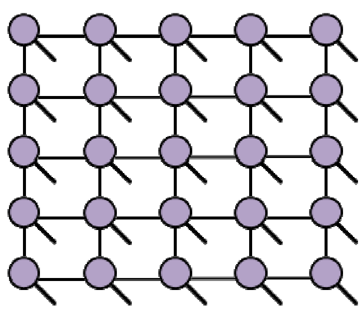


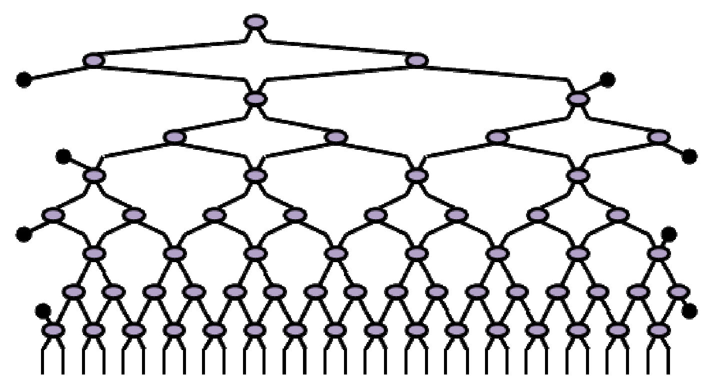


- Tensor Networks

- Computation of expected values

- Optimization of a tensor network
  (energy minimization, time evolution)





# Computation of expected values

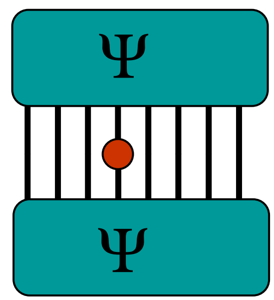
Example: $\langle \Psi_{GS} | \sigma_z^{[4]} | \Psi_{GS} \rangle$

Without a tensor network:

$|\Psi_{GS}\rangle$

$\sigma_z$

$\langle \Psi_{GS}|$




$\exp(N)$ operations

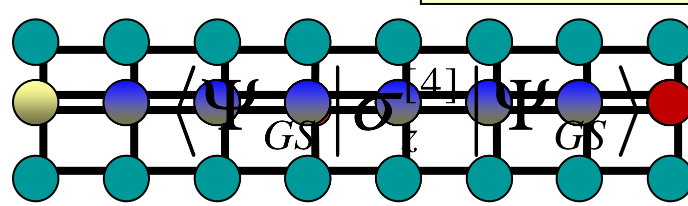
With a MPS:

