The density matrix renormalization group

Adrian Feiguin

L=64; N=48; J=0.5
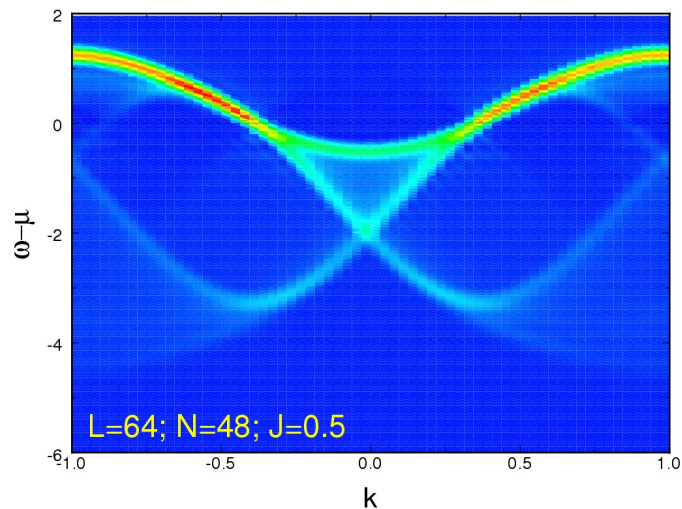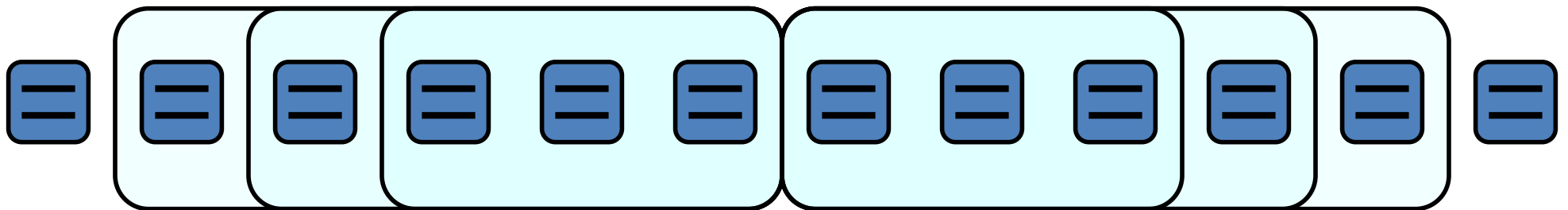
Source code (Python and C++)

These lectures:

http://www.github.com/afeiguin/
http://www.github.com/afeiguin/comp-phys

ALPS libraries and code:

http://alps.comp-phys.org

Some literature

-S. R. White:
. *Density matrix formulation for quantum renormalization groups*, Phys. Rev. Lett. 69, 2863 (1992).
. *Density-matrix algorithms for quantum renormalization groups*, Phys. Rev. B 48, 10345 (1993).

-U. Schollwöck
. *The density-matrix renormalization group*, Rev. Mod. Phys. 77, 259 (2005).

-Karen Hallberg
. *Density Matrix Renormalization: A Review of the Method and its Applications*
in Theoretical Methods for Strongly Correlated Electrons, CRM Series in Mathematical Physics, David Senechal, Andre-Marie Tremblay and Claude Bourbonnais (eds.), Springer, New York, 2003
. *New Trends in Density Matrix Renormalization*, Adv. Phys. **55**, 477 (2006).

-The "DMRG BOOK": *Density-Matrix Renormalization - A New Numerical Method in Physics: Lectures of a Seminar and Workshop held at the Max-Planck-Institut für Physik ... 18th, 1998 (Lecture Notes in Physics)* by Ingo Peschel, Xiaoqun Wang, Matthias Kaulke and Karen Hallberg

-R. Noack and S. Manmana: *Diagonalization- and Numerical Renormalization-Group-Based Methods for Interacting Quantum Systems*
Proceedings of the "IX. Training Course in the Physics of Correlated Electron Systems and High-Tc Superconductors", Vietri sul Mare (Salerno, Italy, October 2004)
AIP Conf. Proc. 789, 93-163 (2005)

-A.E. Feiguin: *The Density Matrix Renormalization Group and its time-dependent variants*
Vietri Lecture Notes, AIP Conference Proceedings **1419**, 5 (2011); https://doi.org/10.1063/1.3667323

- F. Verstraete , V. Murg & J.I. Cirac: Matrix product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems, Advances in Physics, 57:2, 143-224 (2008)

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

- Frank Pollman's lecture notes: Efficient Numerical Simulations Using Matrix-Product States
(https://www.ggi.infn.it/sft/SFT_2016/LectureNotes/Pollmann.pdf) and Efficient numerical simulations with Tensor Networks: Tensor Network Python (TeNPy); Johannes Hauschild, Frank Pollmann; SciPost Phys. Lect. Notes 5 (2018)

- Roman Orus: A practical introduction to tensor networks: Matrix product states and projected entangled pair states, Annals of Physics 349 (2014) 117-158 (2014)

Brief history and milestones

- (1992) Steve White introduces the DMRG.
- (1995-…) Dynamical DMRG. (Hallberg, Ramasesha et al, Kuhner and White, Jeckelmann)
- (1995) Nishino introduces the transfer-matrix DMRG (TMRG) for classical systems.
- (1996-97) Bursill, Wang and Xiang, Shibata, generalize the TMRG to quantum problems.
- (1996) Xiang adapts DMRG to momentum space.
- (2001) Shibata and Yoshioka study FQH systems.
- (2004) Vidal introduces the TEBD. (time-evolving block decimation)
- (2005) Verstraete and Cirac introduce an alternative algorithm for MPS's and explain problem with DMRG and PBC.
- (2006) White and AEF, and Daley, Kollath, Schollwoeck, Vidal generalize the ideas within a DMRG framework: adaptive tDMRG.

