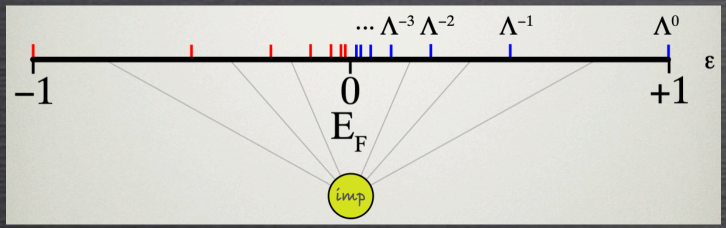
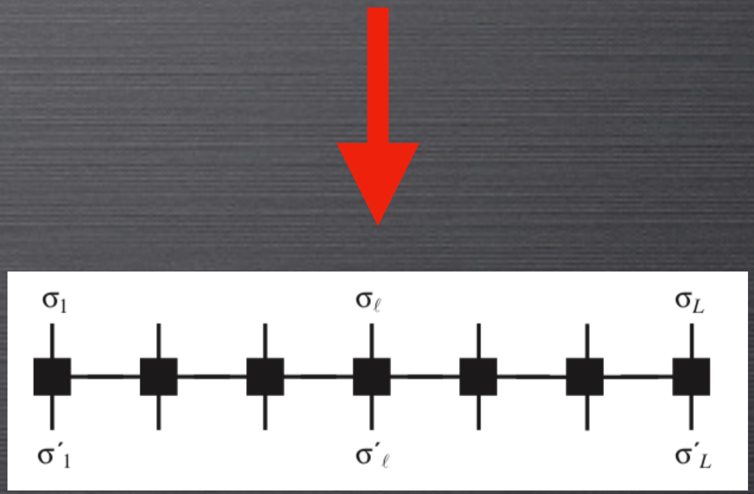
Solvers for quantum impurity problems (with superconducting baths)

Lecture 3: density matrix renormalization group





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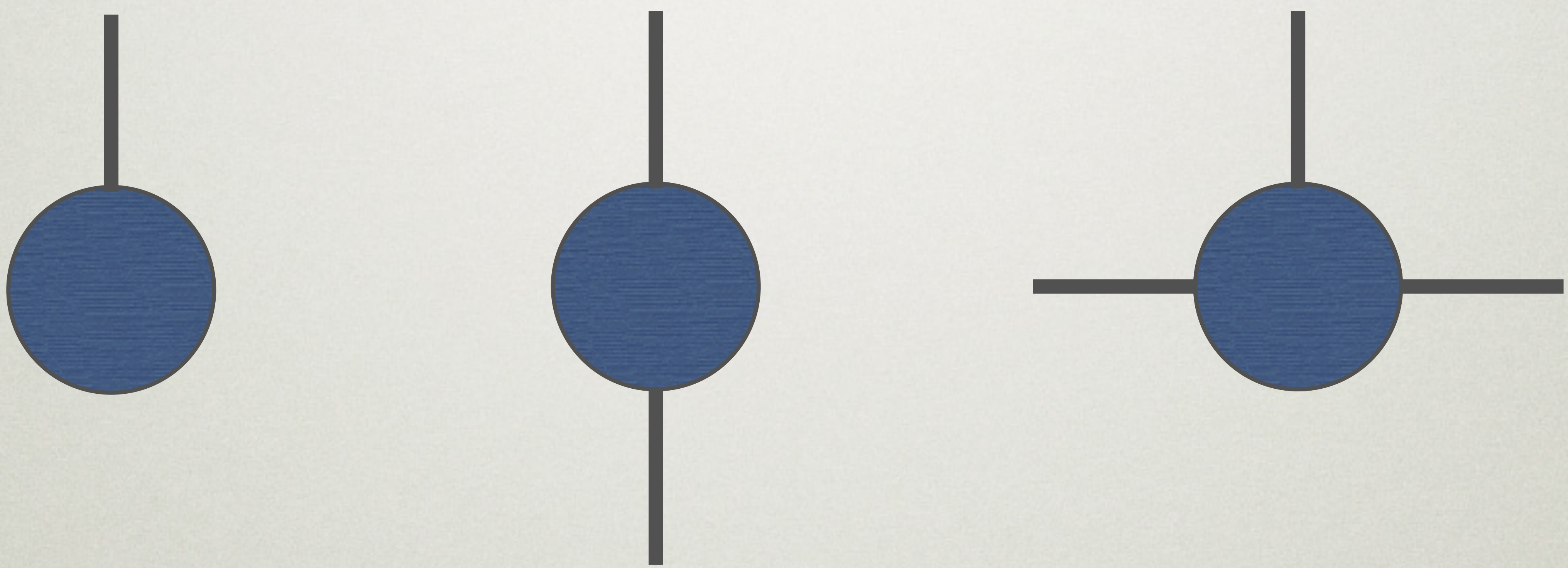
University of Copenhagen, Oct 2021

- Main idea: exponentially big Hilbert space <u>compressed</u> into a subspace of states which carry most of the weight
- Works best for **local** Hamiltonians with a **gap** between the ground state and the first excited state
- Efficient

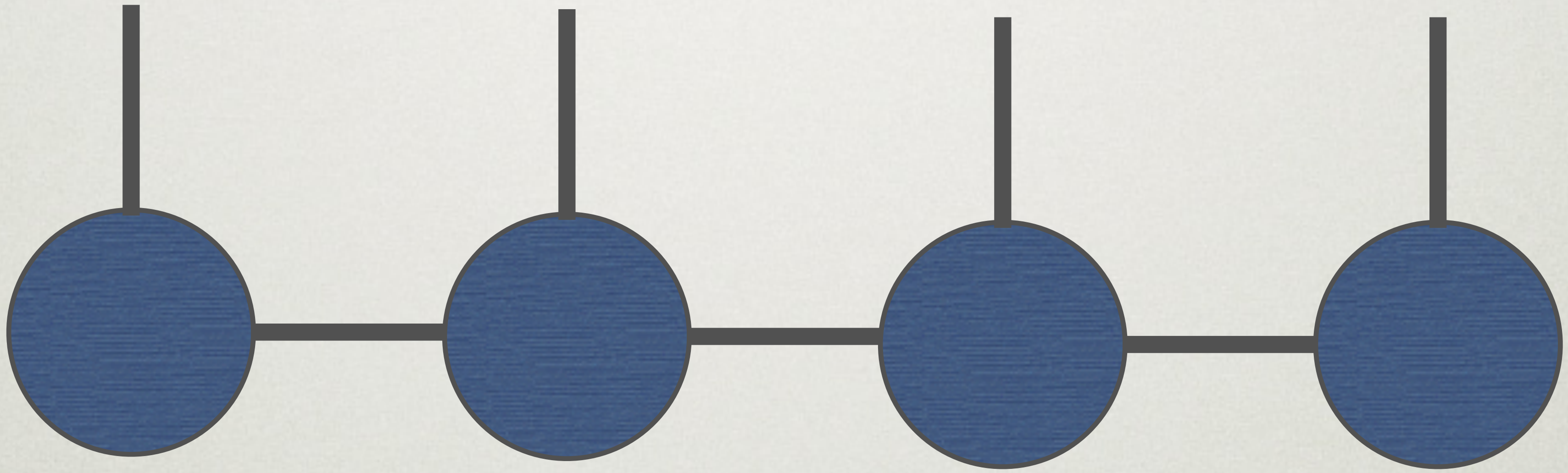
U. Schollwöck, *The density-matrix renormalization group in the age of matrix product states*, Annals of Physics 326, 96 (2011)

