Matrix product states for the absolute beginner

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Brief overview: Why tensor networks?

Graphical notation

Matrix Product States and Matrix Product Operators

Compressing Matrix Product States

Energy optimization

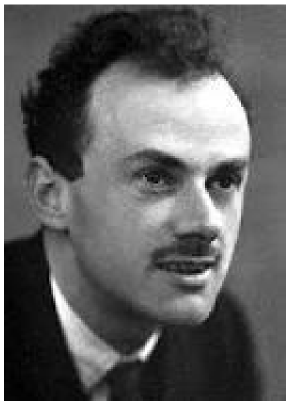
Time evolution

Periodic and infinite MPS

Focus on basic computations and algorithms with MPS

not covered: entanglement area laws, RG, topological aspects, symmetries etc.

Quantum mechanics is complex



Dirac

The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known …

the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.

$$\Psi(r_1, r_2, ...r_n)$$

n electron positions

$$\Psi(s_1, s_2, ...s_L)$$

L spins

$$\Psi(n_1, n_2, ...n_L)$$

L particle occupancies

Exponential complexity to represent wavefunction

This view of QM is depressing

[The Schrodinger equation] cannot be solved accurately when the number of particles exceeds about 10. No computer existing, or that will ever exist, can break this barrier because it is a catastrophe of dimension ...

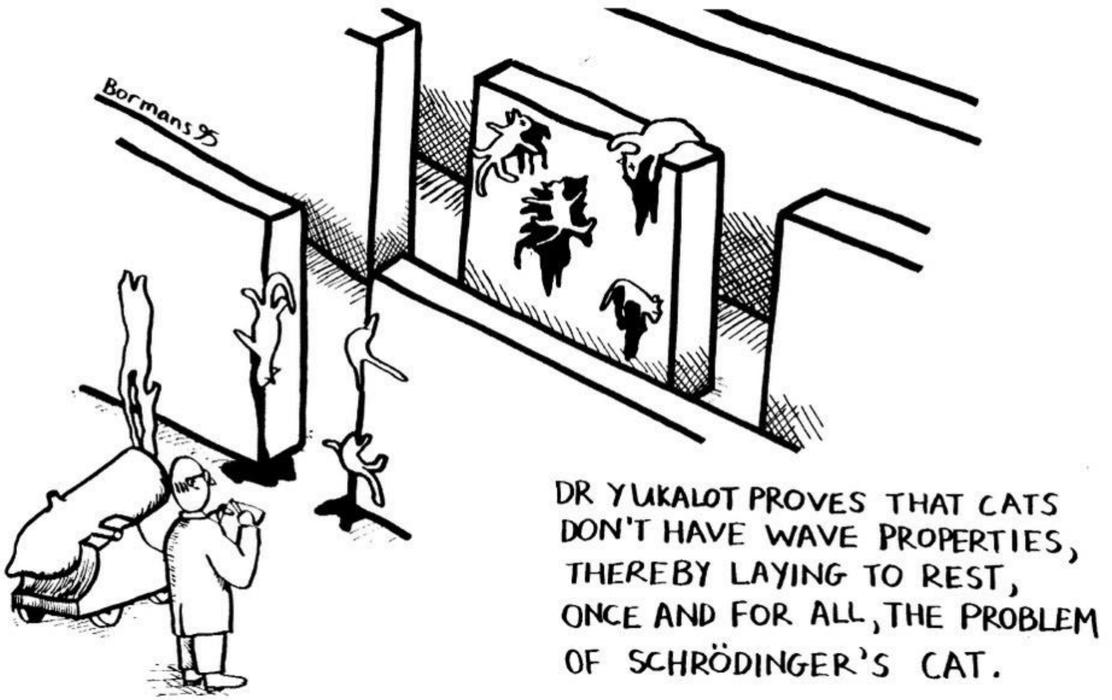
Pines and Laughlin (2000)

in general the many-electron wave function Ψ … for a system of N electrons is not a legitimate scientific concept [for large N]

Kohn (Nobel lecture, 1998)

illusion of complexity

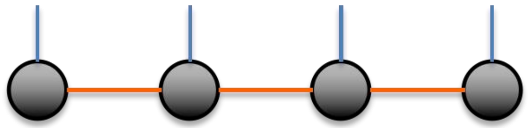
nature does not explore all possibilities



Nature is local: ground-states have **low entanglement**

Language for low entanglement states is tensor networks

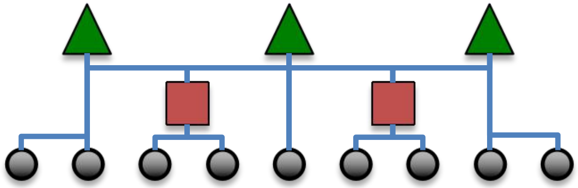
different tensor networks reflect geometry of entanglement



Matrix Product State

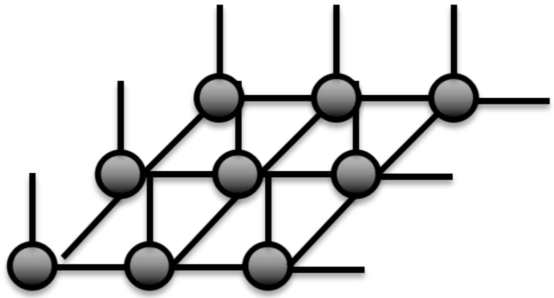
1D entanglement for **gapped** systems

(basis of DMRG - often used in quasi-2D/3D)



MERA

1D/nD entanglement for **gapless** systems



Tensor Product State (PEPS)

nD entanglement for gapped systems

Graphical language

$$|\boldsymbol{\Psi}\rangle = \sum_{n_1 n_2 n_3} \boldsymbol{\Psi}^{n_1 n_2 n_3} |n_1 n_2 n_3\rangle$$

e.g.

$|n\rangle = \{|\uparrow\rangle, |\downarrow\rangle\}$ spin 1/2

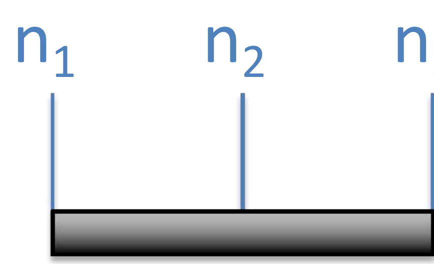
$|n\rangle = \{|0\rangle, |1\rangle\}$ particles

Algebraic form

Graphical form

General state

$\boldsymbol{\Psi}^{n_1 n_2 n_3}$



physical index

thick line = single tensor

Graphical language, cont'd

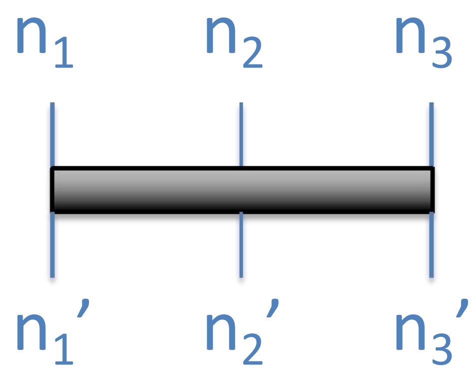
$$\hat{O} = \sum_{nn'} O^{n_1 n_2 n_3}_{n_1' n_2' n_3'} |n_1 n_2 n_3\rangle\langle n_1' n_2' n_3'|$$

Algebraic form

Graphical form

General operator

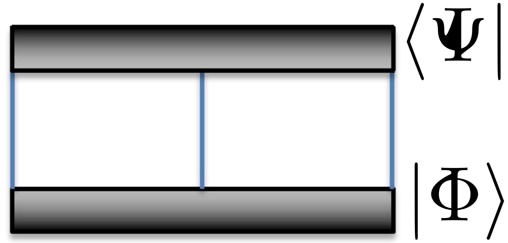
$$O^{n_1 n_2 n_3}_{n_1' n_2' n_3'}$$



Ex: overlap, expectation value

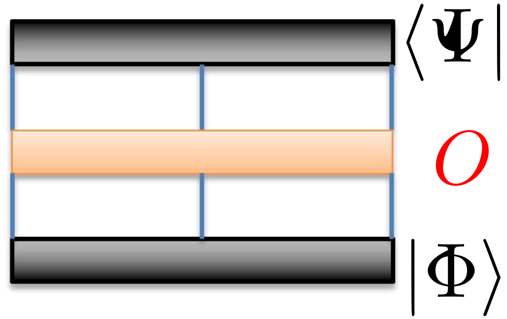
Overlap

$$\langle \mathbf{\Psi} | \Phi \rangle = \sum_{n} \mathbf{\Psi}_{n_1 n_2 n_3} \Phi^{n_1 n_2 n_3}$$



Expectation value

$$\langle \mathbf{\Psi} | {\color{red}O} | \Phi \rangle = \sum_{n,n'} \mathbf{\Psi}_{n_1 n_2 n_3} {\color{red}O}^{n_1 n_2 n_3}_{n_1' n_2' n_3'} \Phi^{n_1 n_2 n_3}$$



Low entanglement states

What does it mean for a state to have low entanglement?