… the DMRG has been used in a variety of fields and contexts, from classical systems to quantum chemistry, to nuclear physics…
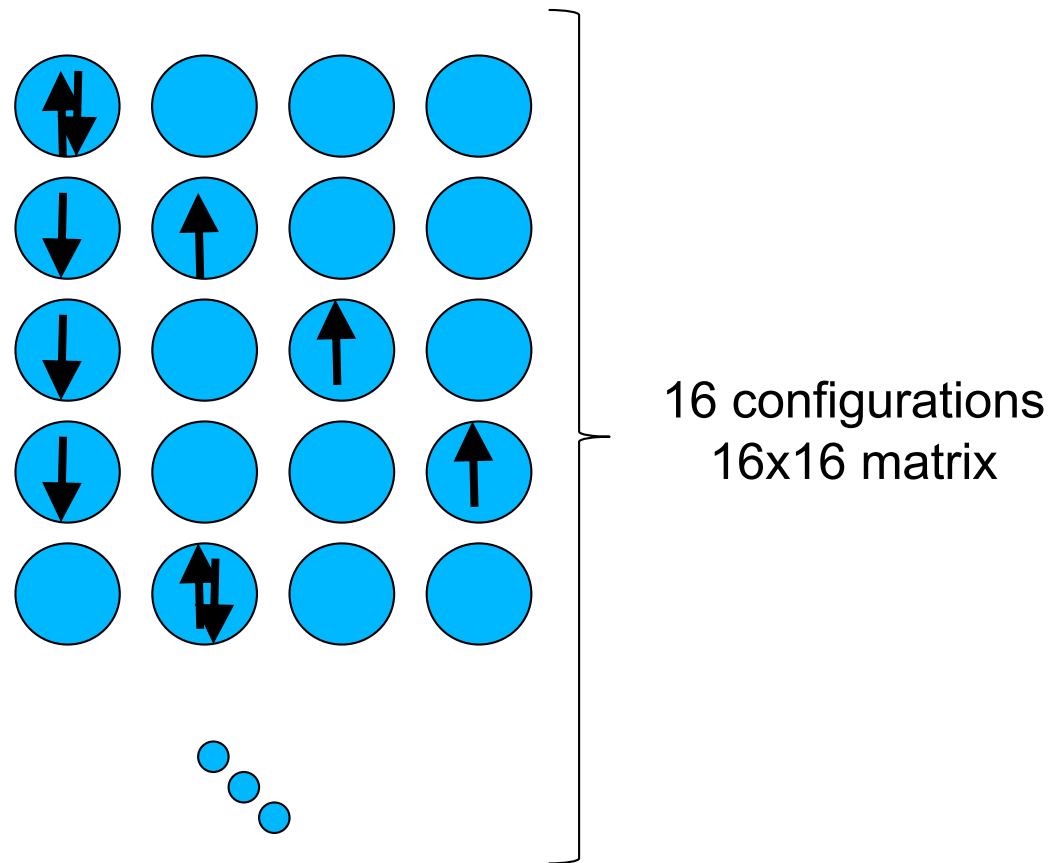
Single particle vs. many body picture

4 configurations
4x4 matrix
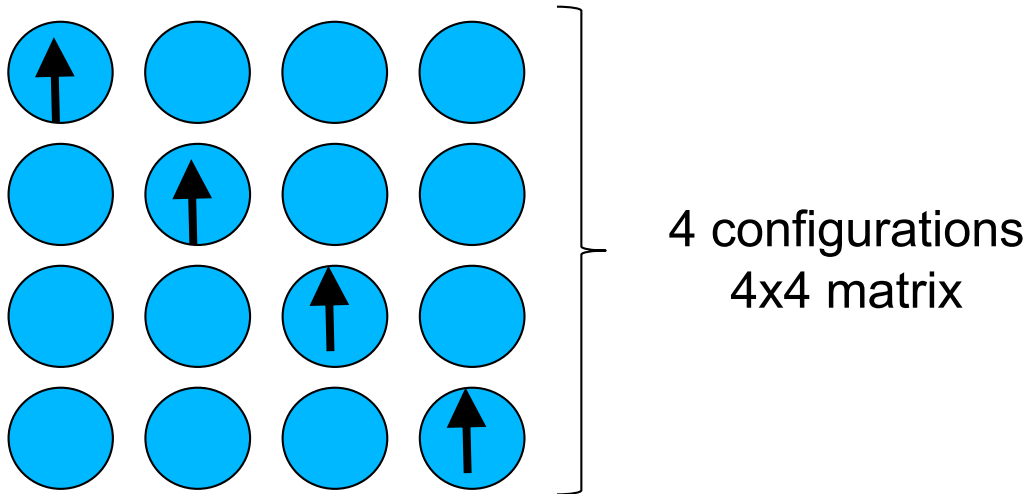
And similarly for the "down" electrons

E_F
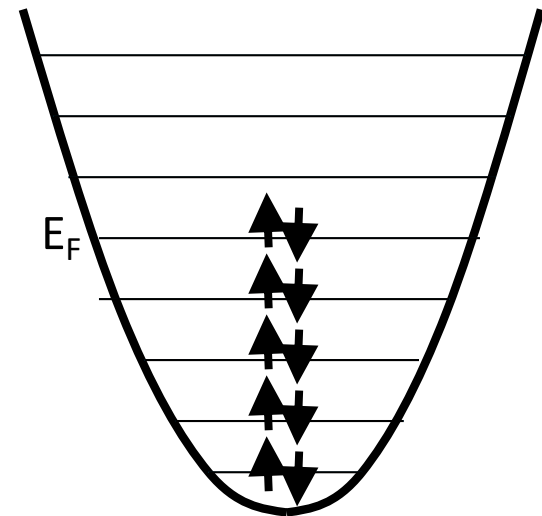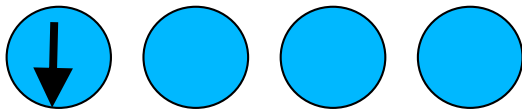
The state of the system is a "product state" of single particle states. We only need to solve the one-particle problem.Think "Hydrogen atom".

Single particle vs. many body picture

16 configurations
16x16 matrix

The state of the system is "highly entangled". It cannot be written as a "product state", and the behavior of each electron is dictated by the behavior of the rest.(Notice that in some case Bethe Ansatz tells us that some many-body states can still be reduced to product states)

Exact diagonalization

"__brute force__" diagonalization of the Hamiltonian matrix.

Schrödinger's Equation:
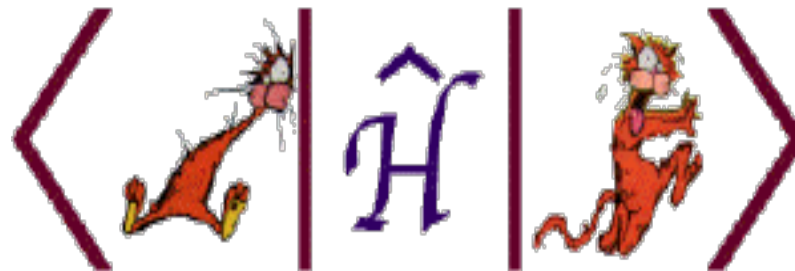
$$H \ket{x} = E \ket{x}$$

H : Hamiltonian operator
$\ket{x}$: eigenstate
E : eigenvalue (ENERGY)

... anything you want to know... **but... only small systems**

All we need to do is to pick a basis and write the Hamiltonian matrix in that basis
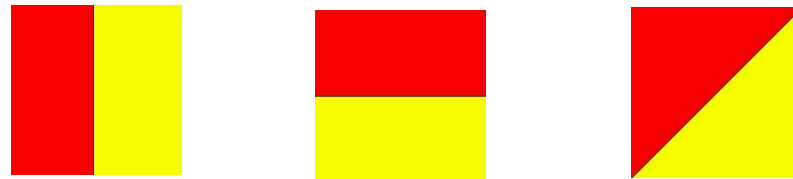
Symmetries *SH=HS*