Tensors

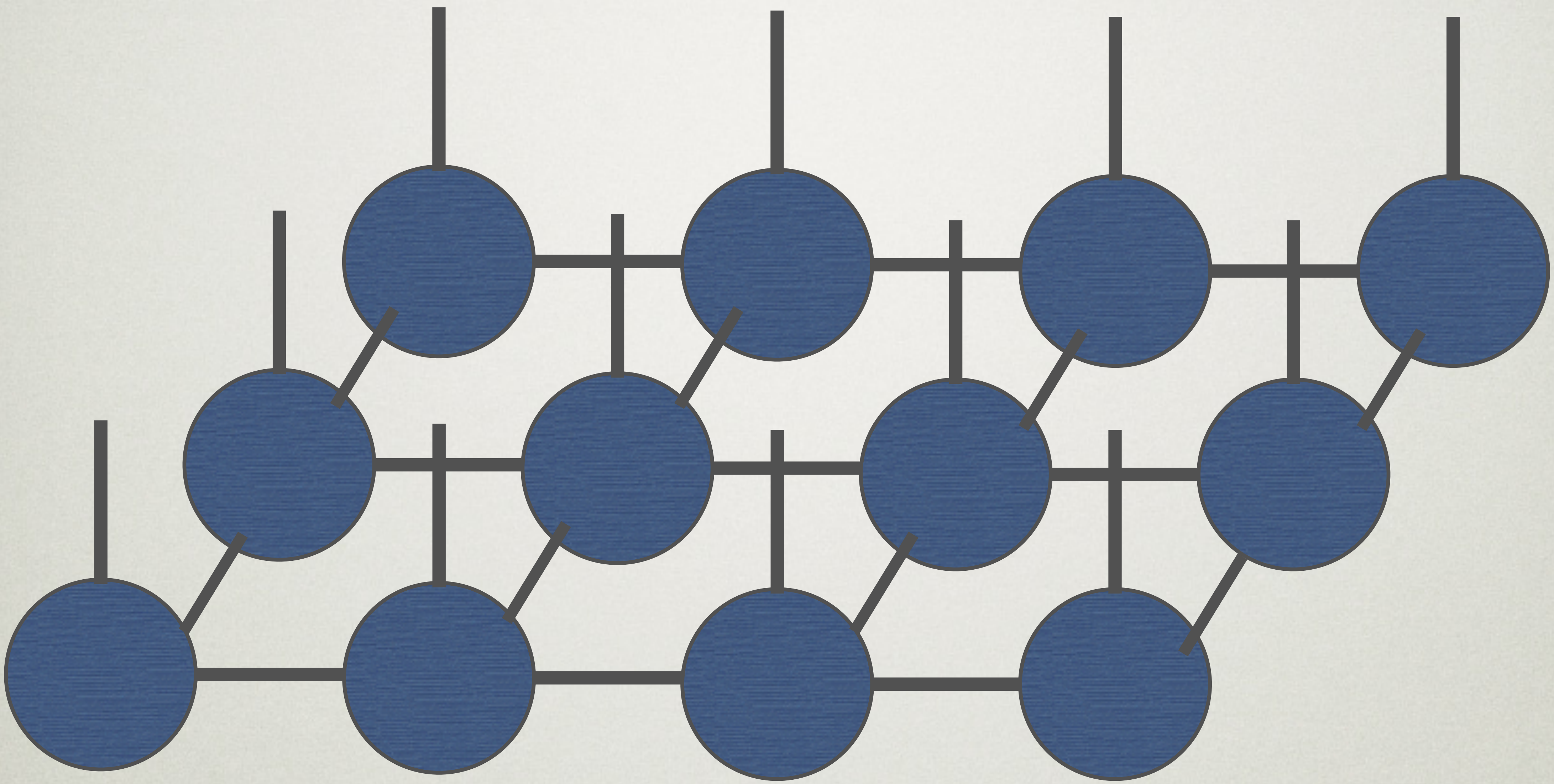


ψ_σ $O_{\sigma\sigma'}$ U_{ij}^{σ}

Tensor networks



matrix product state



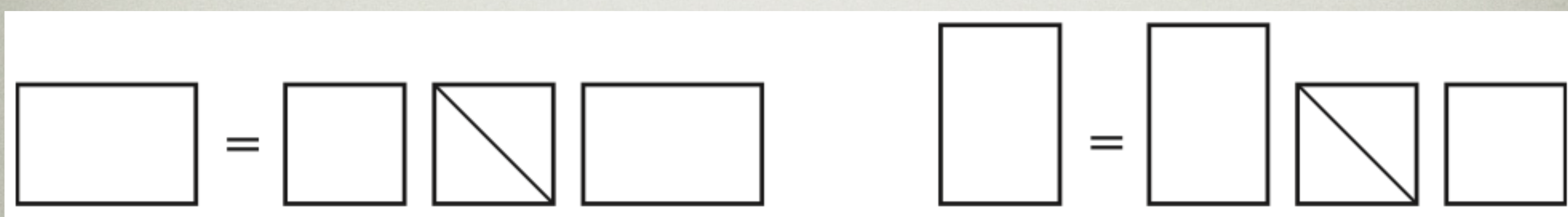
tensor network for a 2D system

Schmidt decomposition

$$|\psi\rangle = \sum_{ij} \Psi_{ij} |i\rangle_A |j\rangle_B$$

$$|\psi\rangle = \sum_{ij} \sum_{a=1}^{\min(N_A,N_B)} U_{ia} S_{aa} V^*_{ja} |i\rangle_A |j\rangle_B = \sum_{a=1}^{\min(N_A,N_B)} \left(\sum_i U_{ia} |i\rangle_A \right) s_a \left(\sum_j V^*_{ja} |j\rangle \right) = \sum_{a=1}^{\min(N_A,N_B)} s_a |a\rangle_A |a\rangle_B$$

singular value decomposition



$$|\psi\rangle = \sum_{a=1}^{r} s_a |a\rangle_A |a\rangle_B$$

$$\hat{\rho}_{\mathrm{A}} = \sum_{a=1}^{r} s_a^2 |a\rangle_{\mathrm{A}}\ {}_{\mathrm{A}}\langle a|, \quad \hat{\rho}_{\mathrm{B}} = \sum_{a=1}^{r} s_a^2 |a\rangle_{\mathrm{B}}\ {}_{\mathrm{B}}\langle a|$$

$$S_{A|B}(|\psi\rangle) = -\mathrm{Tr}\,\hat{\rho}_{\mathrm{A}} \log_2 \hat{\rho}_{\mathrm{A}} = -\sum_{a=1}^{r} s_a^2 \log_2 s_a^2$$

entropy of entanglement

$$\psi_{s_1 s_2} =$$

$$|\Psi\rangle = \sum_{s_1,\alpha,\alpha',s_2} A_{s_1\alpha} D_{\alpha\alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle$$

Matrix product states

L sites, i=1,...,L $\{\sigma_i\}$ $\dim = d$

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c_{\sigma_1,\ldots,\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle$$