Consider system with two parts, 1 and 2

No entanglement

$$\Psi^{n_1 n_2} = A^{n_1} A^{n_2}$$

local measurements on separated system 1, system 2 can be done independently. **Local realism** (classical)

Entangled state

$$\Psi^{n_1 n_2} = \sum_i A_i^{n_1} A_i^{n_2}$$

Low entanglement : small number of terms in the sum

Matrix product states

first and last tensors have one fewer auxiliary index

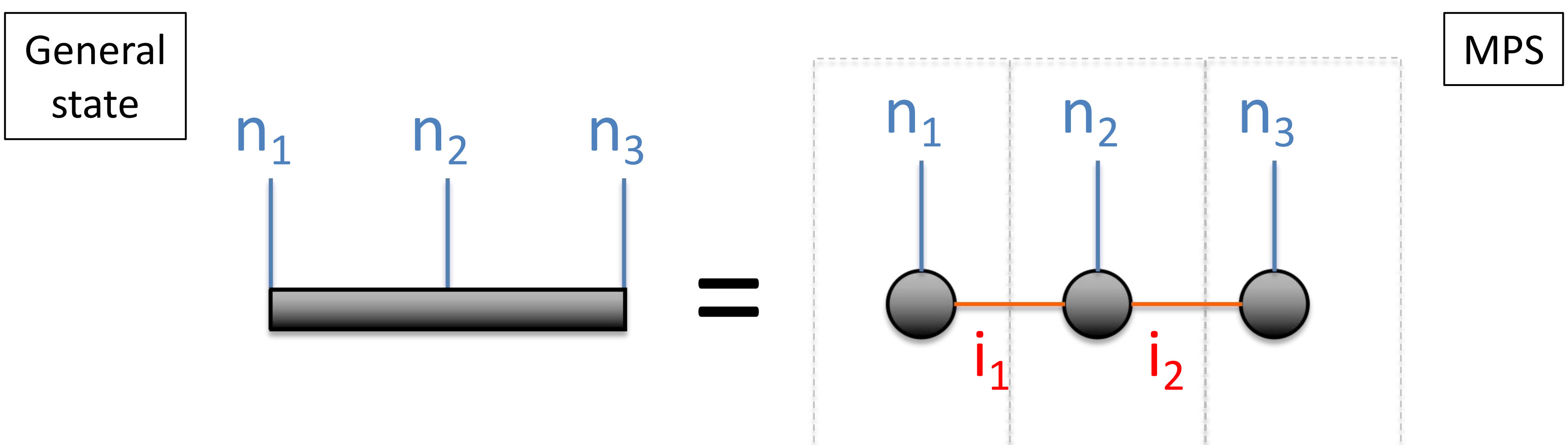
$$\mathbf{\Psi}^{n_1 n_2 n_3 \ldots n_l} = \sum_i A^{n_1}_{i_1} A^{n_2}_{i_1 i_2} A^{n_3}_{i_2 i_3} \cdots A^{n_l}_{i_l}$$

"bond" or "auxiliary" dimension
"M" or "D" or "χ"

1D structure
of entanglement

$$= \mathbf{A}^{n_1} \mathbf{A}^{n_2} \ldots \mathbf{A}^{n_l}$$

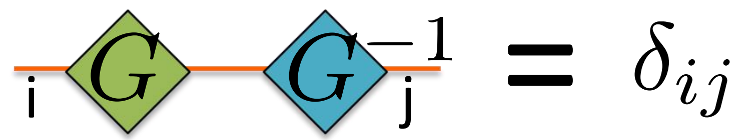
amplitude is obtained as a product of matrices

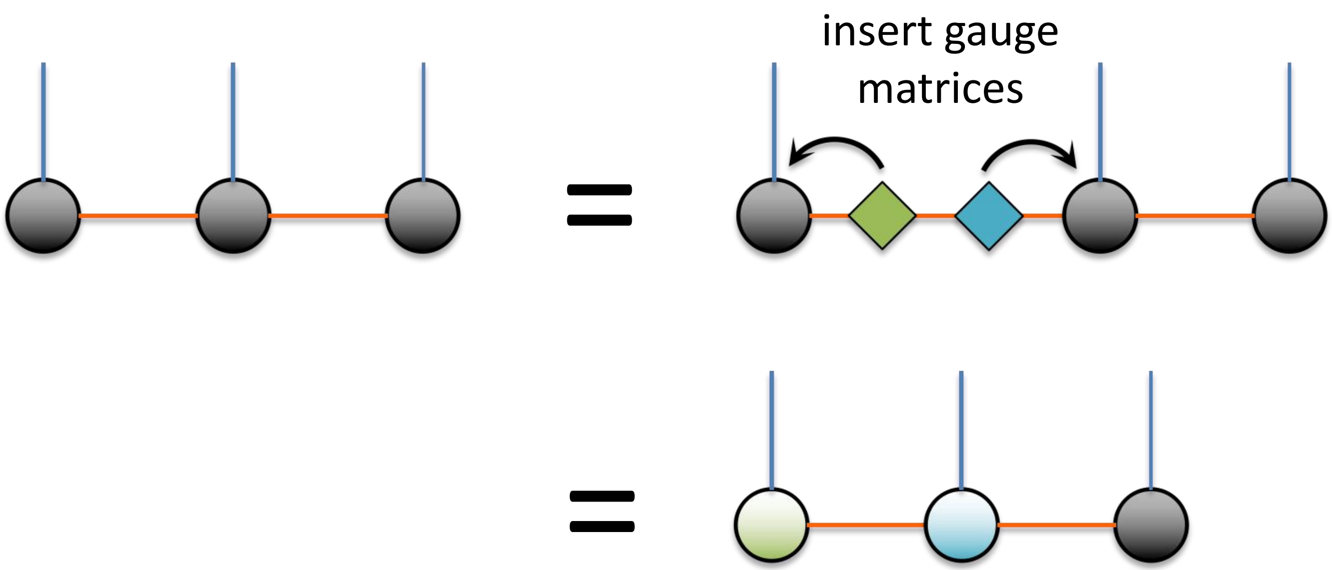


MPS gauge

MPS are not unique: defined up to gauge on the auxiliary indices

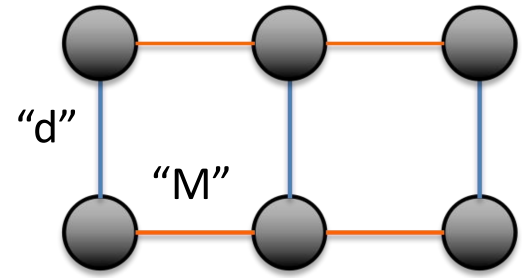
$$\mathbf{GG}^{-1} = \mathbf{1}$$



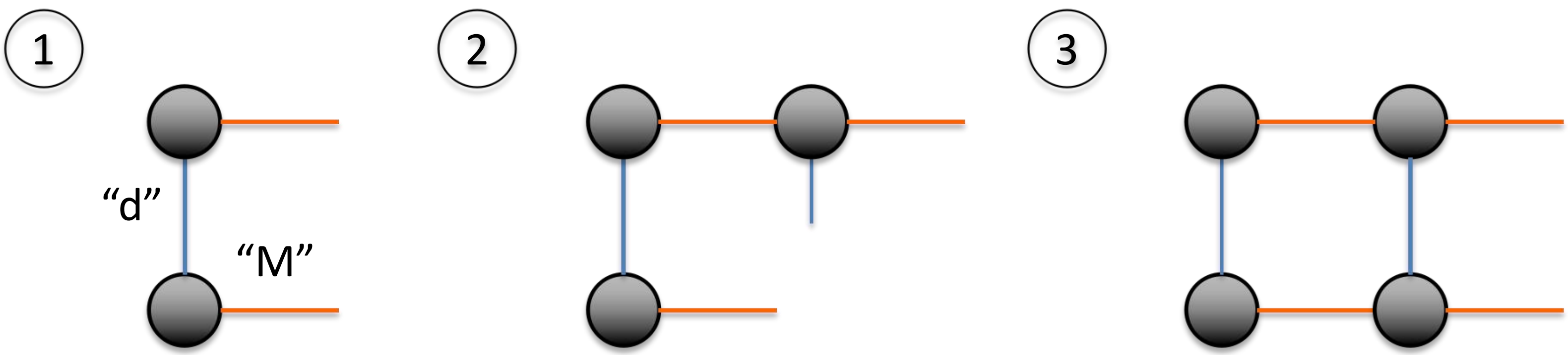


Ex: MPS contraction

Overlap $\langle \Psi | \Phi \rangle$



Efficient computation: contract in the correct order!