Particle number conservation => N_{total}

Spin conservations => S^z_{total}

Spin reversal => $|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle$
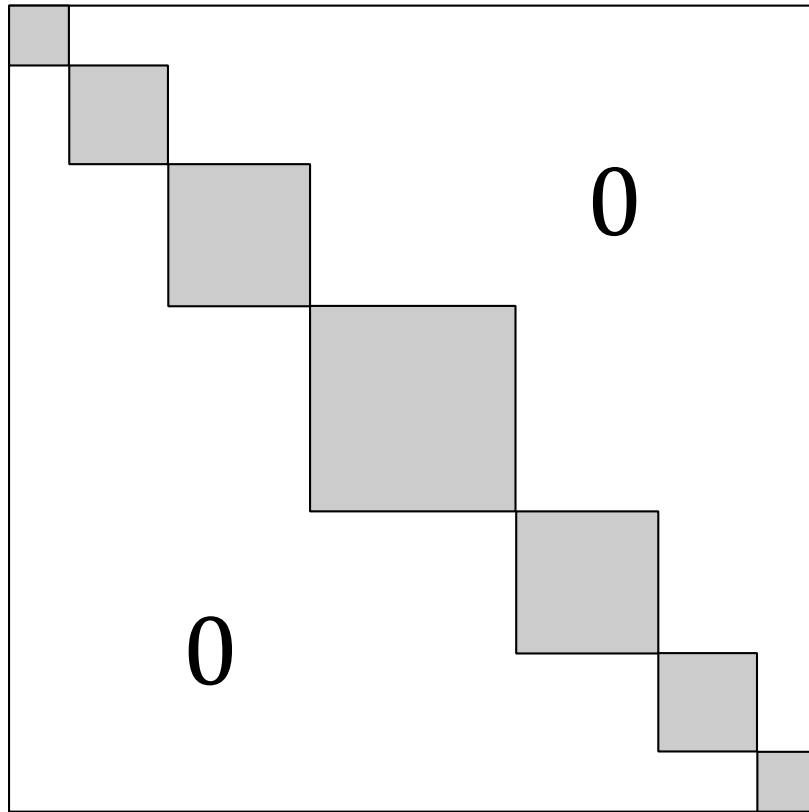
Reflections

$D' = D / 2$

Translations

$D' = D / N$

$$|\psi_{\boldsymbol{k}}\rangle = (1/M) \sum_i a_{\boldsymbol{k}_i} T_i |\phi\rangle; \quad a_{\boldsymbol{k}_i} = \exp(i\boldsymbol{k}x_i)$$
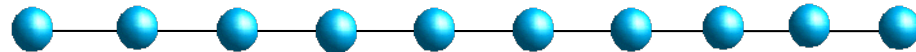
Block diagonalization

ED Example: Heisenberg chain

Model Hamiltonian:

$$H_{Heis} = J \sum_{<i,j>} S_i^z S_j^z + 1/2 \, (S_i^- S_j^+ + S_i^+ S_j^-)$$

Geometry:

1D chain

Basis:

$|\uparrow\downarrow\uparrow\downarrow\rangle; \, |\downarrow\uparrow\downarrow\uparrow\rangle;$

$|\uparrow\uparrow\downarrow\downarrow\rangle; \, |\downarrow\uparrow\uparrow\downarrow\rangle; \, |\downarrow\downarrow\uparrow\uparrow\rangle; \, |\uparrow\downarrow\downarrow\uparrow\rangle$

Translations

Applying translations:

$$|1\rangle = 1/(2\sqrt{2})\{(1+ e^{i2k})|\uparrow\downarrow\uparrow\downarrow\rangle + e^{ik}(1+e^{i2k})|\downarrow\uparrow\downarrow\uparrow\rangle\}$$

$$|2\rangle = 1/2\{|\uparrow\uparrow\downarrow\downarrow\rangle + e^{ik}|\downarrow\uparrow\uparrow\downarrow\rangle + e^{i2k}|\downarrow\downarrow\uparrow\uparrow\rangle + e^{i3k}|\uparrow\downarrow\downarrow\uparrow\rangle\}$$

With $k = 0, -\pi/2, \pi/2, \pi$

$k=0)$

$$|1\rangle = 1/\sqrt{2}\{|\uparrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle\}$$
$$|2\rangle = 1/2\{|\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle\}$$

$k= -\pi/2)$

$$|2\rangle = 1/2\{|\uparrow\uparrow\downarrow\downarrow\rangle + e^{-i\pi/2}|\downarrow\uparrow\uparrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle + e^{i\pi/2}|\uparrow\downarrow\downarrow\uparrow\rangle\}$$

$k= \pi/2)$

$$|2\rangle = 1/2\{|\uparrow\uparrow\downarrow\downarrow\rangle + e^{i\pi/2}|\downarrow\uparrow\uparrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle + e^{-i\pi/2}|\uparrow\downarrow\downarrow\uparrow\rangle\}$$

$k= \pi)$

$$|1\rangle = 1/\sqrt{2}\{|\uparrow\downarrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\uparrow\rangle\}$$
$$|2\rangle = 1/2\{|\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle\}$$

Limitations : small lattices

- Hubbard model: 20 sites at half filling, 10↑ and 10↓, D=20!(10!10!)x20!(10!10!) = 2.4e+10. After symmetries D'=1.1e+8

- *t-J* model (only $|o\rangle$, $|\uparrow\rangle$ and $|\downarrow\rangle$ states): 32 sites with 4 holes, 14↑ and 14↓, D = 32!/(14!18!)x18!/(14!4!) = 1.4e+12; D'=5.6e9

- Heisenberg model (only $|\uparrow\rangle$ and $|\downarrow\rangle$ states): 36 sites, 18↑ and 18↓, D = 36!/(18!18!)=9075135300; D' $=D$/(36x2x2x2x2)=1.5e6 states

Exact diag. is limited by system size… How can we overcome this problem?

Po' man's solution: What about truncating the basis?
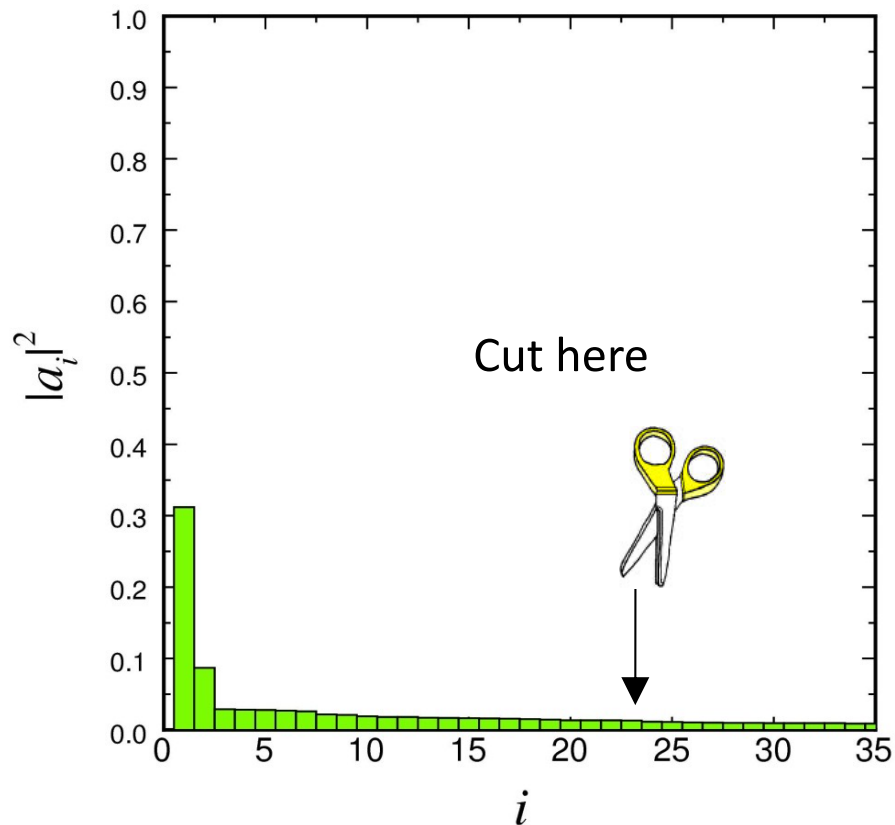
"Classical" analogy
Image compression algorithms (e.g. Jpeg)