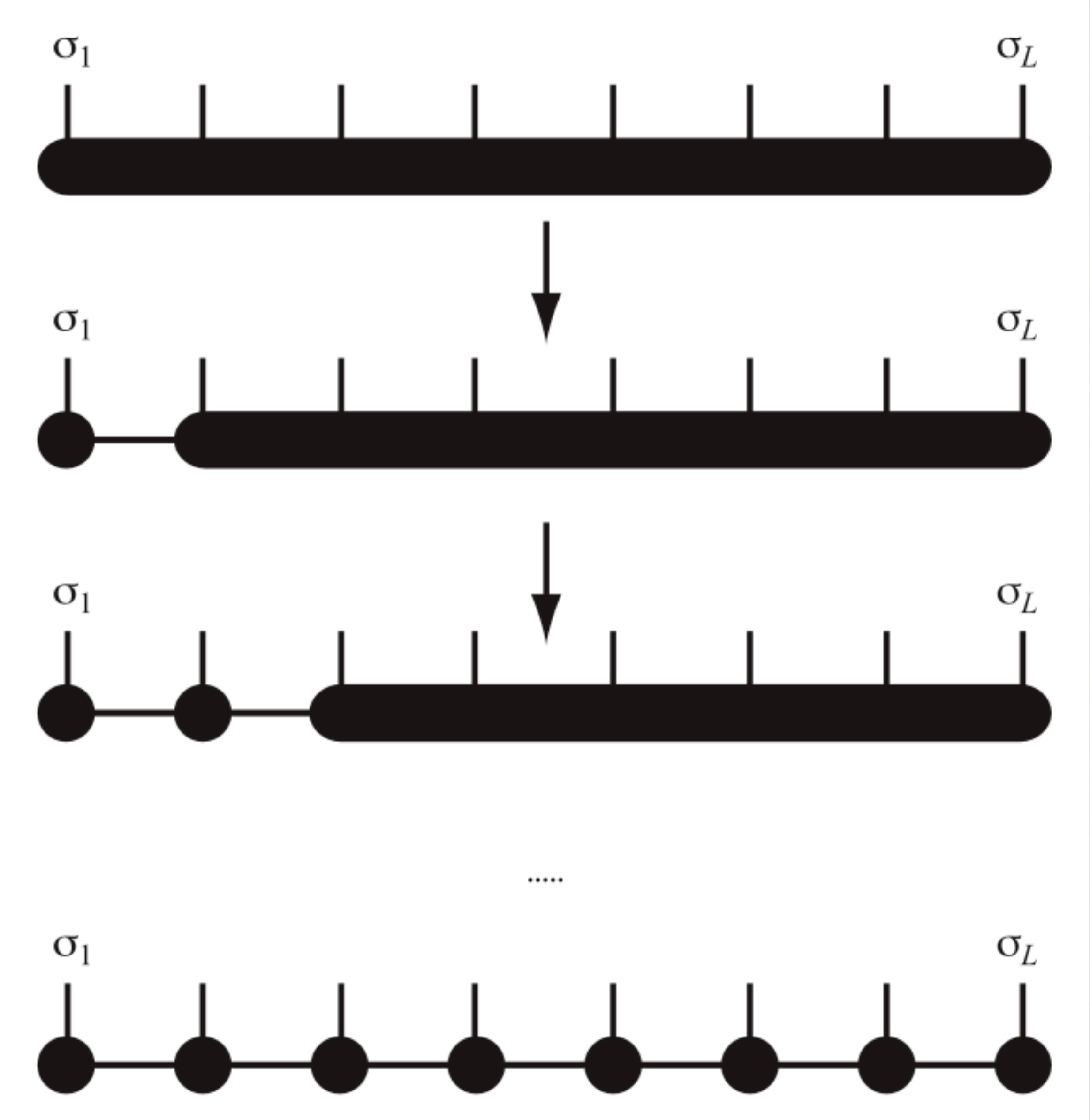
physical degree of freedom

$$c_{\sigma_1,\ldots,\sigma_L} = \sum_{a_1,\ldots,a_{L-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{L_1}}_{a_{L-2},a_{L-1}} A^{\sigma_L}_{a_{L-1}}$$

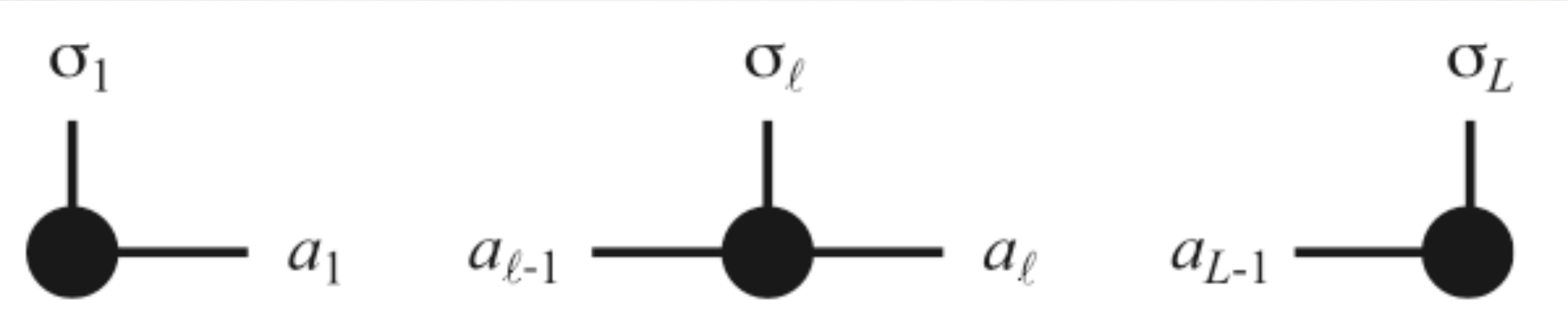
$$c_{\sigma_1,\ldots,\sigma_L} = A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_{L-1}} A^{\sigma_L}$$

auxiliary degree of freedom

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle$$

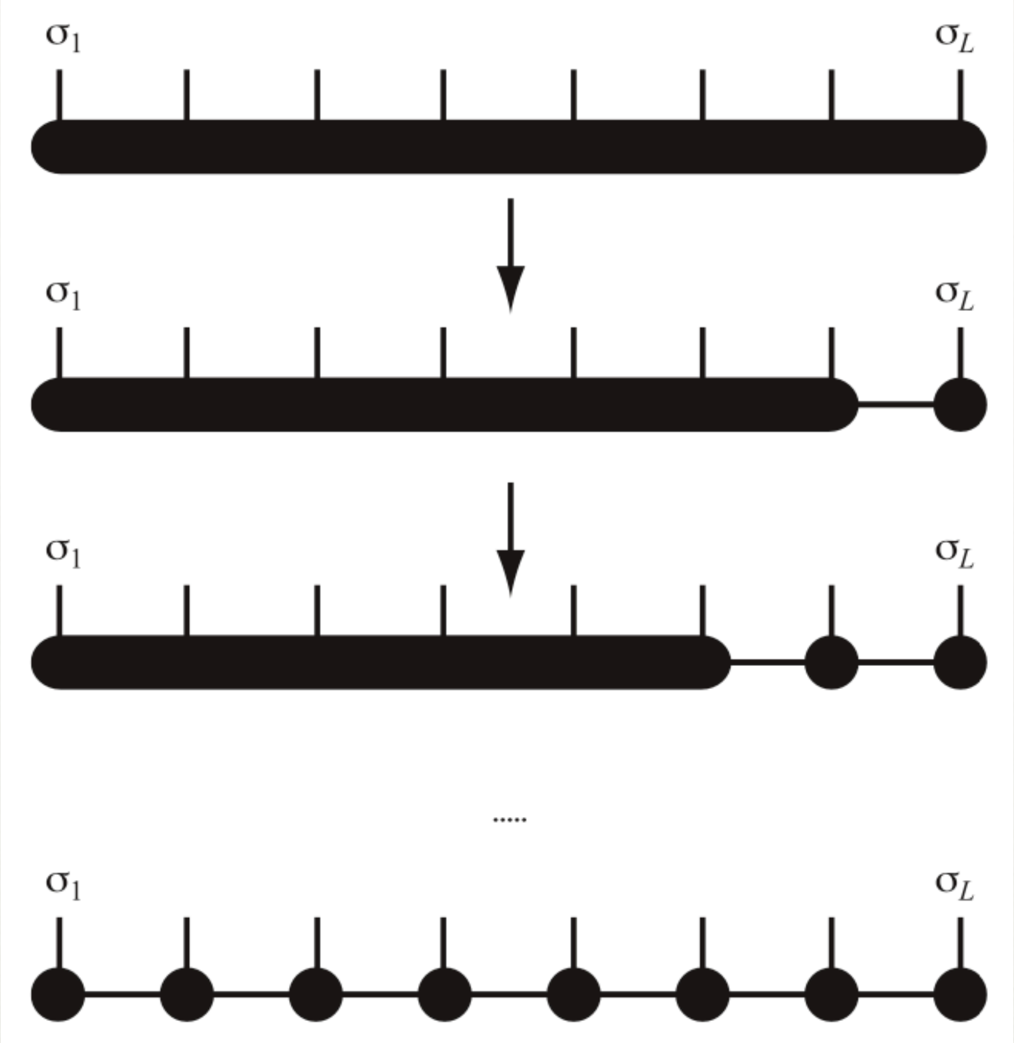


σ1
σL
σ1
σL
σ1
σL
.....
σ1
σL



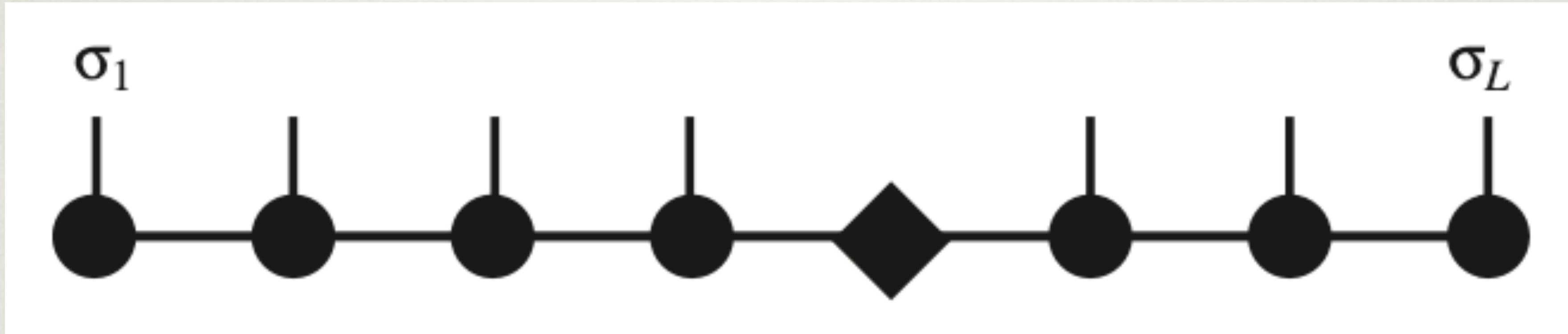
σ1
σℓ
σL
a1
aℓ-1
aℓ
aL-1

Representation is not unique (left-canonical, right-canonical, mixed-canonical).