$O(N\chi^q)$ operations

$|\Psi_{GS}\rangle$

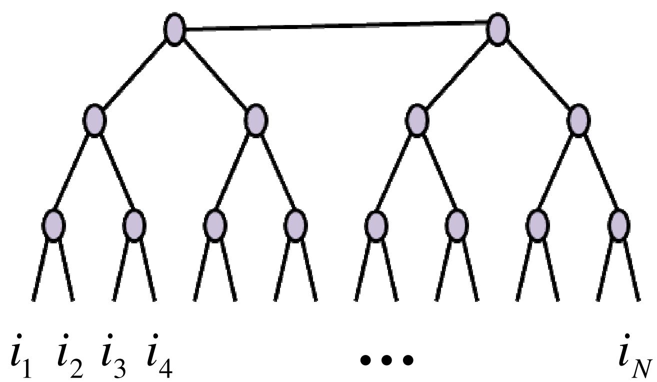
$\sigma_z$

$\langle \Psi_{GS}|$

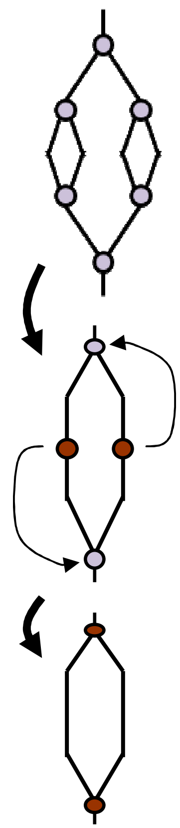


# Computation of expected values

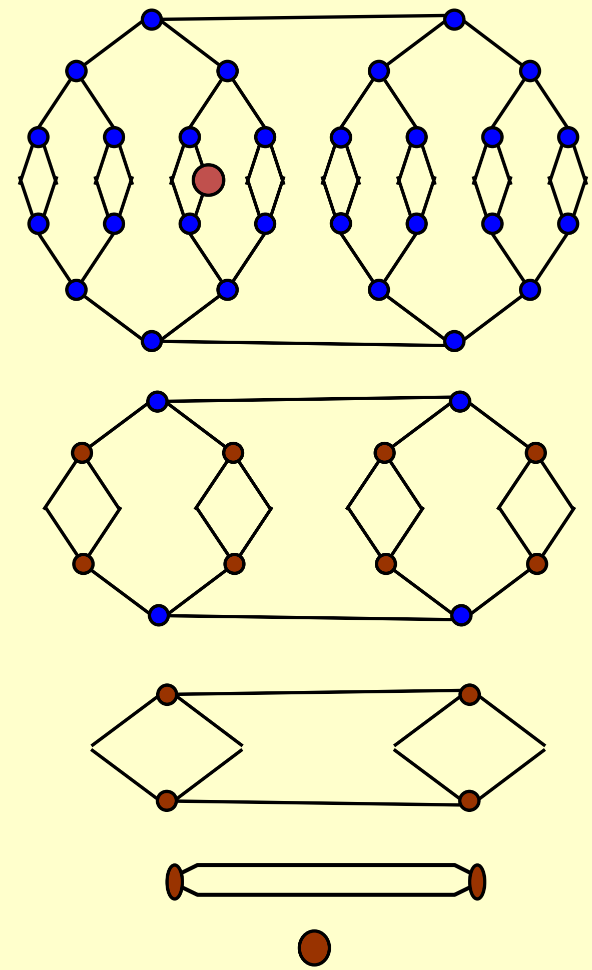
## With a TTN:



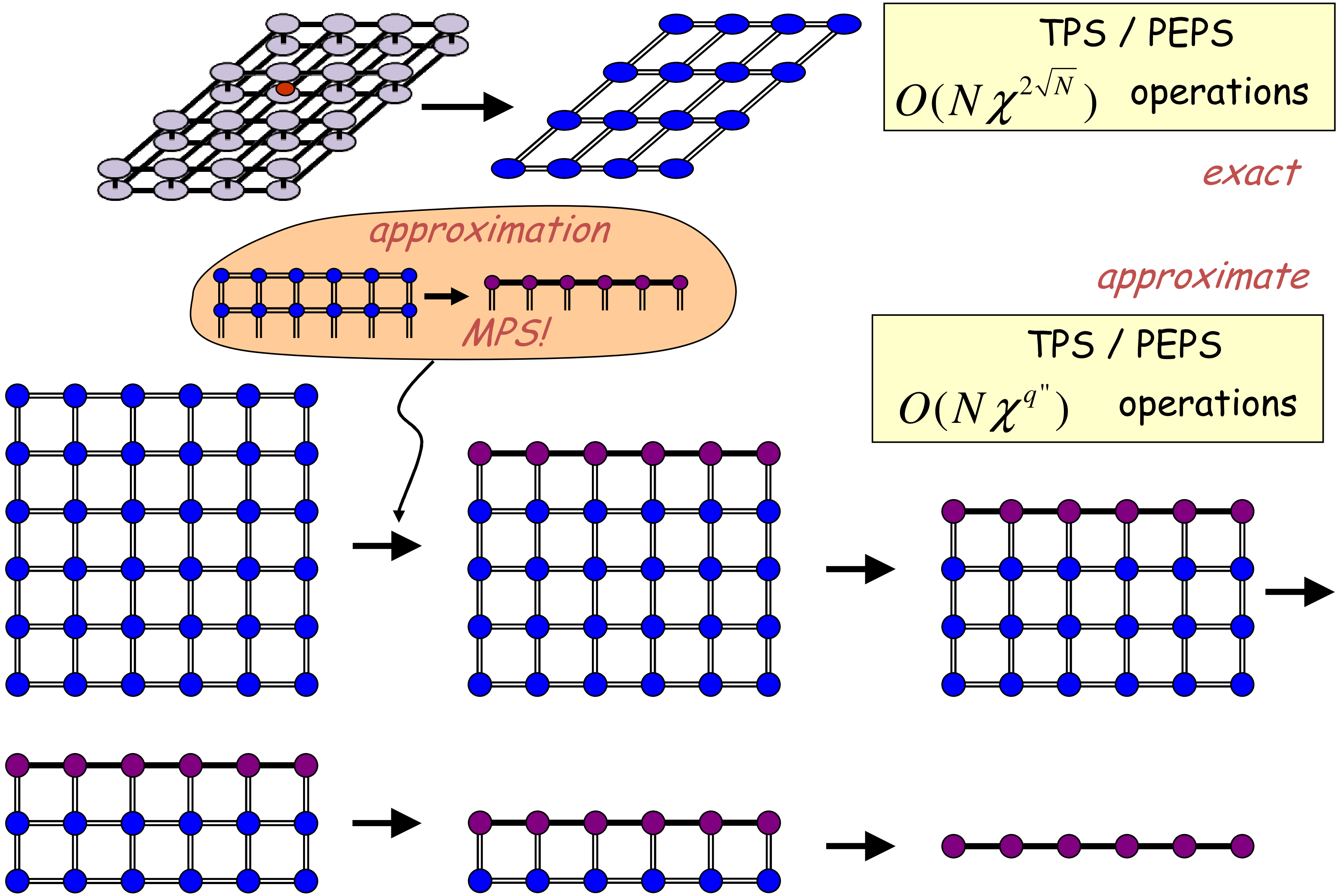

$O(N\chi^{q'})$ operations

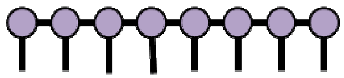


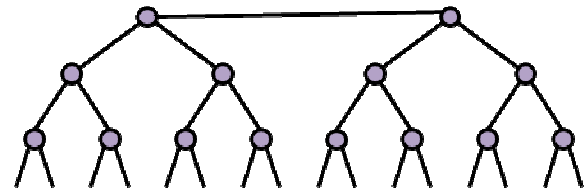
$$p_r = \langle \Psi | \sigma^{[6]} | \Psi \rangle$$



# Computation of expected values with a TPS/PEPS:



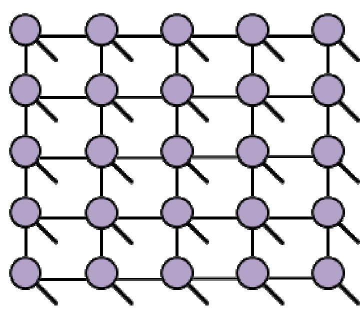


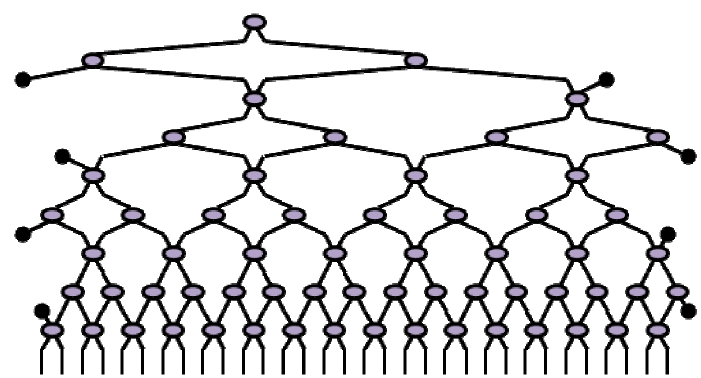


- Tensor Networks

- Computation of expected values

- Optimization of a tensor network
  (energy minimization, time evolution)