$M^2 d$ $\qquad$ $M^3 d$ $\qquad$ $M^3 d$

MPS overlap: total cost $O(M^3 dL)$

MPS from general state

recall singular value decomposition (SVD) of matrix

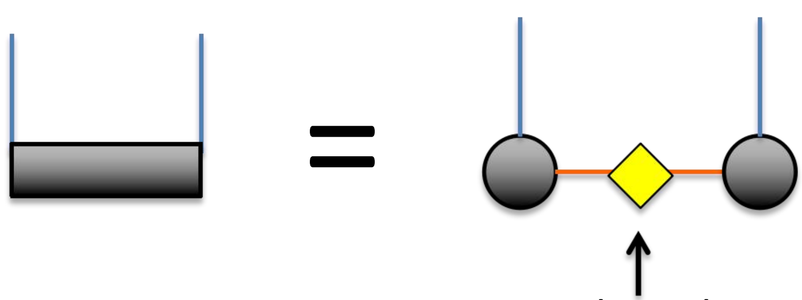
$$\Psi^{nm} = \sum_i L_i^n \sigma_i R_i^m$$

singular values

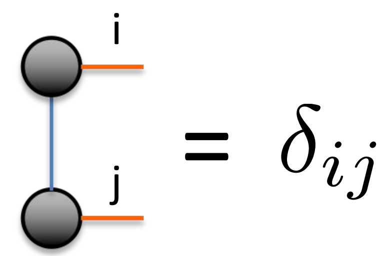
$$\sum_n L_i^n L_j^n = \delta_{ij}$$

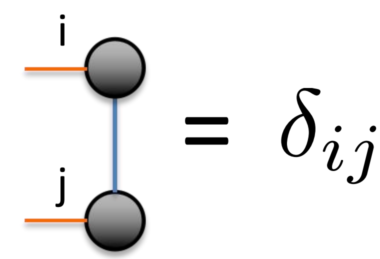
$$\sum_n R_i^n R_j^n = \delta_{ij}$$

orthogonality conditions



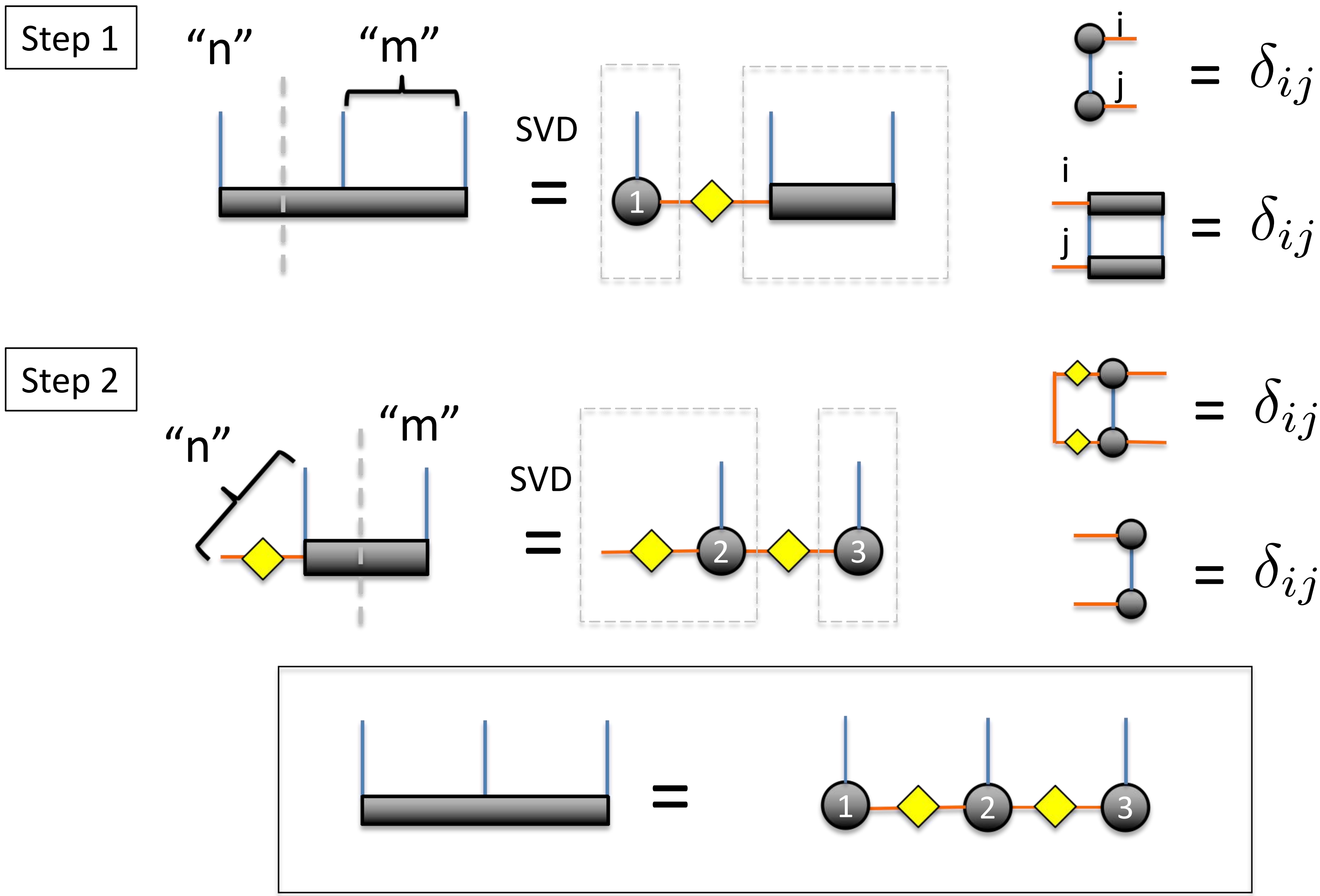
singular values





orthogonality conditions

MPS from general state, cont'd

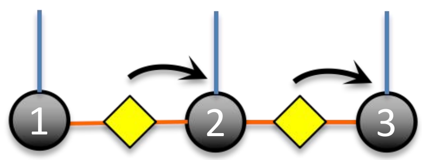


Common canonical forms

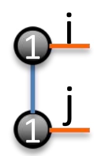
“Vidal” form

different canonical form: absorb singular values into the tensors

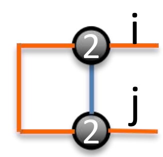
left canonical



all tensors contract to unit matrix from **left**

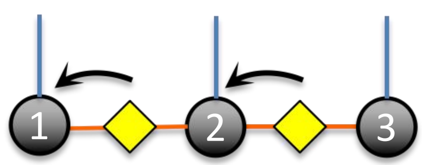


$= \delta_{ij}$

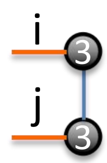


$= \delta_{ij}$ etc

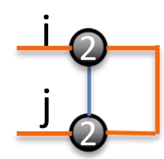
right canonical



all tensors contract to unit matrix from **right**

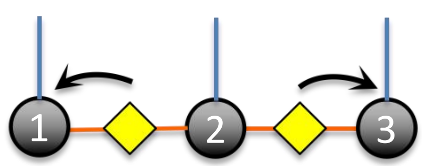


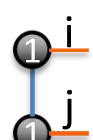
$= \delta_{ij}$



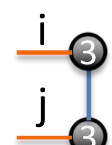
$= \delta_{ij}$ etc

mixed canonical
around site 2
(DMRG form)