$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} B^{\sigma_1} B^{\sigma_2} \cdots B^{\sigma_{L-1}} B^{\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle$$

$$c_{\sigma_1,\ldots,\sigma_L} = A^{\sigma_1} \cdots A^{\sigma_\ell} S B^{\sigma_{\ell+1}} \cdots B^{\sigma_L}$$



$$|\psi\rangle = \sum_{a_\ell} s_a |a_\ell\rangle_{\mathrm{A}} |a_\ell\rangle_{\mathrm{B}}$$

Truncation error: $\| |\psi\rangle - |\psi_{\mathrm{trunc}}\rangle \|_2^2 \leqslant 2 \sum_{i=1}^{L} \epsilon_i(D)$

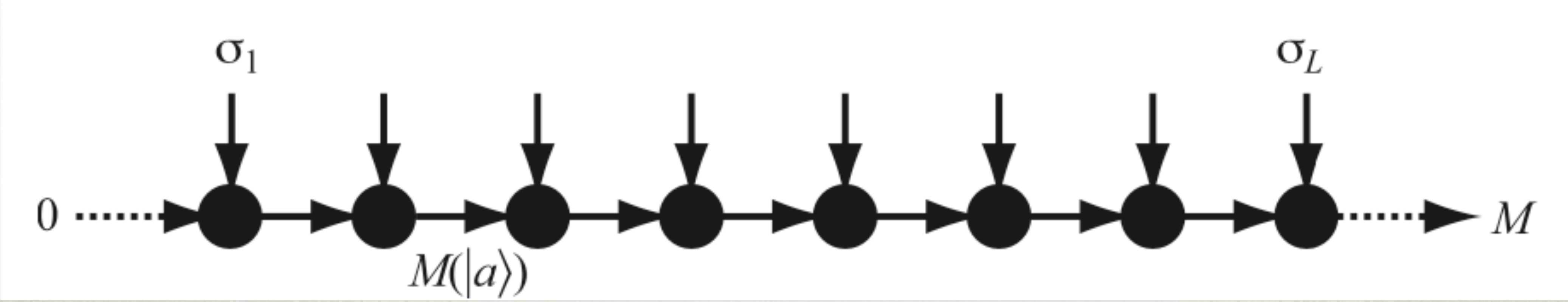
Compression: $d^L \rightarrow LD^2$

D=1: product state. D≥2: entangled state.

Symmetries

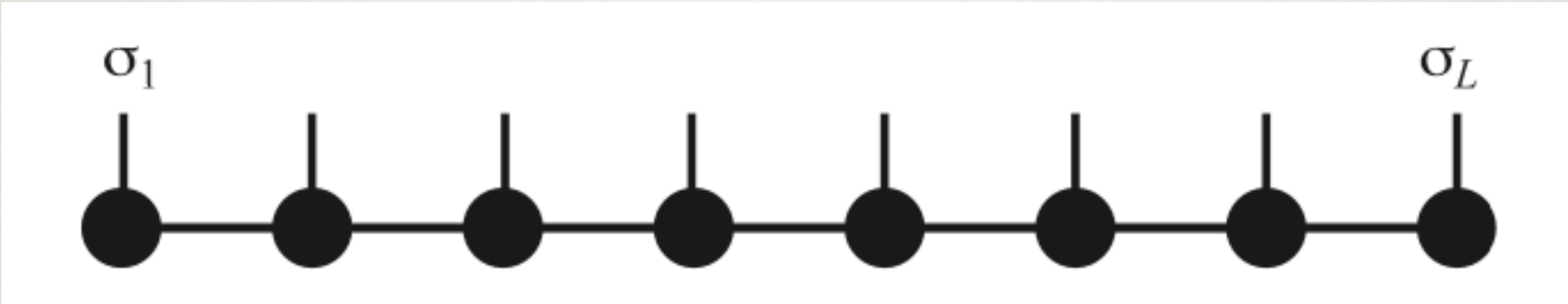
Abelian quantum numbers easy to implement.

$$M = \sum_i M_i$$

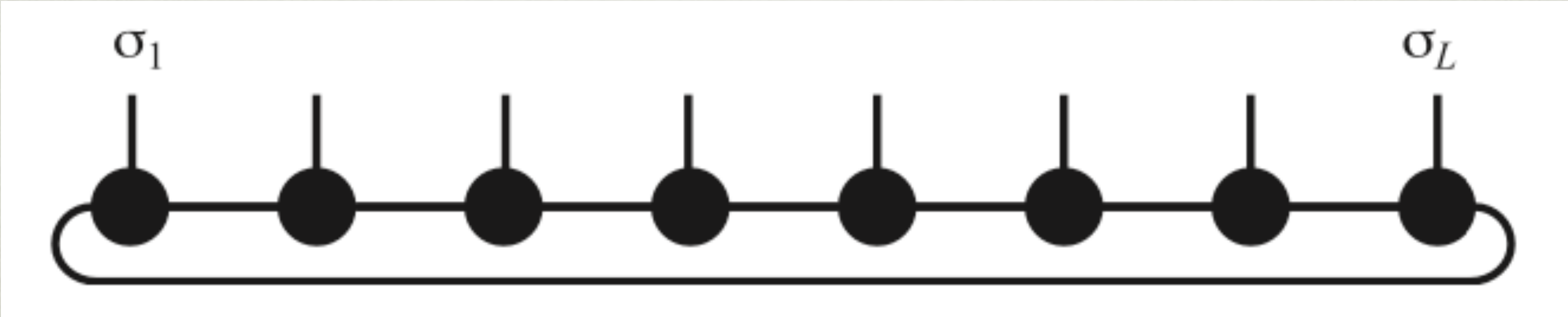


Imposes block structure upon matrices.

BOUNDARY CONDITIONS



$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} M^{\sigma_1} \cdots M^{\sigma_L} |\boldsymbol{\sigma}\rangle \quad \text{(MPS for OBC)}$$



$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{Tr}(M^{\sigma_1} \cdots M^{\sigma_L}) |\boldsymbol{\sigma}\rangle \quad \text{(MPS for PBC)}$$

AKLT states (Affleck-Kennedy-Lieb-Tasaki)