We want to achieve "lossless compression"
... or at least minimize *the loss of information*

Idea 1: Truncated diagonalization

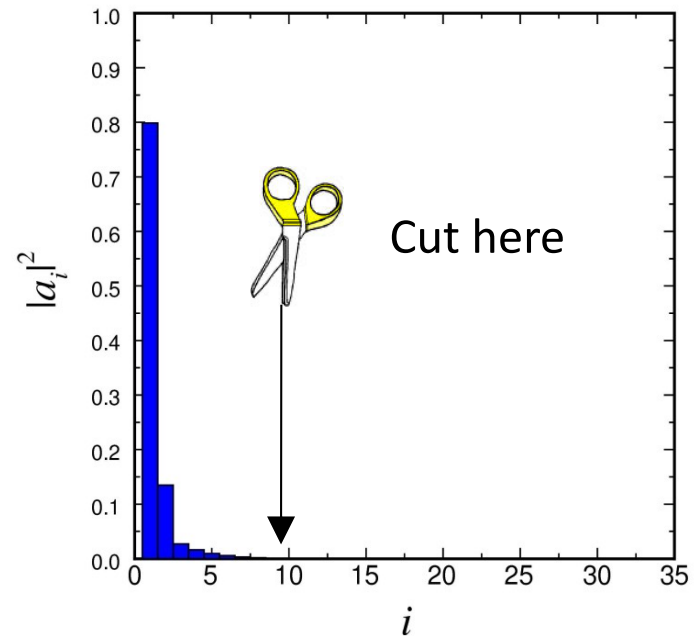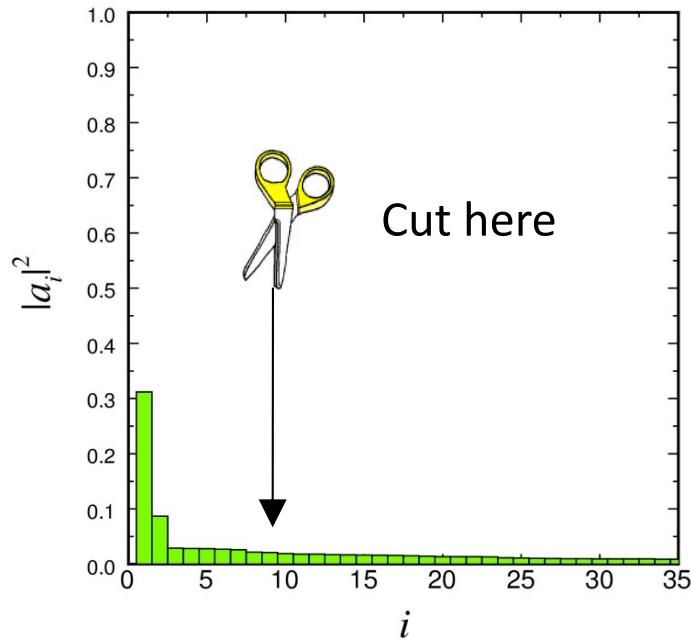$$|gs\rangle = \sum a_i |x_i\rangle \quad , \sum |a_i|^2 = 1$$

Cut here

Usually, only a few important states possess most of the weight

$$\leftarrow Error = 1 - \sum{}' |a_i|^2$$

Idea 2: Change of basis

Can we rotate our basis to one where the weights are more concentrated, to minimize the error?

$$|gs\rangle = \sum a_i |x_i\rangle \ , \ \sum |a_i|^2 = 1 \implies Error = 1 - \sum' |a_i|^2$$

The case of spins

The two-site basis is given by the states

$$|\sigma\sigma'\rangle = \{|\uparrow\uparrow\rangle; |\uparrow\downarrow\rangle; |\downarrow\uparrow\rangle; |\downarrow\downarrow\rangle\}$$

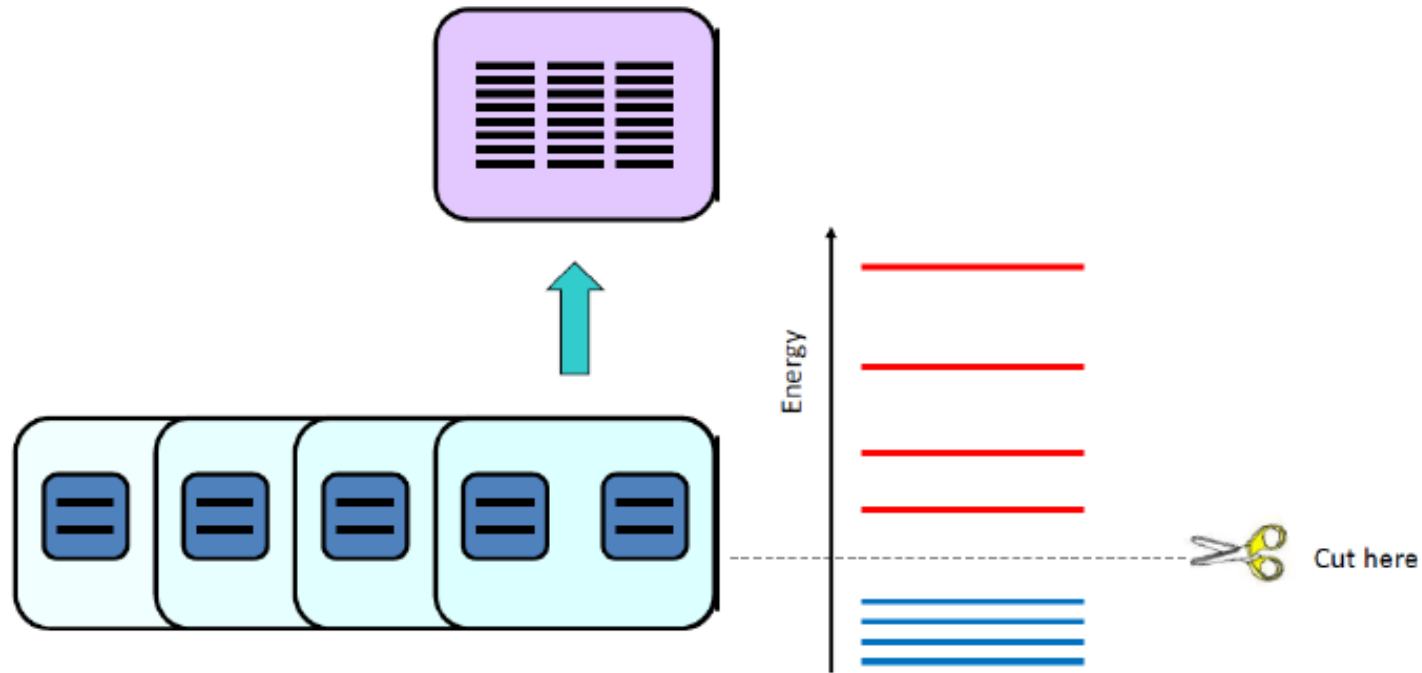We can easily diagonalize the Hamiltonian by rotating with the matrix:

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

That yields the eigenstates:

$$|s\rangle = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]$$

$$|t\rangle = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle]$$

Numerical Renormalization Group

Let's consider the 1d Heisenberg model

$$H = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} = \sum_i S_i^z S_{i+1}^z + \frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)$$

For a single site ⬤ , the operator matrices are:

$$S_0^z = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}; S_0^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}; S_0^- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

We also need to define the identity on a block of l sites

$$I_l = \begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}; \text{ with dimensions } 2^l \times 2^l$$
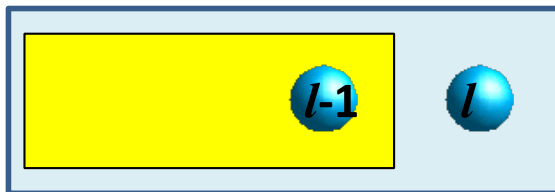
Building the Hamiltonian a la NRG

$$H_2 = S_0^z \otimes S_0^z + \frac{1}{2} S_0^+ \otimes S_0^- + \frac{1}{2} S_0^- \otimes S_0^+$$

$$H_3 = H_2 \otimes I_1 + I_1 \otimes \left[S_0^z \otimes S_0^z + \frac{1}{2} S_0^+ \otimes S_0^- + \frac{1}{2} S_0^- \otimes S_0^+ \right]$$

$$\rightarrow H_l = H_{l-1} \otimes I_l + I_{l-2} \otimes H_2$$

This recursion will generate a $2^l \times 2^l$ Hamiltonian matrix that we can easily diagonalize
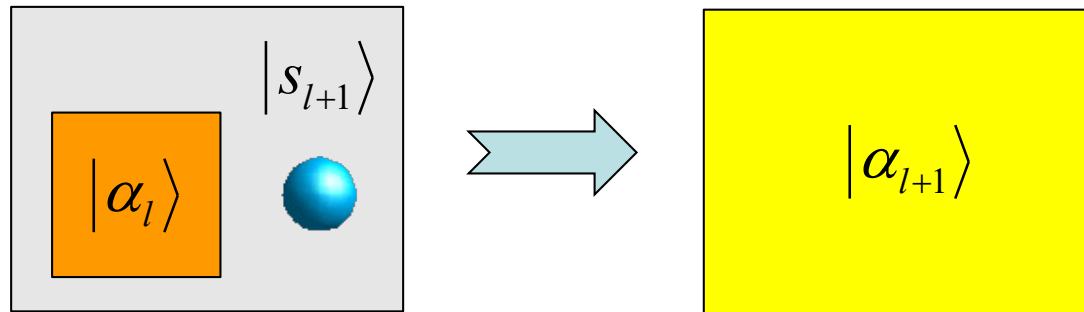
Another way to put it…

$$H_l = H_{l-1} \otimes I_1 + I_{l-2} \otimes \left[S_0^z \otimes S_0^z + \frac{1}{2} S_0^+ \otimes S_0^- + \frac{1}{2} S_0^- \otimes S_0^+ \right]$$

$$= H_{l-1} \otimes I_1 + \left(I_{l-2} \otimes S_0^z \right) \otimes S_0^z + \frac{1}{2} \left(I_{l-2} \otimes S_0^+ \right) \otimes S_1^- + \frac{1}{2} \left(I_{l-2} \otimes S_0^- \right) \otimes S_0^+$$

$$= H_{l-1} \otimes I_1 + S_{l-1}^z \otimes S_0^z + \frac{1}{2} S_{l-1}^+ \otimes S_0^- + \frac{1}{2} S_{l-1}^- \otimes S_0^+$$

with $\qquad O_l = I_{l-1} \otimes O_0$

Adding a single site to the block

Before truncating we build the new basis as:

$$\left|\alpha_{l+1}\right\rangle = \left|\alpha_l\right\rangle \otimes \left|s_{l+1}\right\rangle$$

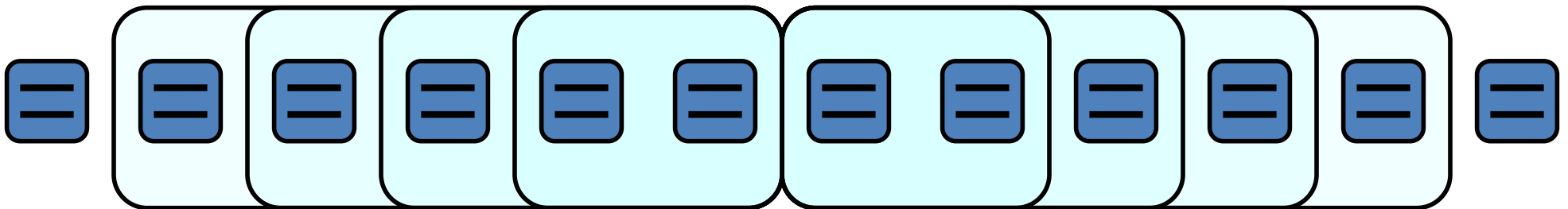And the Hamiltonian for the new block as

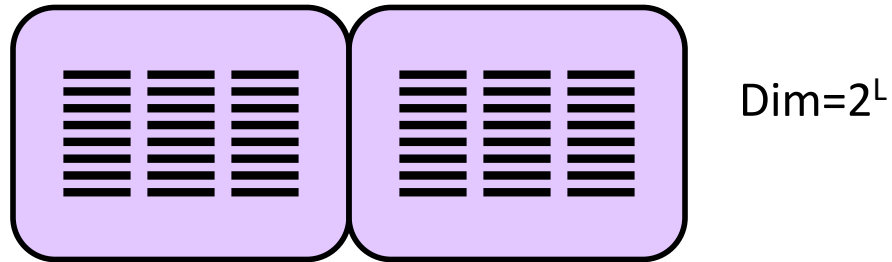$$H_{L,l+1} = H_{L,l} \otimes I_1 + I_l \otimes H_0 + O_{L,l} \otimes O'_0 + \ldots$$