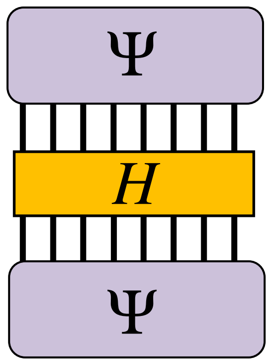
# Optimization of a tensor network

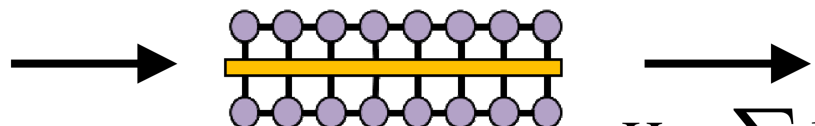
• Ground state $|\Psi_{GS}\rangle$ obtained from $\boxed{\min_{\Psi} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}}$

$|\Psi_{GS}\rangle$

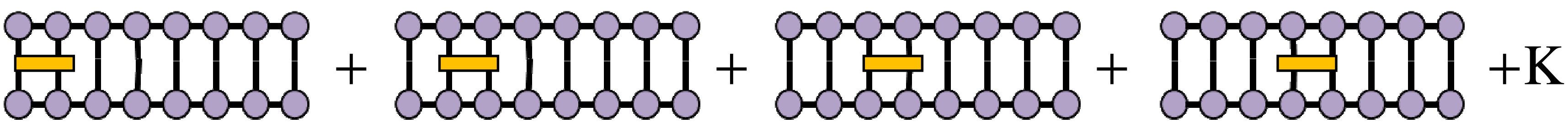
$H$

$\langle \Psi_{GS}|$



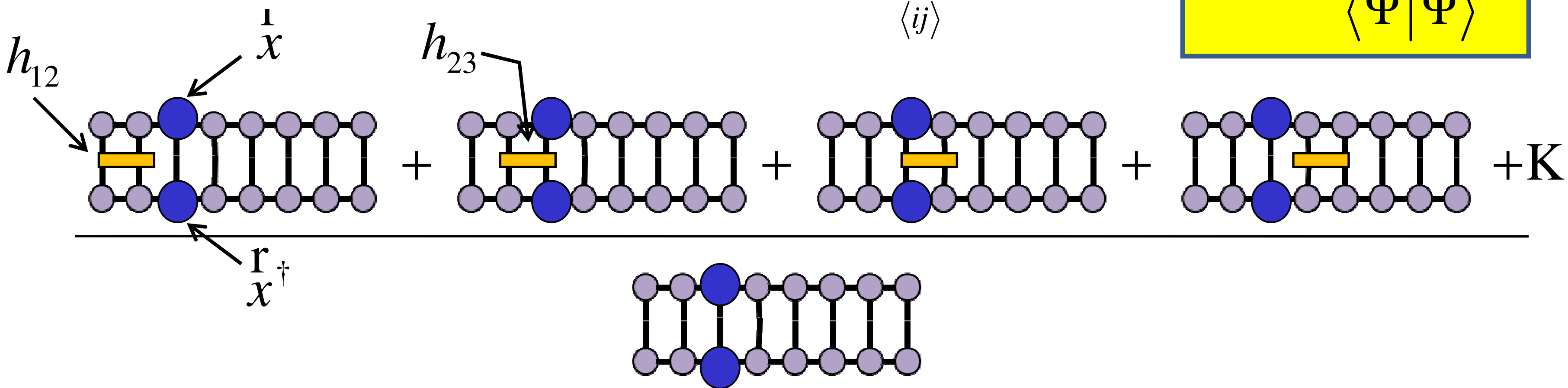
$$H = \sum_{\langle ij \rangle} h_{ij}$$