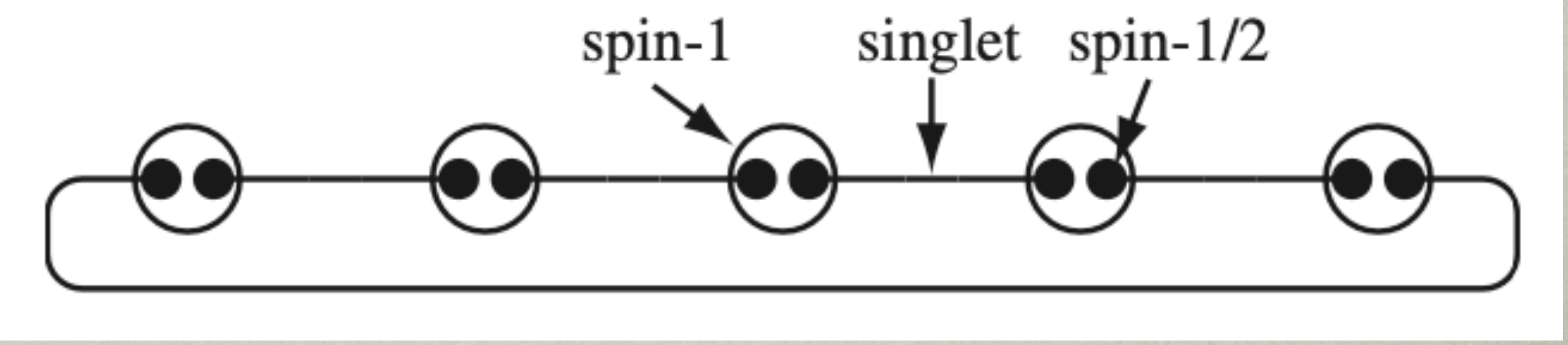
$$H = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$$

$$|+\rangle = |\uparrow\uparrow\rangle,$$
$$|0\rangle = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}},$$
$$|-\rangle = |\downarrow\downarrow\rangle.$$

$$M^{\sigma}_{ab}|\sigma\rangle\langle ab|$$

$$M^{+} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad M^{0} = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \quad M^{-} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$



$$|\psi\rangle = \sum_{\mathbf{a}} \sum_{\mathbf{b}} c_{\mathbf{ab}} |\mathbf{ab}\rangle$$

$|\mathbf{a}\rangle = |a_1, \ldots, a_L\rangle$ and $|\mathbf{b}\rangle = |b_1, \ldots, b_L\rangle$ representing the first and second spin-$\frac{1}{2}$ on each site.

$$|\Sigma^{[i]}\rangle = \sum_{b_i a_{i+1}} \Sigma_{ba} |b_i\rangle |a_{i+1}\rangle,$$

$$\Sigma = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

$$|\psi_\Sigma\rangle = \sum_{\mathbf{a}} \sum_{\mathbf{b}} \Sigma_{b_1 a_2} \Sigma_{b_2 a_3}, \ldots, \Sigma_{b_{L-1} a_L} \Sigma_{b_L a_1} |\mathbf{ab}\rangle$$

$$\sum_{\boldsymbol{\sigma}} \sum_{\mathbf{ab}} M^{\sigma_1}_{a_1 b_1} M^{\sigma_2}_{a_2 b_2} \cdots M^{\sigma_L}_{a_L b_L} |\boldsymbol{\sigma}\rangle\langle \mathbf{ab}|$$

$$\sum_{\boldsymbol{\sigma}} \sum_{\mathbf{ab}} M^{\sigma_1}_{a_1 b_1} \Sigma_{b_1 a_2} M^{\sigma_2}_{a_2 b_2} \Sigma_{b_2 a_3}, \ldots, \Sigma_{b_{L-1} a_L} M^{\sigma_L}_{a_L b_L} \Sigma_{b_L a_1} |\boldsymbol{\sigma}\rangle$$

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{Tr}(M^{\sigma_1} \Sigma M^{\sigma_2} \Sigma \cdots M^{\sigma_L} \Sigma])|\boldsymbol{\sigma}\rangle,$$

$$\widetilde{A}^{+} = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{bmatrix} \quad \widetilde{A}^{0} = \begin{bmatrix} -\frac{1}{2} & 0 \\ 0 & +\frac{1}{2} \end{bmatrix} \quad \widetilde{A}^{-} = \begin{bmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{Tr}(\widetilde{A}^{\sigma_1} \widetilde{A}^{\sigma_2} \cdots \widetilde{A}^{\sigma_L})|\boldsymbol{\sigma}\rangle$$

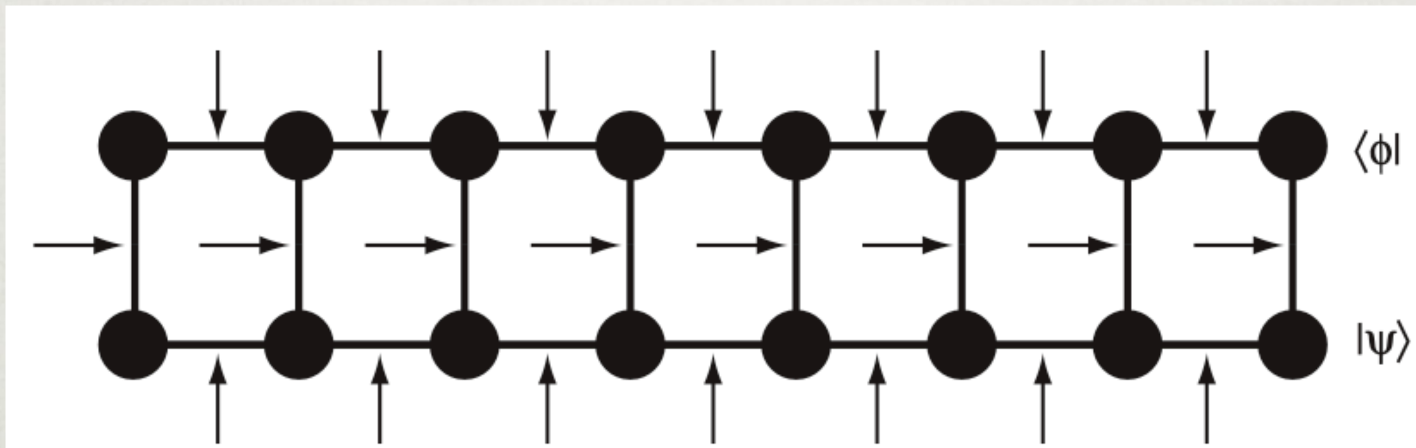
$$\left\langle S_i^z S_j^z \right\rangle \propto (-1/3)^{i-j}$$

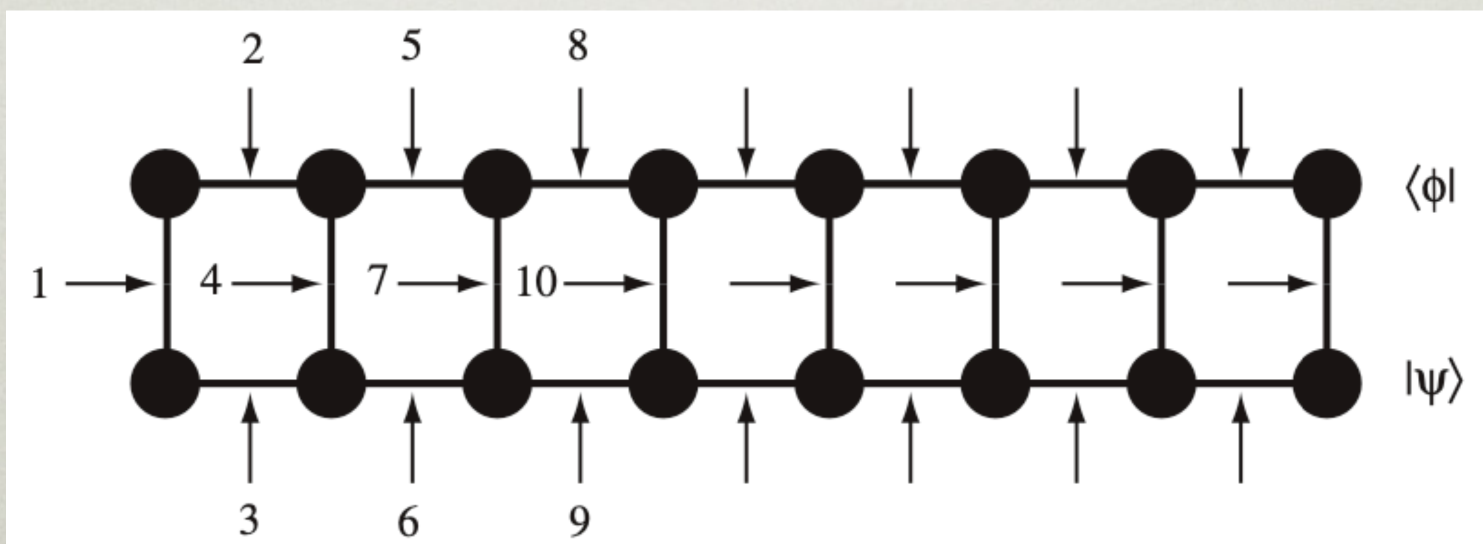
$$\left\langle S_i^z e^{i\pi \sum_{i<k<j} S_k^z} S_j^z \right\rangle = -4/9 \text{ for } j - i > 2$$

hidden order

Overlaps

$$\langle\phi|\psi\rangle = \sum_{\boldsymbol{\sigma}} \widetilde{M}^{\sigma_L\dagger} \cdots \widetilde{M}^{\sigma_1\dagger} M^{\sigma_1} \cdots M^{\sigma_L}$$