with $\qquad O_{L,l} = I_{l-1} \otimes O_0$

Idea 3: Density Matrix Renormalization Group

$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle$$

Dim=2^L

Dimension of the block grows exponentially

Block decimation

$$|\psi\rangle = \sum_{ij}\psi_{ij}|i\rangle|j\rangle$$
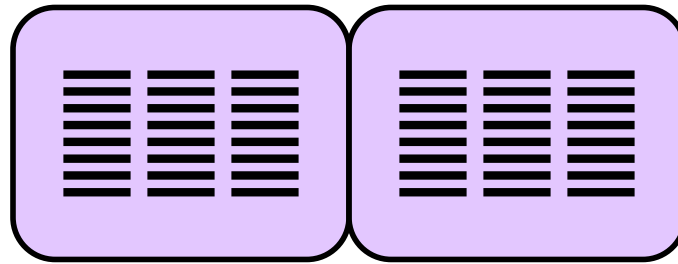
Dim=2^N $\longrightarrow$ Dim=m

constant

The density matrix projection

Universe

system

$|i\rangle$

environment

$|j\rangle$
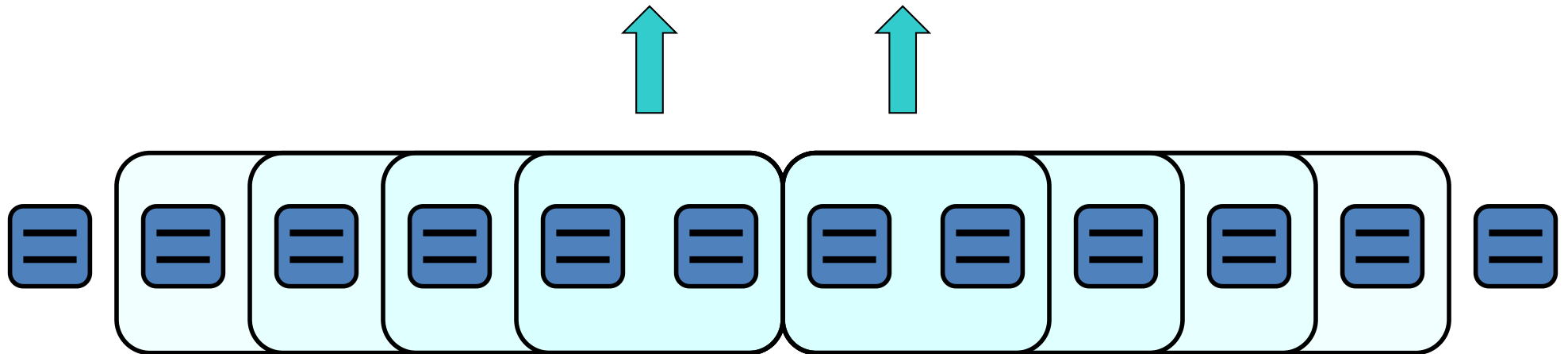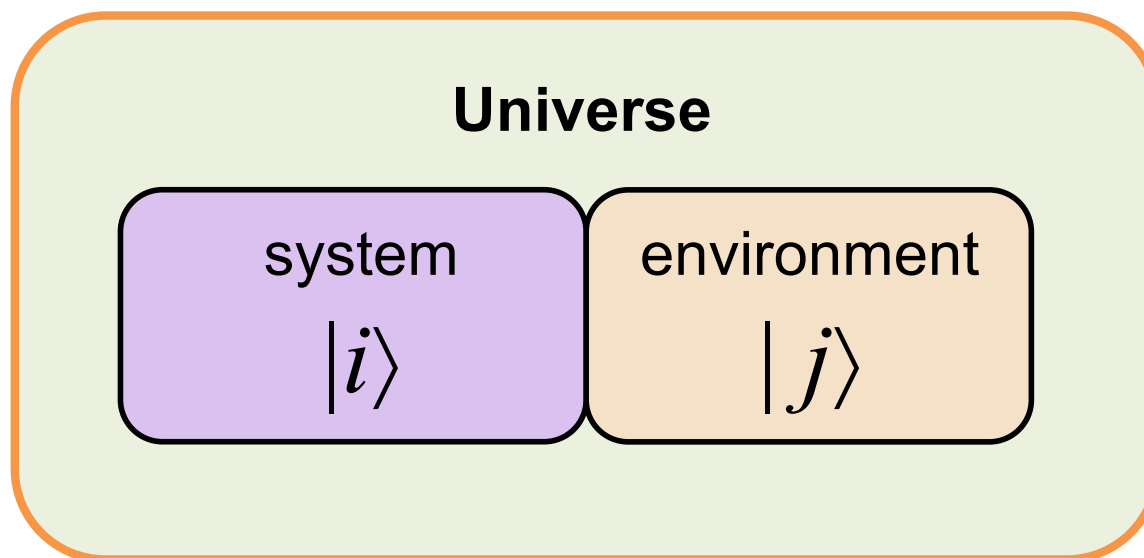
Solution: The optimal states are the eigenvectors of the reduced density matrix

$$\rho_{ii'} = \sum_j \psi^*_{ij} \psi_{i'j} \qquad \text{Tr } \rho = 1$$

with the m largest eigenvalues ω_α

Understanding the density-matrix projection
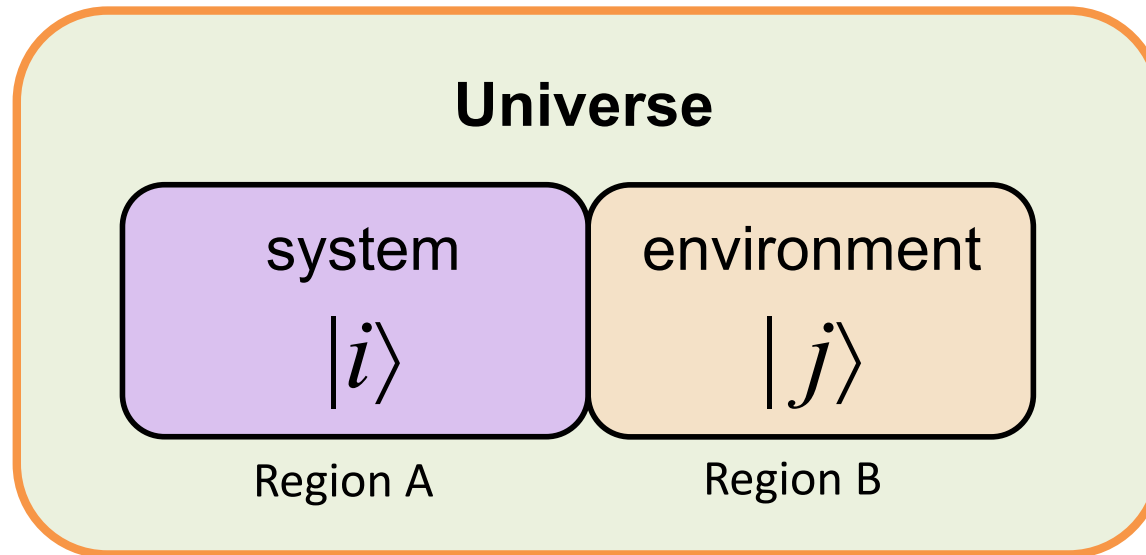
$$|\psi\rangle_{AB} = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B$$