δ_{ij}

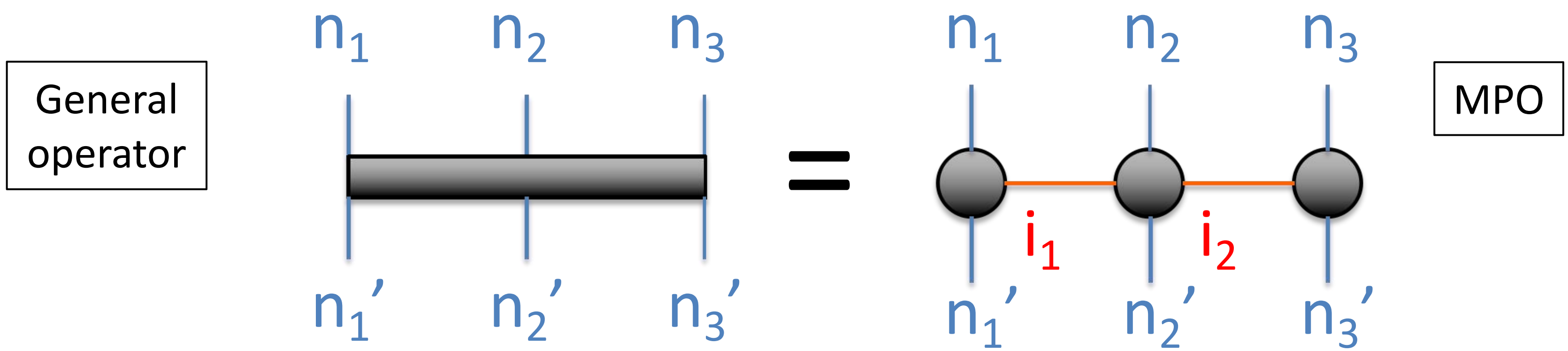


$= \delta_{ij}$

Matrix product operators

$$O^{n_1 n_2 n_3 \ldots n_l}_{n'_1 n'_2 n'_3 \ldots n'_l} = \sum_i W^{n_1, n'_1}_{i_1} \boxed{W^{n_2, n'_2}_{i_1 i_2}} W^{n_3 n'_3}_{i_2 i_3} \ldots W^{n_l n'_l}_{i_l}$$

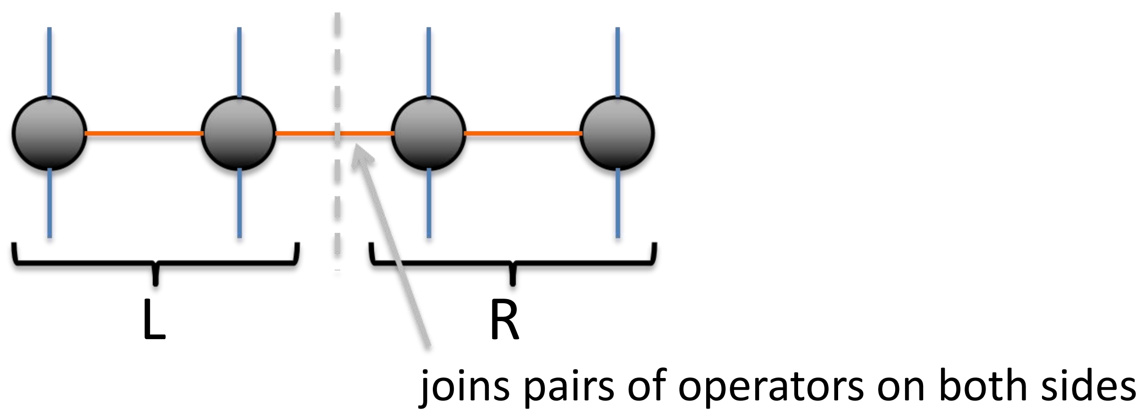
each tensor has a bra and ket physical index



Typical MPO's

$$H = \sum_{\langle ij \rangle} S_i \cdot S_j$$

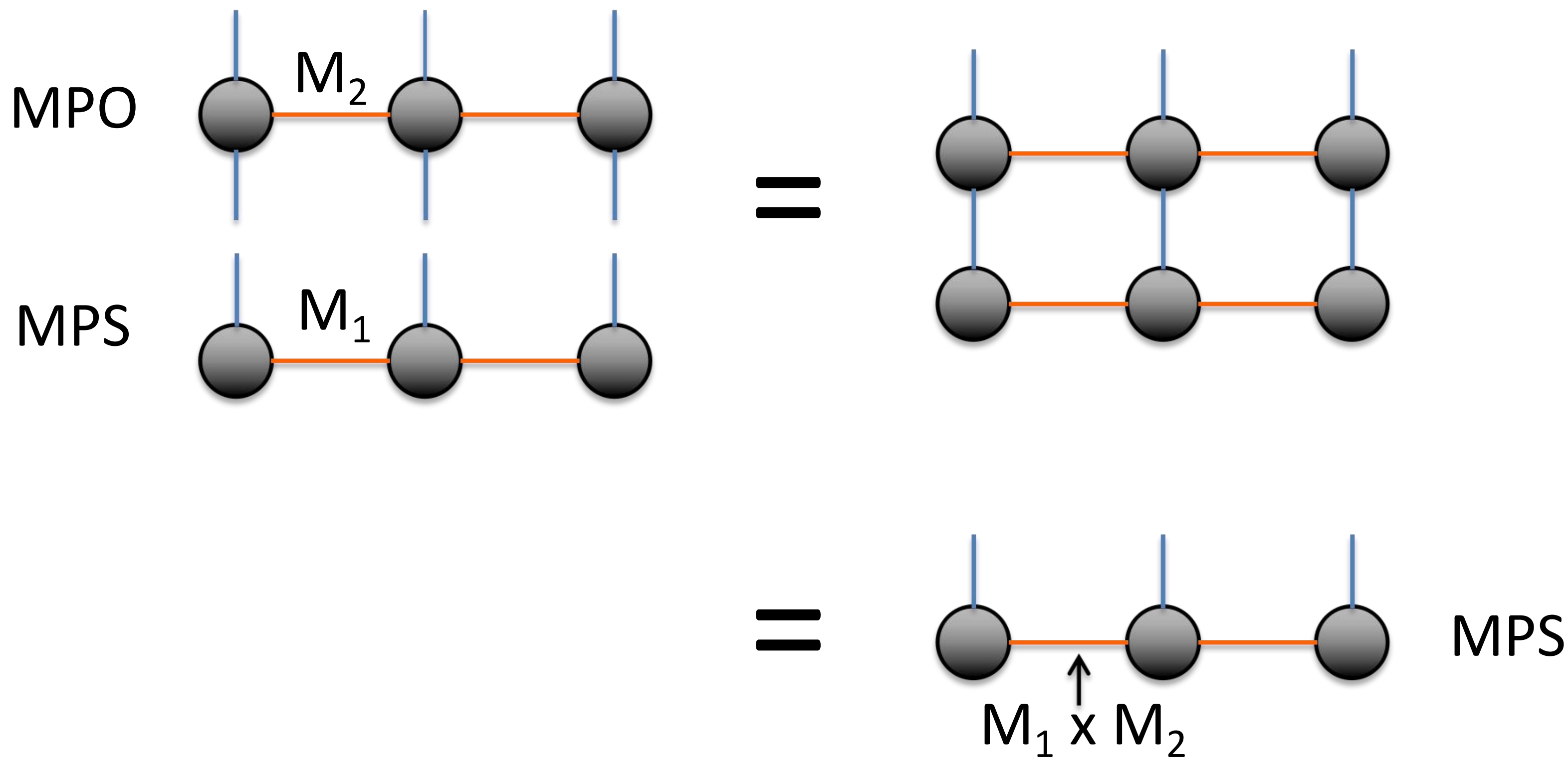
What is bond dimension as an MPO?



$$H_L \otimes \mathbf{1}_R + \mathbf{1}_L \otimes H_R + \sum_{\alpha=x,y,z} S_{\mathbf{2}}^{\alpha} \cdot S_3^{\alpha}$$

MPO bond dimension = 5

MPO acting on MPS



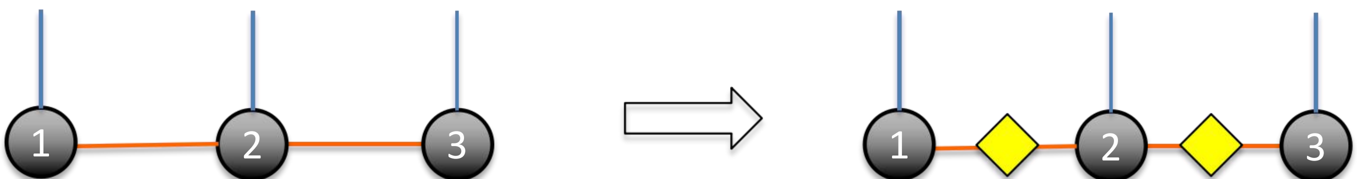
MPO on MPS leads to new MPS with **product** of bond dimensions

MPS compression: SVD

many operations (e.g. MPOxMPS, MPS+MPS) increase bond dim.

compression: best approximate MPS with smaller bond dimension.

write MPS in Vidal gauge via SVD's

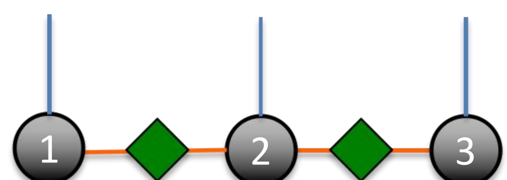


$$\mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_{M_1})$$

M_1 singular values

truncate bonds with small singular values

Each site is compressed independently of new information of other sites:
"Local" update: non-optimal.