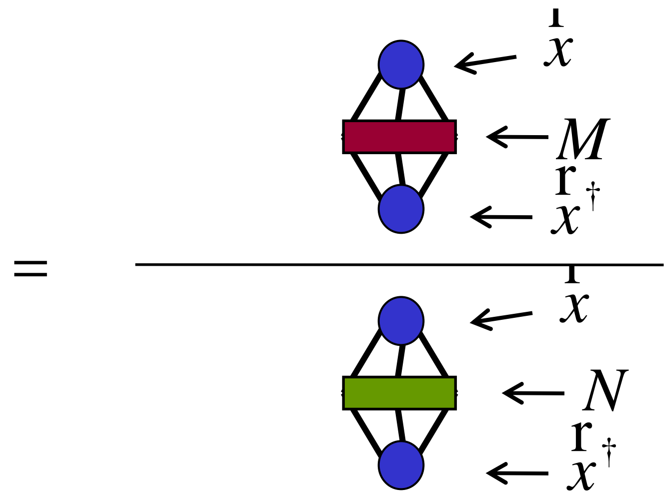


# Optimization of a tensor network

- Ground state $\left|\Psi_{GS}\right\rangle$ $\quad H=\sum_{\langle ij\rangle} h_{ij}$

$$\boxed{\min_{\Psi} \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}}$$

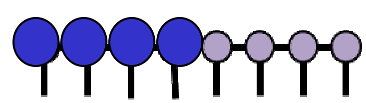



$$\min_{\vec{x}} \frac{\vec{x}^{\dagger} M \vec{x}}{\vec{x}^{\dagger} N \vec{x}} \Rightarrow M\vec{x} = \lambda N \vec{x}$$

generalized eigenvalue problem

- sweep over tensor network

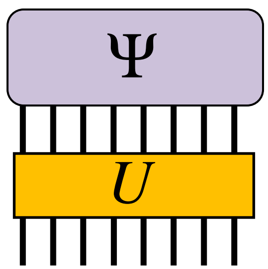


# Optimization of a tensor network

- time evolution $|\Psi'\rangle = U|\Psi\rangle$

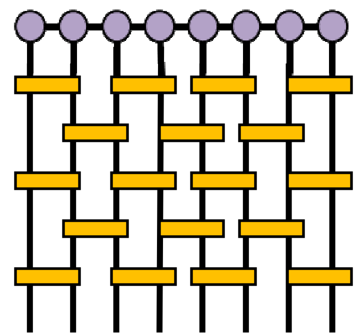
$|\Psi\rangle$

$U$




$$U = \exp - iHt$$

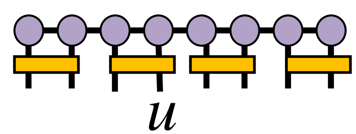
$$H = \sum_{\langle ij \rangle} h_{ij}$$