The reduced density matrix is defined as:

$$\rho_A = \mathrm{tr}_B |\psi\rangle_{AB}\,_{AB}\langle\psi|$$

$$\rightarrow (\rho_A)_{ii'} = \,_A\langle i|\rho_A|i'\rangle_A = \sum_j \psi_{ij}\psi_{i'j}^*$$

Properties of the density matrix

$$\rho_A = \text{tr}_B |\psi\rangle_{AB}\,_{AB}\langle\psi|$$

- Hermitian -> eigenvalues are real
- Eigenvalues are non-negative
- The trace equals to unity-> Tr ρ_A=1
- Eigenvectors form an orthonormal basis.

$$\rho_A = \sum_\alpha \omega_\alpha |\alpha\rangle_{A}\,_{A}\langle\alpha|; \quad \text{with } \omega_\alpha \geq 0 \text{ and } \sum_\alpha \omega_\alpha = 1$$

The singular value decomposition (SVD)

Consider a matrix

$$\Psi_{ij}=$$

dim$_B$

dim$_A$

(we are choosing dim$_B$ < dim$_A$ for convenience)

We can decompose it into the product of three matrices U,D,V:

$$\psi = UDV^\dagger$$

- U is a (dim$_A$xdim$_B$) matrix with orthonormal columns-> $UU^\dagger=1$; $U=U^\dagger$
- D is a (dim$_B$xdim$_B$) diagonal matrix with non-negative elements λ_α
- V is a (dim$_B$xdim$_B$) unitary matrix -> $VV^\dagger=1$

$$\left(\Psi \right) = \left(U \right) \times \left(D \right) \times \left(V \right)$$

$$\psi_{ij} = \sum_{\alpha}^{\dim B} U_{i\alpha} \lambda_\alpha \left(V^t\right)_{\alpha j} = \sum_{\alpha}^{\dim B} U_{i\alpha} \lambda_\alpha V_{\alpha j}^*$$

$$\left|\psi\right\rangle_{AB} = \sum_{ij} \sum_{\alpha}^{\dim B} U_{i\alpha} \lambda_\alpha V_{\alpha j}^* \left|i\right\rangle_A \left|j\right\rangle_B$$

$$= \sum_{\alpha}^{\dim B} \left(\sum_i U_{i\alpha} \left|i\right\rangle_A\right) \lambda_\alpha \left(\sum_j V_{\alpha j}^* \left|j\right\rangle_B\right) = \sum_{\alpha}^{\dim B} \left(\left|\alpha\right\rangle_A\right) \lambda_\alpha \left(\left|\alpha\right\rangle_B\right)$$

$$\rightarrow \left|\psi\right\rangle_{AB} = \sum_{\alpha}^{\dim B} \lambda_\alpha \left|\alpha\right\rangle_A \left|\alpha\right\rangle_B$$

Here the bases $\left\{\left|\alpha\right\rangle_A\right\}, \left\{\left|\alpha\right\rangle_B\right\}$ are orthonormal!

This is also called the "Schmidt decomposition" of the state

The SVD and the density matrix

In general:

$$\left|\psi\right\rangle_{AB} = \sum_{\alpha}^{r} \lambda_{\alpha}\left|\alpha\right\rangle_{A}\left|\alpha\right\rangle_{B} \quad \text{with } r = \min(\dim_A, \dim_B)$$

In the Schmidt basis, the reduced density matrix is

$$\rho_A = \text{tr}_B \left|\psi\right\rangle_{AB\ AB}\left\langle\psi\right| = \sum_{\alpha}^{r} \lambda_{\alpha}^2 \left|\alpha\right\rangle_{A\ A}\left\langle\alpha\right|$$

$$\text{and } \rho_B = \sum_{\alpha}^{r} \lambda_{\alpha}^2 \left|\alpha\right\rangle_{B\ B}\left\langle\alpha\right|$$

- The singular values are the eigenvalues of the reduced d.m. squared $\omega_i = \lambda_i^2$
- The two reduced density matrices share the spectrum
- the singular vectors are the eigenvectors of the density matrix.

Optimizing the wave-function

We want to minimize the distance between the two states

$$S = \left| \, |\psi'\rangle - |\psi\rangle \, \right|^2$$

where $|\psi\rangle$ is the actual ground state, and $|\psi'\rangle$ is the variational approximation after rotating to a new basis and truncating

$$|\psi'\rangle = \sum^m{}_{\alpha j} a_{\alpha j} |\alpha\rangle |j\rangle$$

We reformulate the question as: Given a matrix ψ, what is the optimal matrix ψ' with fixed rank r that minimizes the Frobenius distance between the two matrices.
It turn out, this is a well known problem, called the "low rank matrix approximation" or "prical component approximation" (PCA) in machine learning.
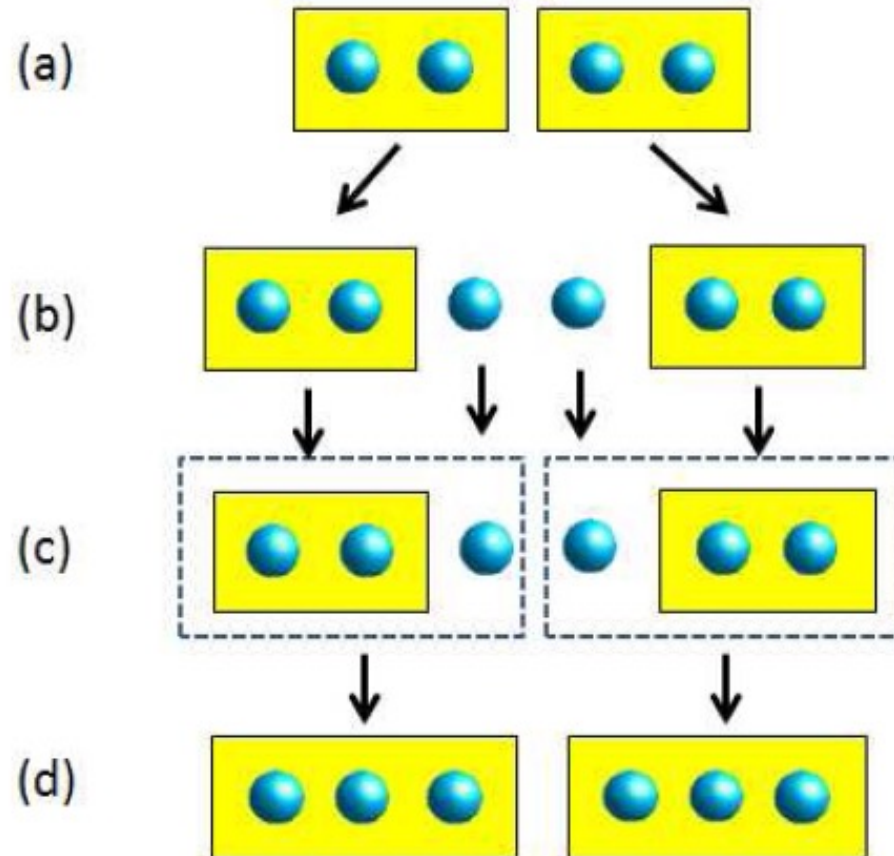If we order the eigenvalues of the density matrix in descending order $\omega_1, \omega_2, ..., \omega_m, ..., \omega_r$ we obtain