$$\mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_{M_2})$$

truncated M_2 singular values

MPS: variational compression

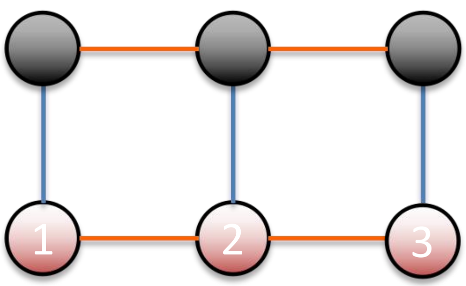
solve minimization problem

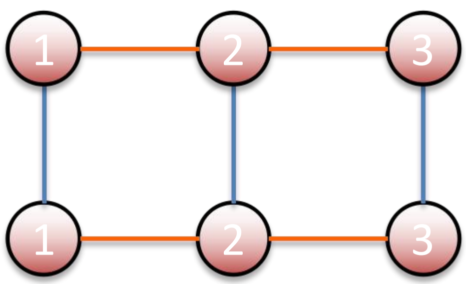
$$\min_{\Phi} \langle \Psi - \Phi | \Psi - \Phi \rangle = \min_{\Phi} [-2\langle \Phi | \Psi \rangle + \langle \Phi | \Phi \rangle]$$

original (fixed) MPS

new MPS

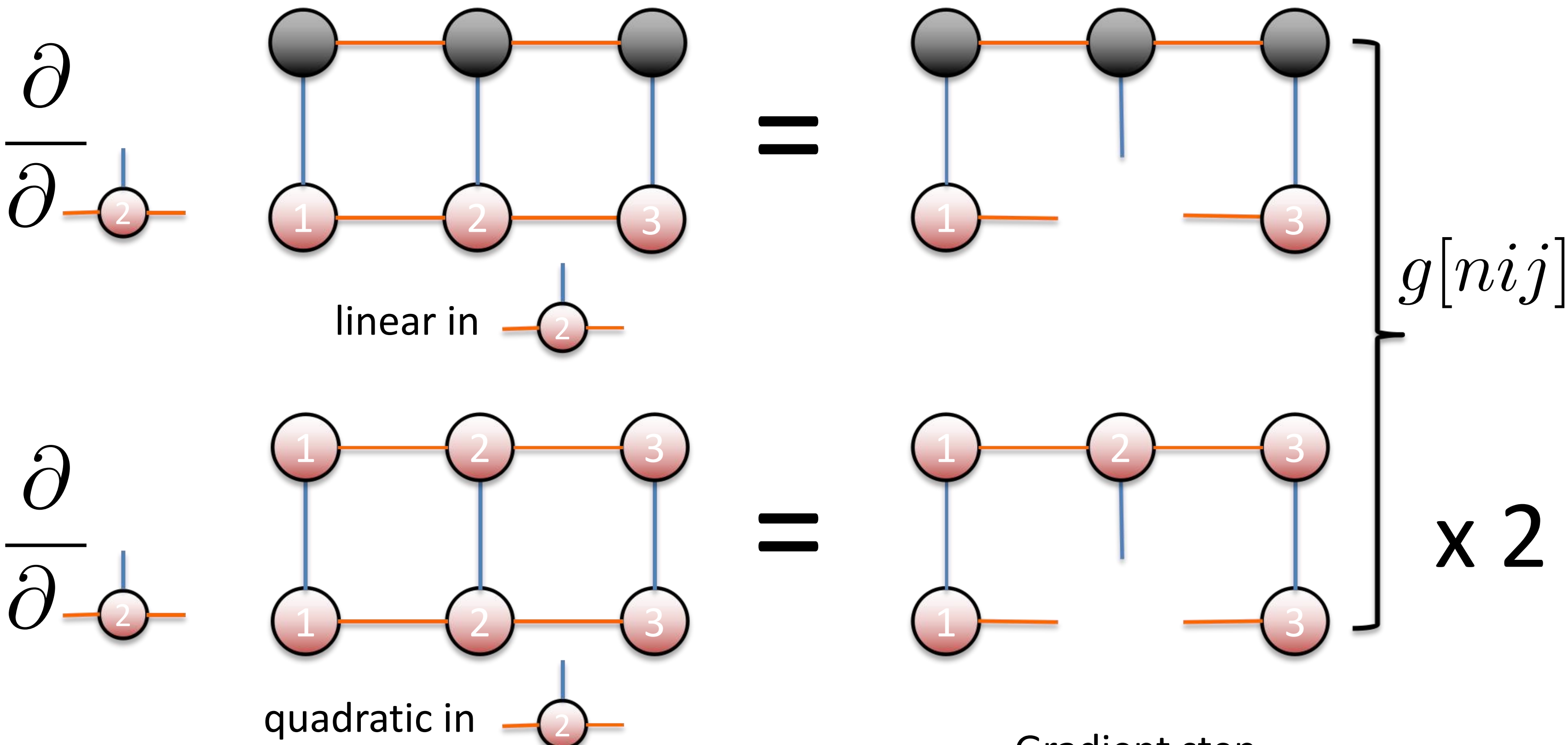
-2



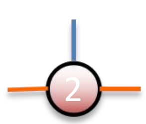


Gradient algorithm

To minimize quantity, follow its gradient until it vanishes



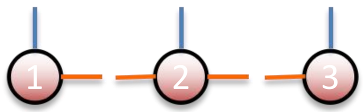
Gradient step

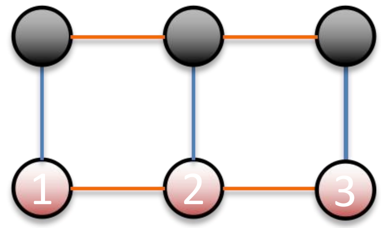


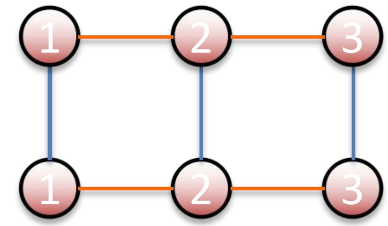
$$A^n_{ij} \equiv a[nij] \qquad a[nij] \rightarrow a[nij] + \epsilon g[nij]$$

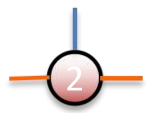
Sweep algorithm (DMRG style)

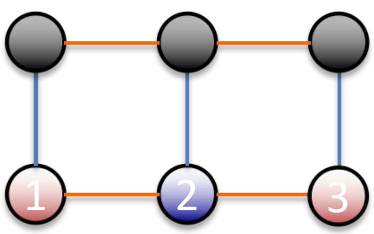
$$\langle \boldsymbol{\Psi} - {\color{red}\boldsymbol{\Phi}} | \boldsymbol{\Psi} - {\color{red}\boldsymbol{\Phi}} \rangle$$