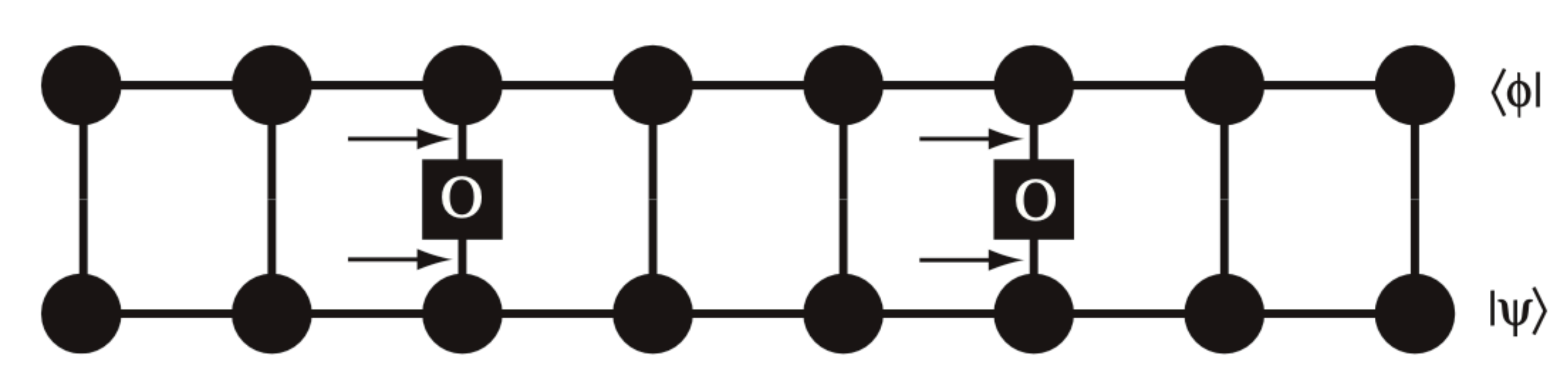


(2L-1)d multiplications, $O(D^3)$ each

Expectation values

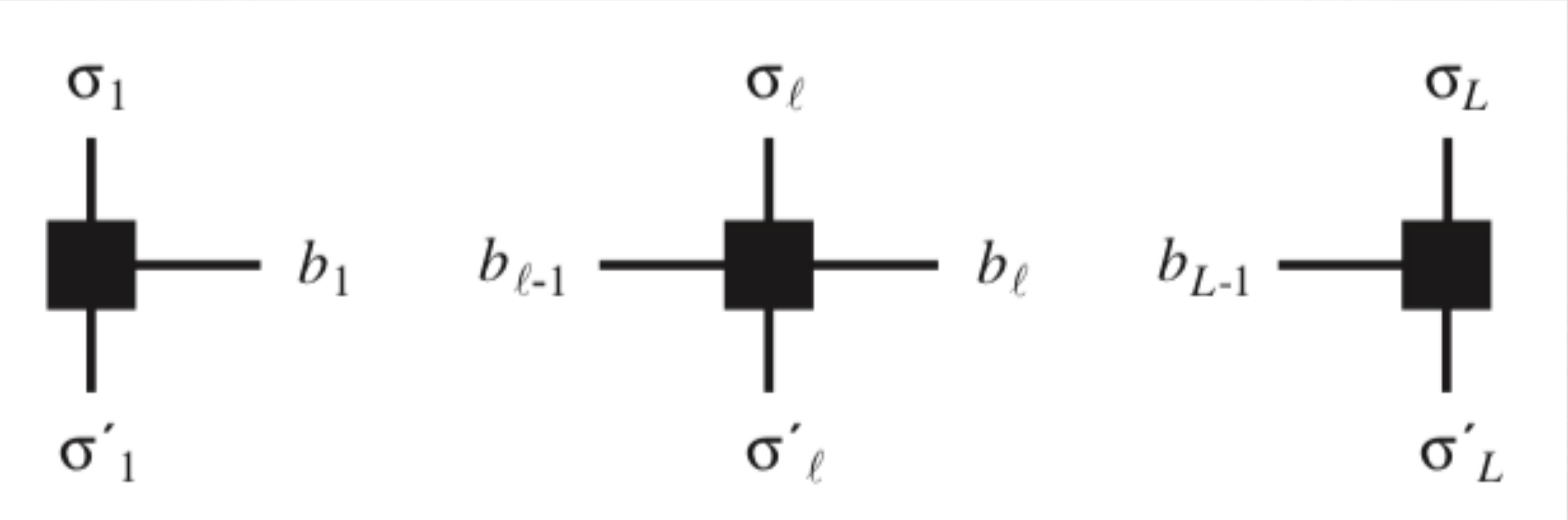
$$\left\langle \phi \middle| \widehat{O}^{[i]} \widehat{O}^{[j]} \cdots \middle| \psi \right\rangle$$

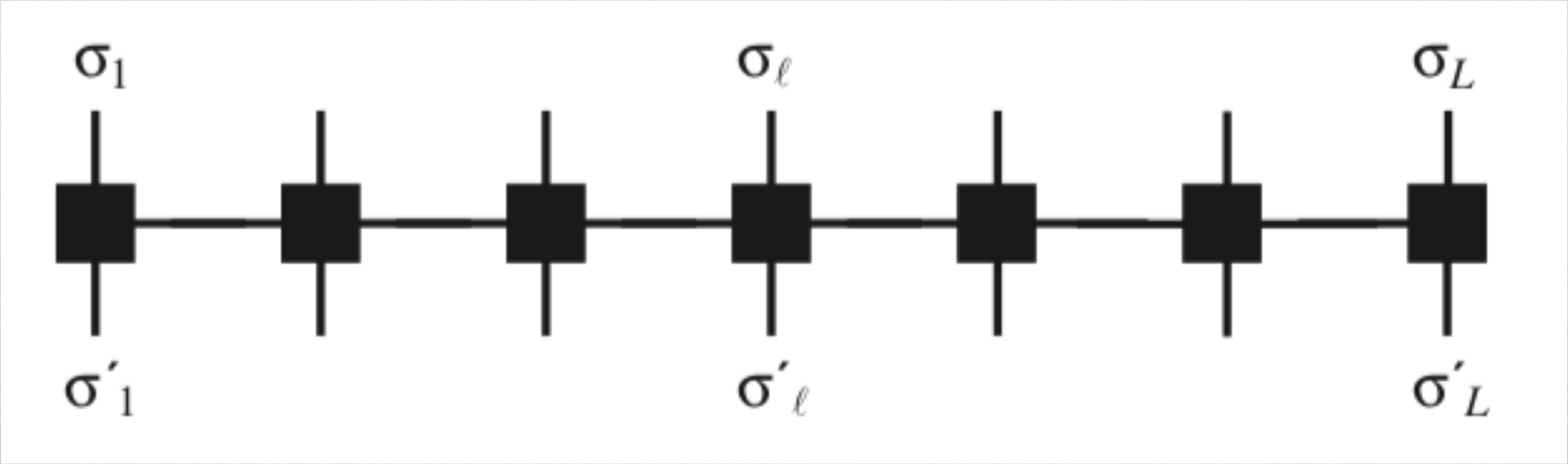
$$\widehat{O}^{[\ell]} = \sum_{\sigma_\ell, \sigma'_\ell} O^{\sigma_\ell, \sigma'_\ell} |\sigma_\ell\rangle\langle\sigma'_\ell|$$