- break into steps of the form

$$|\Psi'\rangle = u|\Psi\rangle$$

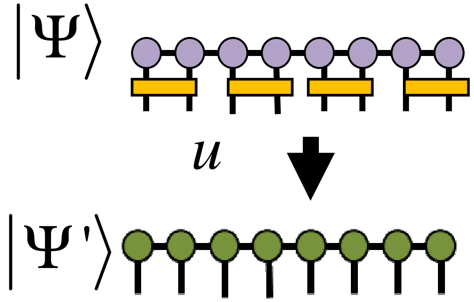
$|\Psi\rangle$



# Optimization of a tensor network

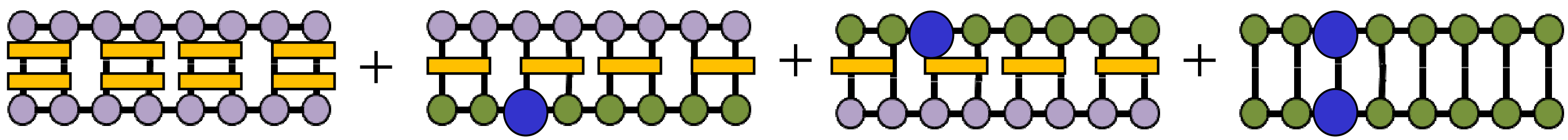
- time evolution

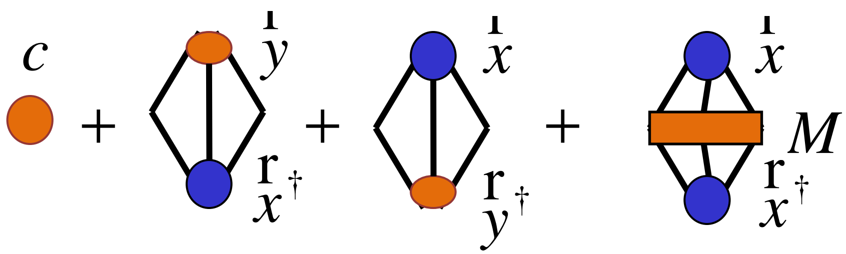
$|\Psi'\rangle = u|\Psi\rangle$




$$\min_{\psi'} \| u|\Psi\rangle - |\Psi'\rangle \|^2$$

$$\| u|\Psi\rangle - |\Psi'\rangle \|^2 = \langle\Psi|u^\dagger u|\Psi\rangle - \langle\Psi'|u|\Psi\rangle - \langle\Psi|u^\dagger|\Psi'\rangle + \langle\Psi'|\Psi'\rangle$$

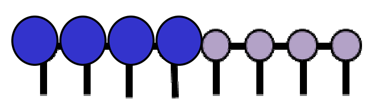



$$\min_{\vec{x}} c - \vec{x}^\dagger \vec{y} - \vec{y}^\dagger \vec{x} + \vec{x}^\dagger M \vec{x}$$

$$\Rightarrow \quad M\vec{x} = \vec{y}$$

- sweep over tensor network



# Optimization of a tensor network

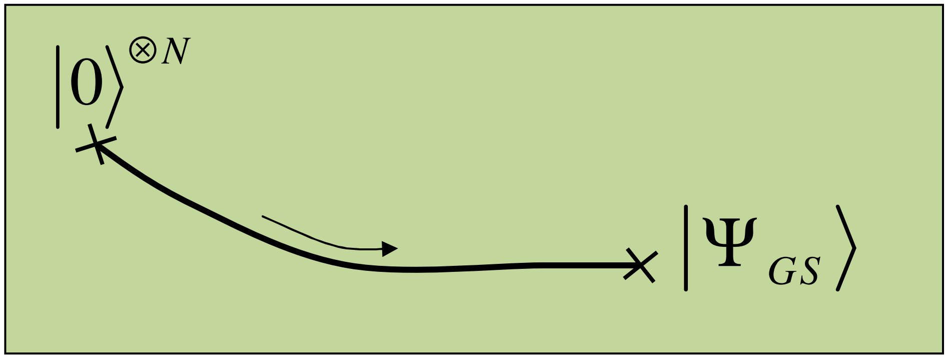
Therefore the ground state $|\Psi_{GS}\rangle$ can be obtained in two ways:

• minimization of energy

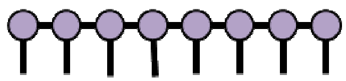
$$\min_{\Psi} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

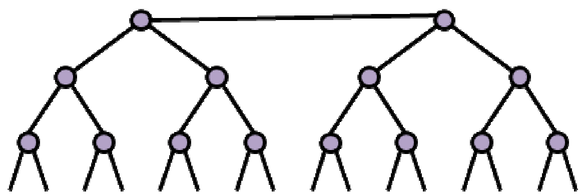
• simulation of evolution in “Euclidian” or “imaginary” time

$$|\Psi_{GS}\rangle = \lim_{\tau \to \infty} \frac{e^{-H\tau} |0\rangle^{\otimes N}}{\| e^{-H\tau} |0\rangle^{\otimes N} \|}$$



# Summary





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