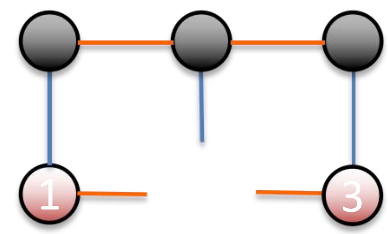
bilinear in 

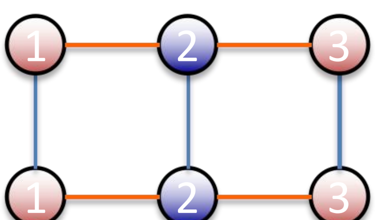


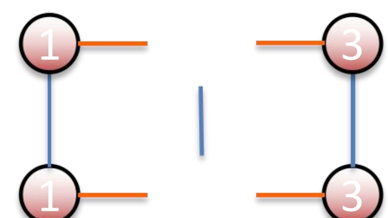


consider  as vector $A_{ij}^{n} \equiv a[nij]$



$= b^T a$ where $b^T =$ 

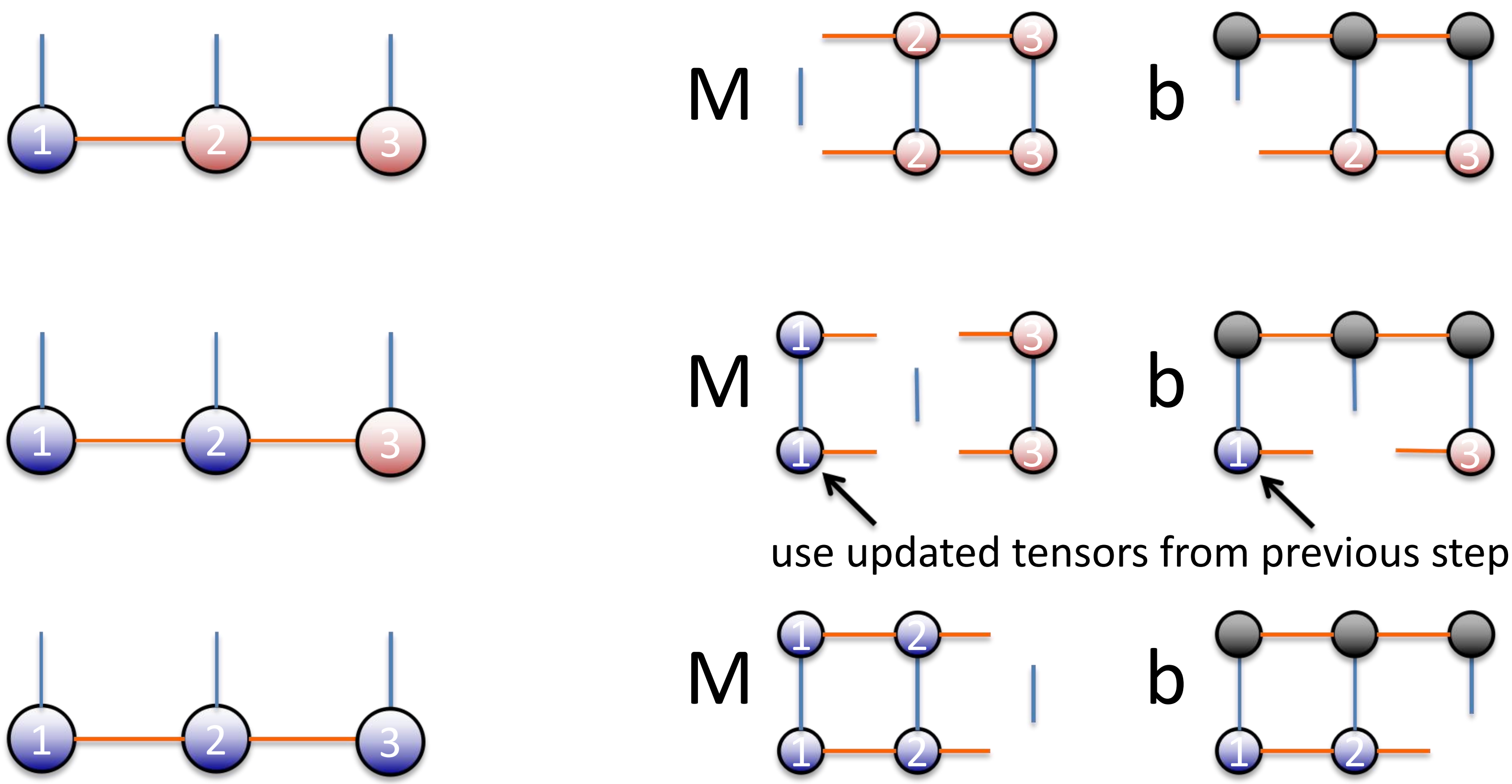


$= a^T M a$ where $M =$ 

$$\min_a (a^T M a - b^T a) \Rightarrow M a = b$$

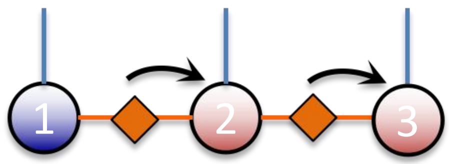
Sweep algorithm cont' d

Minimization performed site by site by solving $Ma = b$

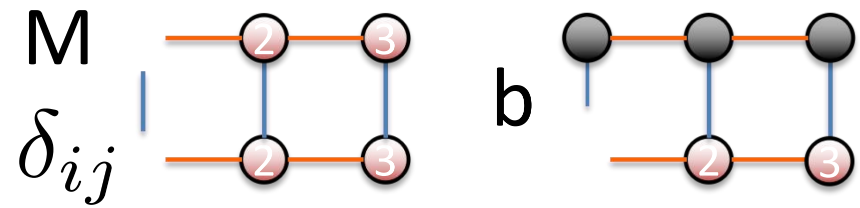


Sweep and mixed canonical form

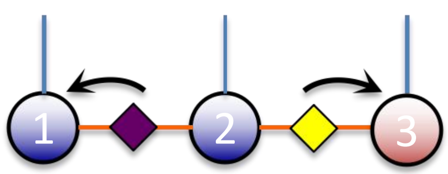
in mixed canonical form $Ma = b \Rightarrow a = b$



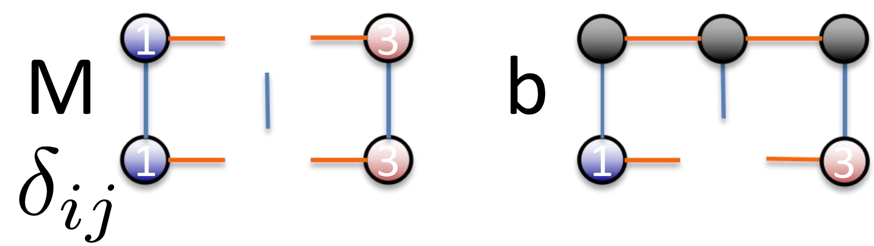
mixed canonical around site 1



change canonical form



mixed canonical around site 2
note: updated singular values



SVD vs. variational compression

variational algorithms – optimization for each site depends on all other sites. Uses “**full environment**”

SVD compression: “**local update**”. Not as robust, but cheap!

MPS: full environment / local update **same computational scaling**, only differ by number of iterations.

General tensor networks (e.g. PEPS): full environment may be expensive to compute or need further approximations.

Energy optimization

$$\min_{\Psi}[\langle\Psi|H|\Psi\rangle - E\langle\Psi|\Psi\rangle]$$

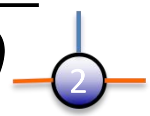
bilinear form: similar to compression problem

$\boxed{\text{commonly used algorithms}}$

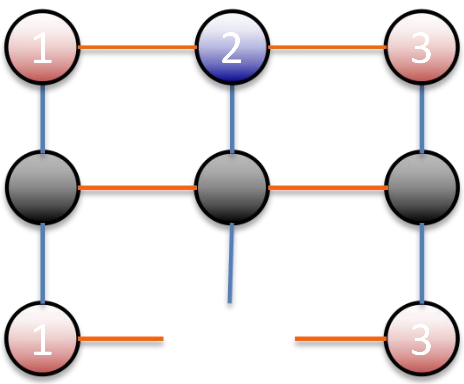
DMRG: variational sweep with full environment

imag. TEBD: local update, imag. time evolution + SVD compression

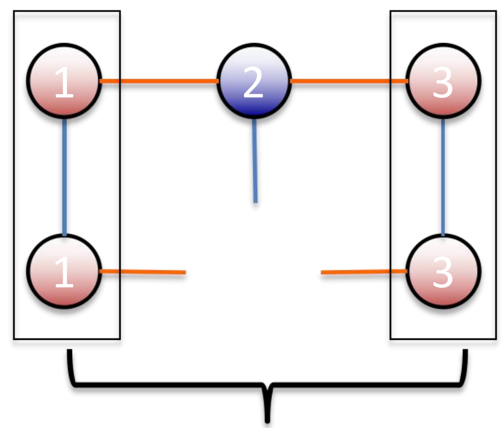
DMRG energy minimization

$$\frac{\partial}{\partial}$$  $$\langle \Psi | H | \Psi \rangle - E \langle \Psi | \Psi \rangle = 0$$

use mixed canonical form around site 2



$-E$



$= 0$

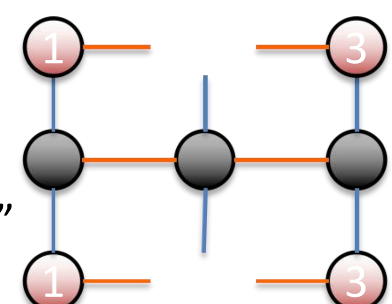
unit matrix

$$Ha = Ea$$

where

eigenvalue problem for each site, in mixed canonical form

$H =$



DMRG “superblock” Hamiltonian

Time evolution

real time evolution

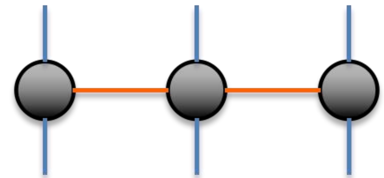
$$|\Psi(\delta t)\rangle = \exp(-iH\delta t)|\Psi(0)\rangle$$

imaginary time evolution: replace i by 1.