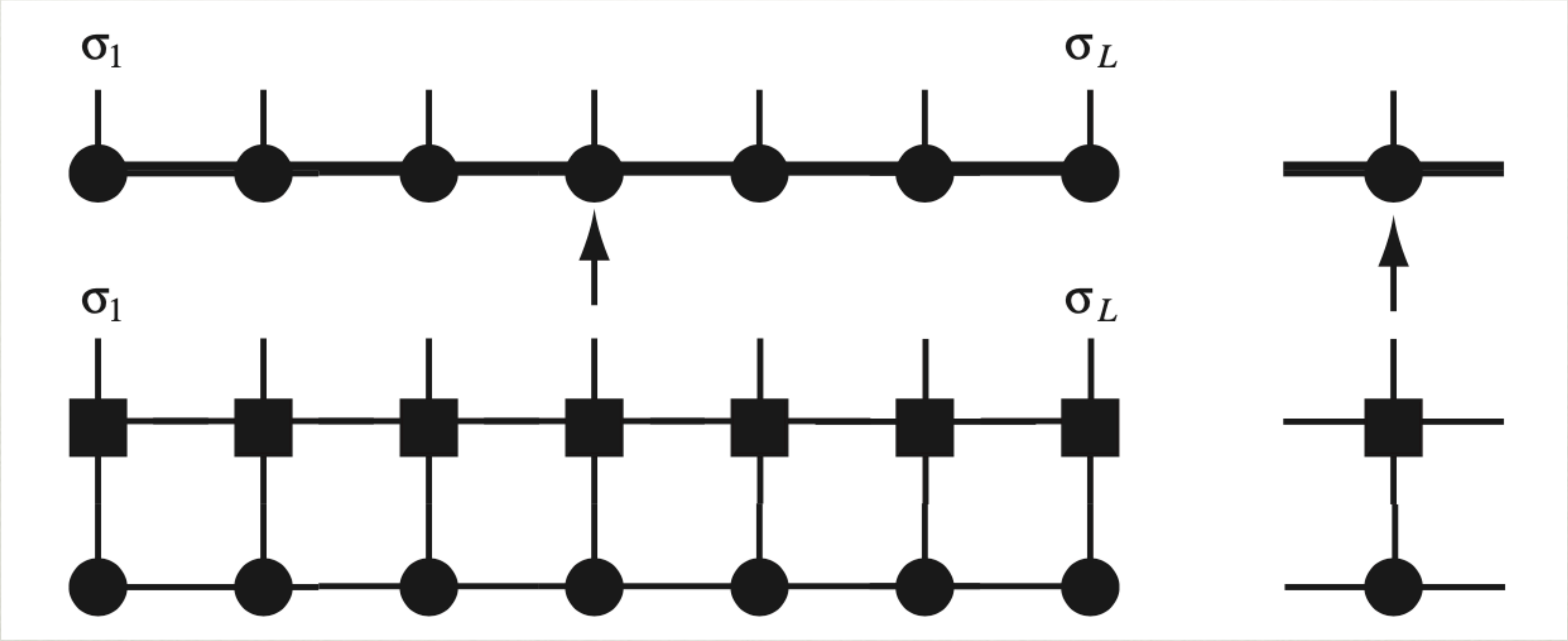
Matrix product operators

$$\hat{O} = \sum_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} W^{\sigma_1\sigma_1'} W^{\sigma_2\sigma_2'} \ldots W^{\sigma_{L-1}\sigma_{L-1}'} W^{\sigma_L\sigma_L'} |\boldsymbol{\sigma}\rangle\langle\boldsymbol{\sigma}'|$$





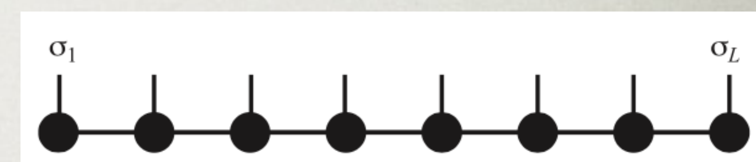
Schollwöck, Ann. Phys. (2011)



σ_1
σ_L
σ_1
σ_L

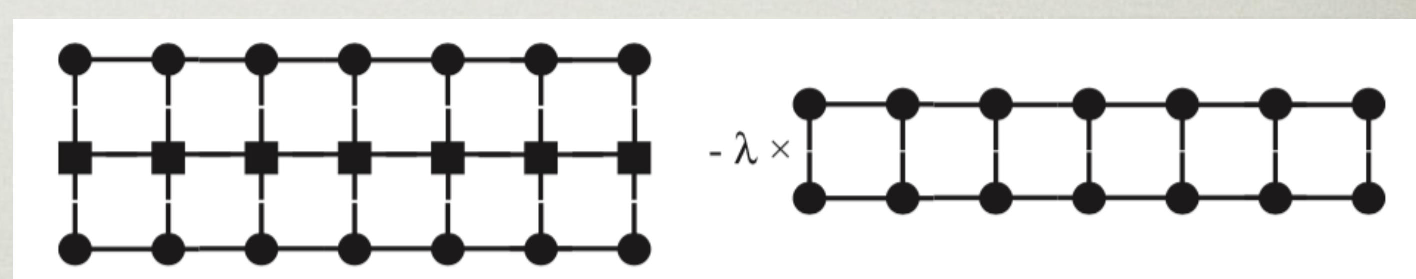
Density matrix renormalization group

matrix product state: $|\psi\rangle = \sum_{\boldsymbol{\sigma}} M^{\sigma_1} \cdots M^{\sigma_L} |\boldsymbol{\sigma}\rangle$



$$E = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$$

$$\langle\psi|\widehat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle.$$



https://itensor.org/

Schollwöck, Ann. Phys. (2011)

Sweeping

Consider all matrices except one fixed. Vary the elements of this matrix so as to extremize $\langle\psi|H|\psi\rangle - \lambda\langle\psi|\psi\rangle$.
Equivalent to a generalized eigenvalue problem $H\nu - \lambda N\nu = 0$

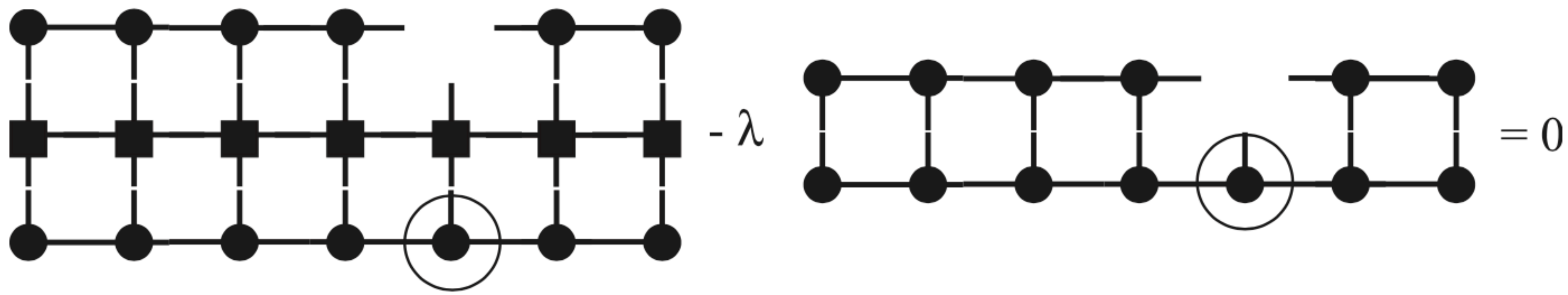


Fig. 41. Generalized eigenvalue problem for the optimization of $M^{\sigma_\ell}_{a_{\ell-1},a_\ell}$. The unknown matrix is circled on the left and right networks.

Eigenproblem becomes standard for open b.c.
Iterative eigensolvers (Jacobi-Davidson or Lanczos) needs to be used.

Sweep left to right and back.
Energy can only decrease--variational problem.
Good test: $\langle\psi|H^2|\psi\rangle - \left(\langle\psi|H|\psi\rangle\right)^2 \to 0$

Initial approximation may be bad. Compensate by doing many sweeps with small matrix sizes, then increase dimension D, and sweep further.

Avoiding metastable states

General problem, exacerbated if starting with small matrix sizes D.

Cause: conservation of the distribution of contributions to conserved quantum numbers in L and R blocks.