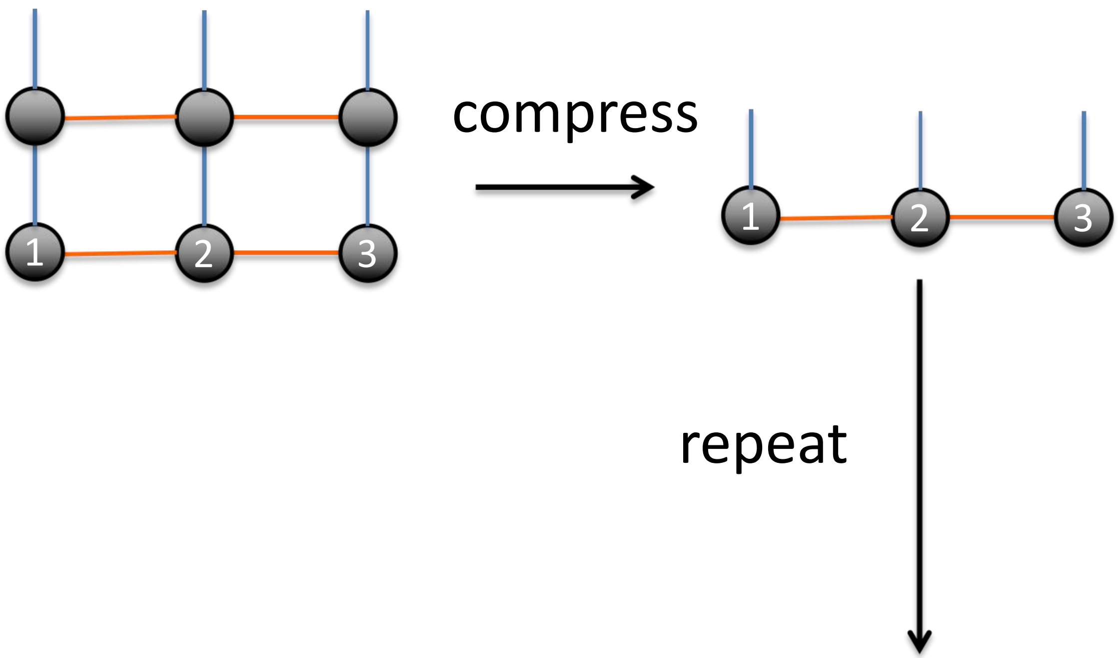
projects onto ground-state at long times.

General time-evolution

$$1 - iH\delta t =$$



$$1 - iH\delta t$$



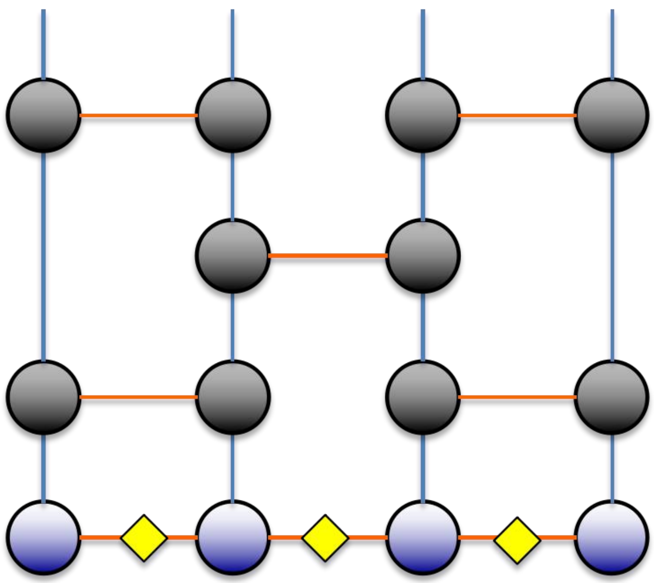
Short range H: Trotter form

$$H = \sum_{ij} S_i \cdot S_j$$

$$e^{-\delta H} = e^{-\delta S_1 \cdot S_2} e^{-\delta S_2 \cdot S_3} \ldots + O(\delta^2)$$

evolution on pairs of bonds

Even-odd evolution



$$e^{-\delta S_1 \cdot S_2} e^{-\delta S_3 \cdot S_4}$$

$$e^{-\delta S_2 \cdot S_3}$$

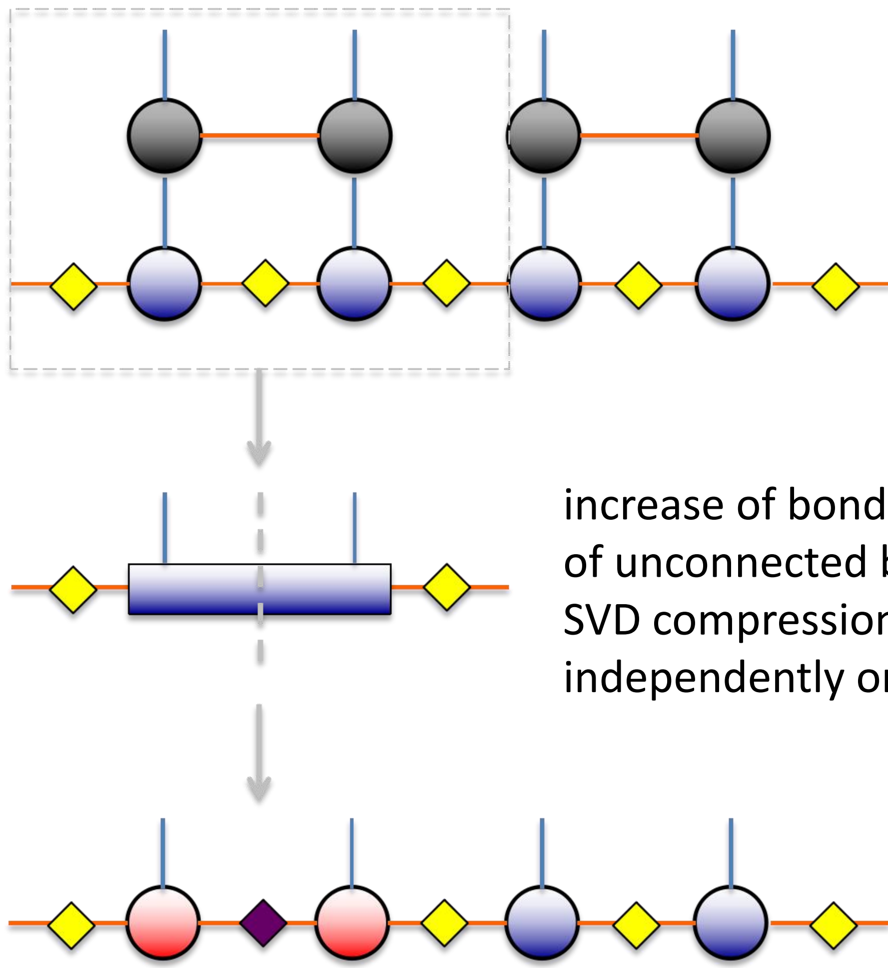
$$e^{-\delta S_1 \cdot S_2} e^{-\delta S_3 \cdot S_4}$$

time evolution can be broken up into even and odd bonds

Time-evolving block decimation

even/odd evolution easy to combine with SVD compression: TEBD

SVD

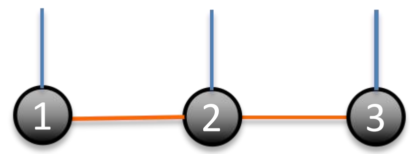


increase of bond dimension
of unconnected bonds:
SVD compression can be done
independently on each bond.

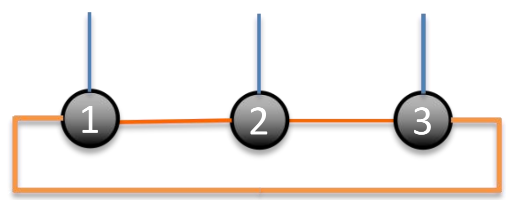
Periodic and infinite MPS

MPS easily extended to PBC and thermodynamic limit

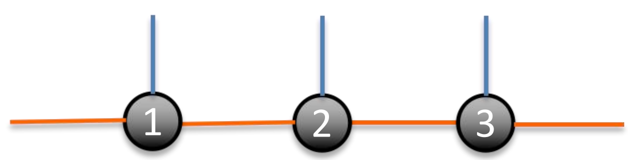
Finite MPS (OBC)