Solution: perturbation that expands the search space (and changes the distribution of quantum numbers).

White, PRB **72** 180403 (2005)

Excited states

a) If in different sector, then excited state is just a ground state in that different symmetry sector.

b) In the same sector, then i-th lowest state. All states must be orthogonal with respect to each other. We compute excited states one by one.

Time-dependent variation principle

$$e^{-iHt} \text{ or } e^{-\beta H}$$

Usually evaluated using Trotter decomposition.
But only applicable for short range (nearest-neighbours) interactions.

TDVP applicable to problems with long-range interaction.

Time-dependent variational principle with ancillary Krylov subspace

Mingru Yang and Steven R. White
Phys. Rev. B **102**, 094315 – Published 29 September 2020

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About ITensor

ITensor

Introduction

ITensor—Intelligent Tensor—is a library for implementing tensor network calculations. See the list of recent papers using ITensor.

Features include:

- Permuting indices is handled automatically when adding or contracting tensors
- Full-featured matrix product state / tensor train and DMRG layer
- Quantum number conserving (block-sparse) tensors; same interface as dense tensors
- Complex numbers handled automatically and efficiently
- Easy to install, with a friendly and productive interface
- Multi-threaded contraction over sparse tensor blocks
- Automatically convert sums of local operators to MPOs (AutoMPO)
- Efficiently apply local operators to MPS (quantum circuits, time evolution)

Latest Julia version is v0.2.9
View source on github
Documentation for the Julia version

Latest C++ version is v3.1.10
Clone from github (preferred)
Download: tar.gz or zip

On Twitter @ITensorLib
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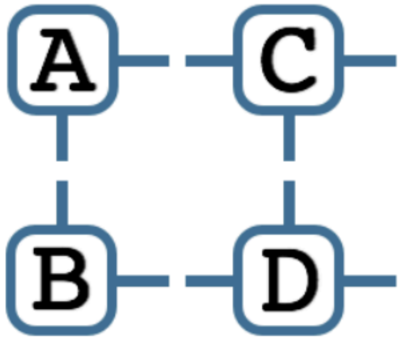
Recent News

ITensors have an interface resembling tensor diagram notation, making them nearly as easy to multiply as scalars: tensors indices have unique identities and matching indices automatically contract when two ITensors are multiplied. This type of interface makes it simple to transcribe tensor network diagrams into correct, efficient code.

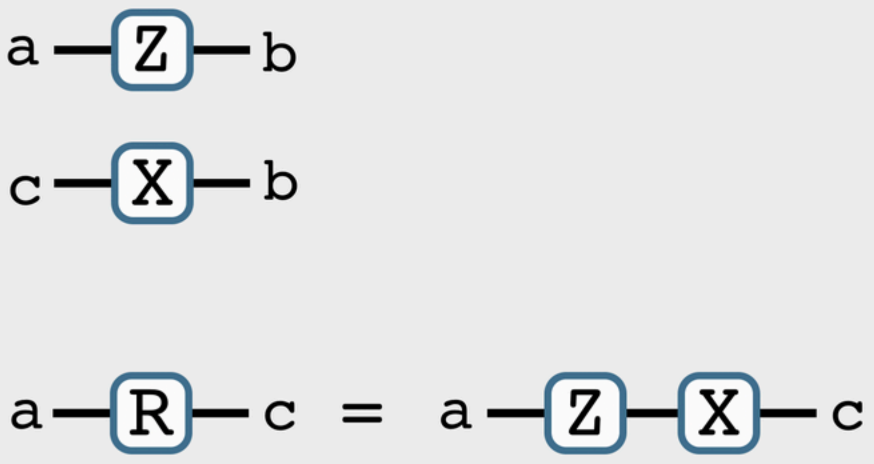
For example, the diagram below (resembling the overlap of matrix product states) can be converted to code as




```
= A*B*C*D
```

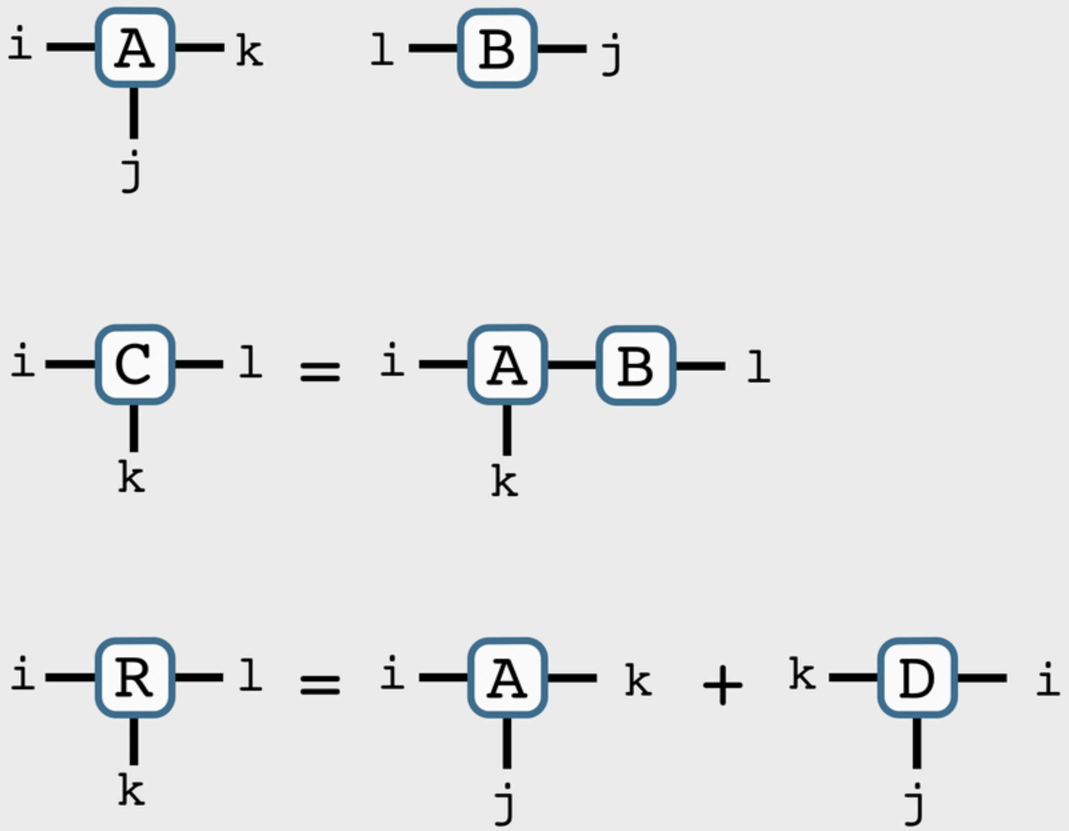
Contract Two Matrix-Like ITensors

```
auto a = Index(2),
auto b = Index(2),
auto c = Index(2);

auto Z = ITensor(a,b),
auto X = ITensor(c,b);

Z.set(a=1,b=1, +1.0);
Z.set(a=2,b=2, -1.0);

X.set(b=1,c=2, +1.0);
X.set(b=2,c=1, +1.0);

//the * operator finds and
//contracts common index 'b'
//regardless of index order:

ITensor R = Z * X;

Print( elt(R,a=2,c=1) );

//output:
// elt(R,a=2,c=1) = -1
```



Contract and Add ITensors

```
auto i = Index(3);
auto j = Index(5);
auto k = Index(2);
auto l = Index(7);

auto A = ITensor(i,j,k);
auto B = ITensor(l,j);

A.set(i=1,j=1,k=1, 11.1);
A.set(i=2,j=1,k=2, -21.2);
A.set(k=1,i=3,j=1, 31.1);
A.set(k=1,i=1,j=2, 11.2);

B.set(j=2,l=4, 2.+4._i);

auto C = A * B;
PrintData(C);

auto D = randomITensor(k,j,i);

auto R = A + D;
```



Factorize an ITensor (Using SVD)

```
auto i = Index(3,"i");
auto j = Index(7,"j");
auto k = Index(2,"k");
auto l = Index(4,"l");

auto T = randomITensor(i,j,k,l);

auto [U,S,V] = svd(T,i,k);

Print(norm(T - U*S*V));

//output:
// norm(T - U*S*V) = 4.7458E-14
```