Periodic MPS



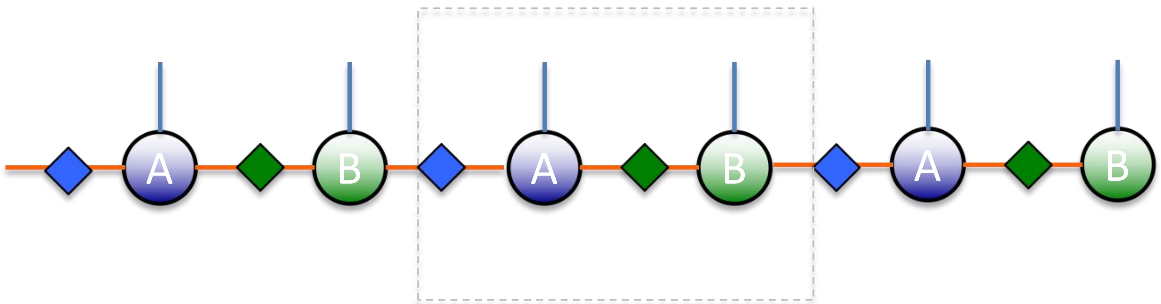
Infinite MPS



Infinite TEBD

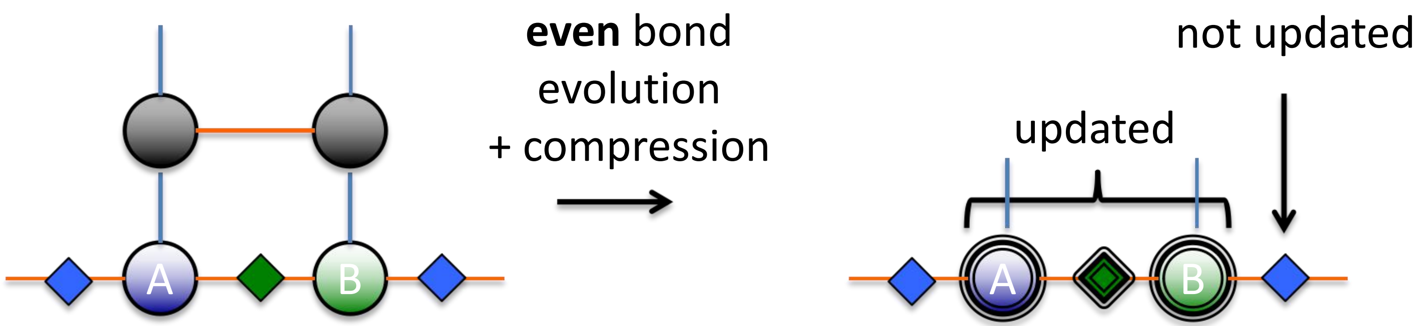
local algorithms such as TEBD easy to extend to infinite MPS

Unit cell = 2 site infinite MPS

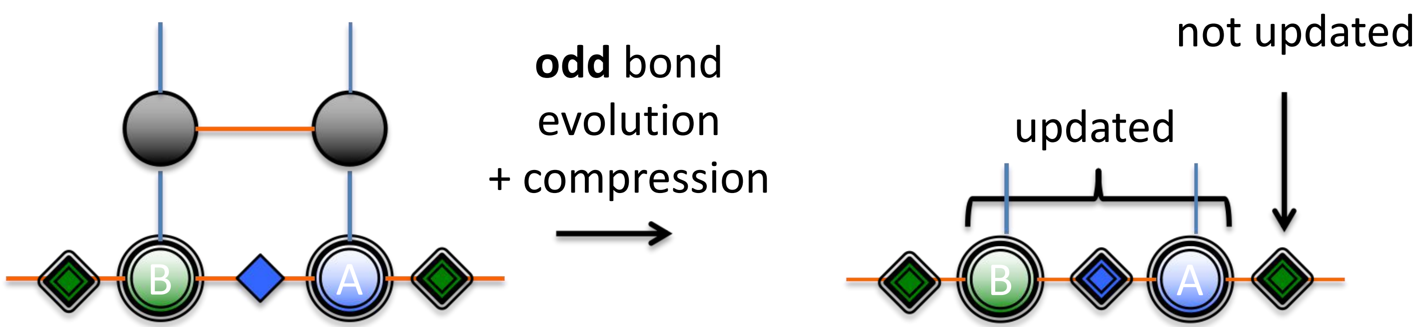


i-TEBD cont' d

Step 1



Step 2



Repeat

Symmetries

Given global symmetry group, local site basis can be labelled by irreps of group – **quantum numbers**

U(1) – site basis labelled by integer n (particle number) $|n\rangle$

n=0, 1, 2 etc...

SU(2) symmetry – site basis labelled by j, m (spin quanta) $|jm\rangle$

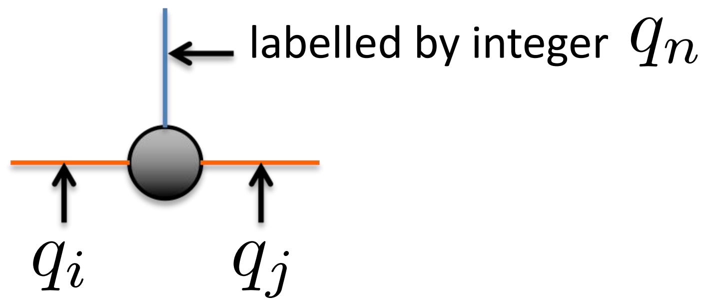
Total state associated with good quantum numbers

$$|\mathbf{\Psi}\rangle = |\mathbf{\Psi}(n, j, m...)\rangle$$

MPS and symmetry

bond indices can be labelled by same symmetry labels as physical sites

e.g. particle number symmetry

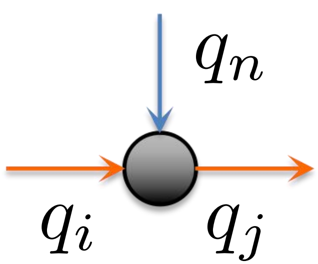


MPS: well defined Abelian symmetry, each tensor fulfils rule

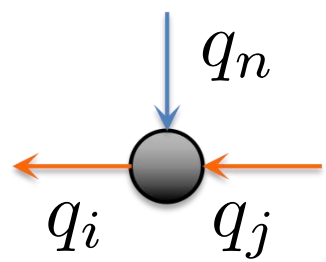
$$\sum q_{in} = \sum q_{out}$$

tensor with no arrows leaving gives total state quantum number

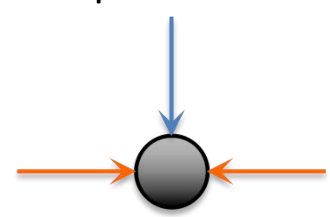
Choice of convention:



$$q_i + q_n = q_j$$



$$q_j + q_n = q_i$$



$$Q = q_n + q_i + q_j$$

Brief overview: Why tensor networks?

Graphical notation

Matrix Product States and Matrix Product Operators

Compressing Matrix Product States

Energy optimization

Time evolution

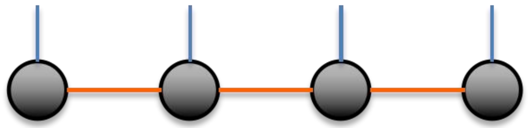
Periodic and infinite MPS

Focus on basic computations and algorithms with MPS

not covered: entanglement area laws, RG, topological aspects, symmetries etc.

Language for low entanglement states is tensor networks

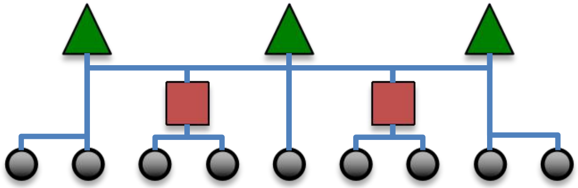
different tensor networks reflect geometry of entanglement



Matrix Product State

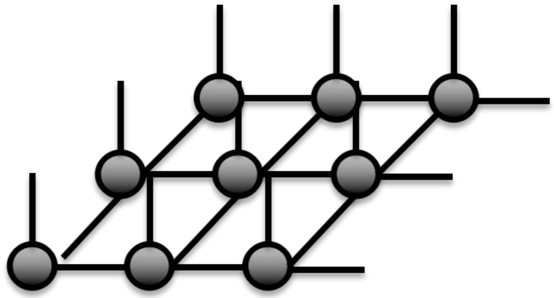
1D entanglement for **gapped** systems

(basis of DMRG - often used in quasi-2D/3D)



MERA

1D/nD entanglement for **gapless** systems



Tensor Product State (PEPS)

nD entanglement for gapped systems

Questions

1. What is the dimension of MPS (M_1) + MPS (M_2)?
2. How would we graphically represent the DM of an MPS, (tracing out sites n_3 to n_L?)
3. What is the dimension of the MPO of an electronic Hamiltonian with general quartic interactions?
4. What happens when we use an MPS to represent a 2D system?
5. What happens to the bond-dimension of an MPS as we evolve it in time? Do we expect the MPS to be compressible? How about for imaginary time evolution?
6. How would we alter the discussion of symmetry for non-Abelian symmetry e.g. SU(2)?