$$S = \left| \, |\psi'\rangle - |\psi\rangle \, \right|^2 = \sum_{m+1}^{r} \omega_i \qquad \text{Truncation error!}$$

DMRG: The Algorithm

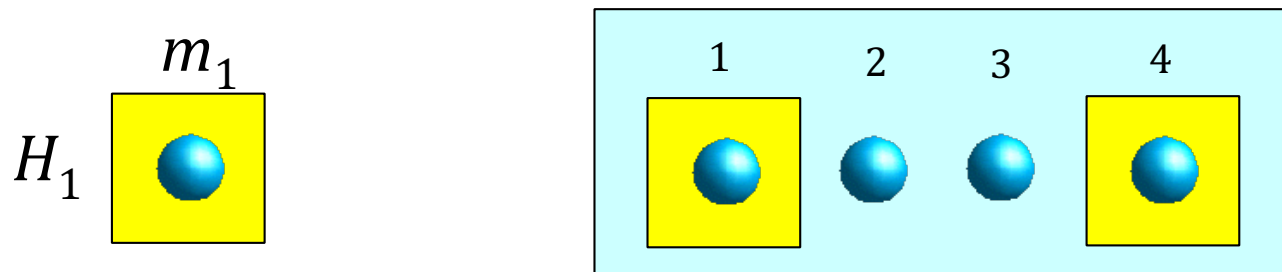**How do we build the reduced basis of states?**
We grow our basis systematically, adding sites to our system at each step, and using the density matrix projection to truncate

The Algorithm

1) We start from a small superblock with 4 sites/blocks, each with a dimension m_i, small enough to be easily diagonalized
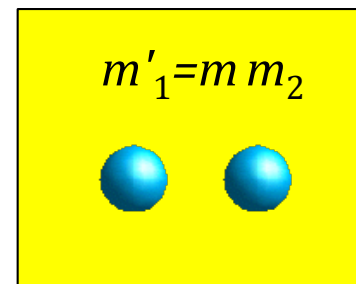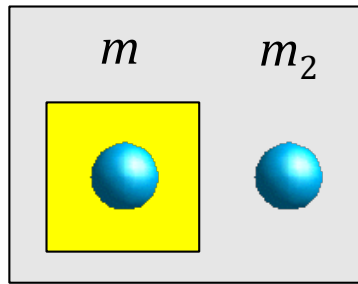

2) We diagonalize the system and obtain the ground state

$$|gs\rangle = \sum \psi_{1234}|\alpha_1\rangle|s_2\rangle|s_3\rangle|\beta_4\rangle$$

3) We calculate the reduced density matrix ρ for blocks 1-2 and 3-4.

$$\left\langle \alpha_1 s_2 \left| \rho_1 \right| \alpha'_1 s'_2 \right\rangle = \sum_{s_3 \beta_4} \psi_{1234} \psi^*_{1'2'34}$$

4) We diagonalize ρ obtaining the eigenvectors and eigenvalues ω_i

5) We add a new site to blocks 1 and 4, expanding the basis for each block to $m'_1 = m\, m_2$ and $m'_4 = m_3\, m$

6) We rotate the Hamiltonian and operators to the new basis keeping the m states with larger eigenvalues *(notice that we no longer are in the occupation number representation)*

7) We repeat starting from 2) replacing H_1 by H'_1 and H_4 by H'_4
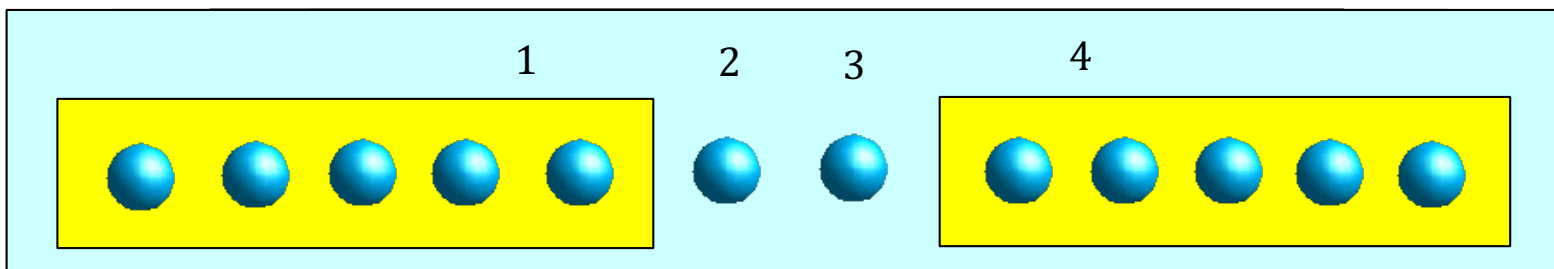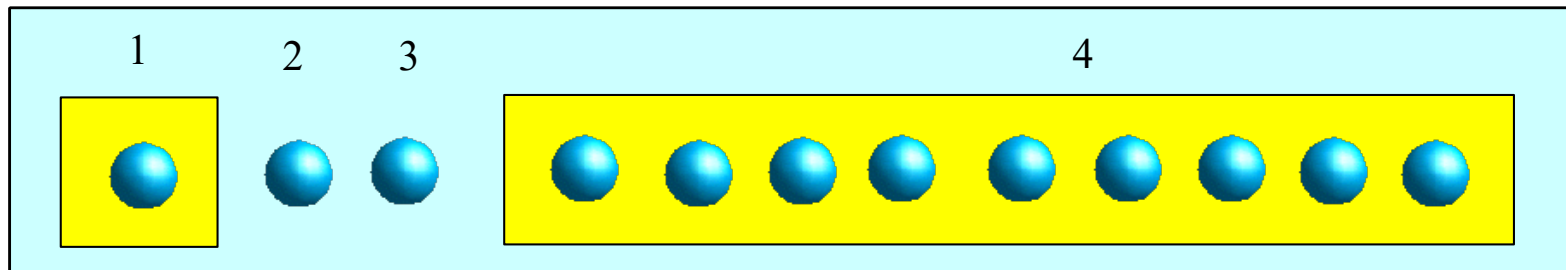
The finite size algorithm

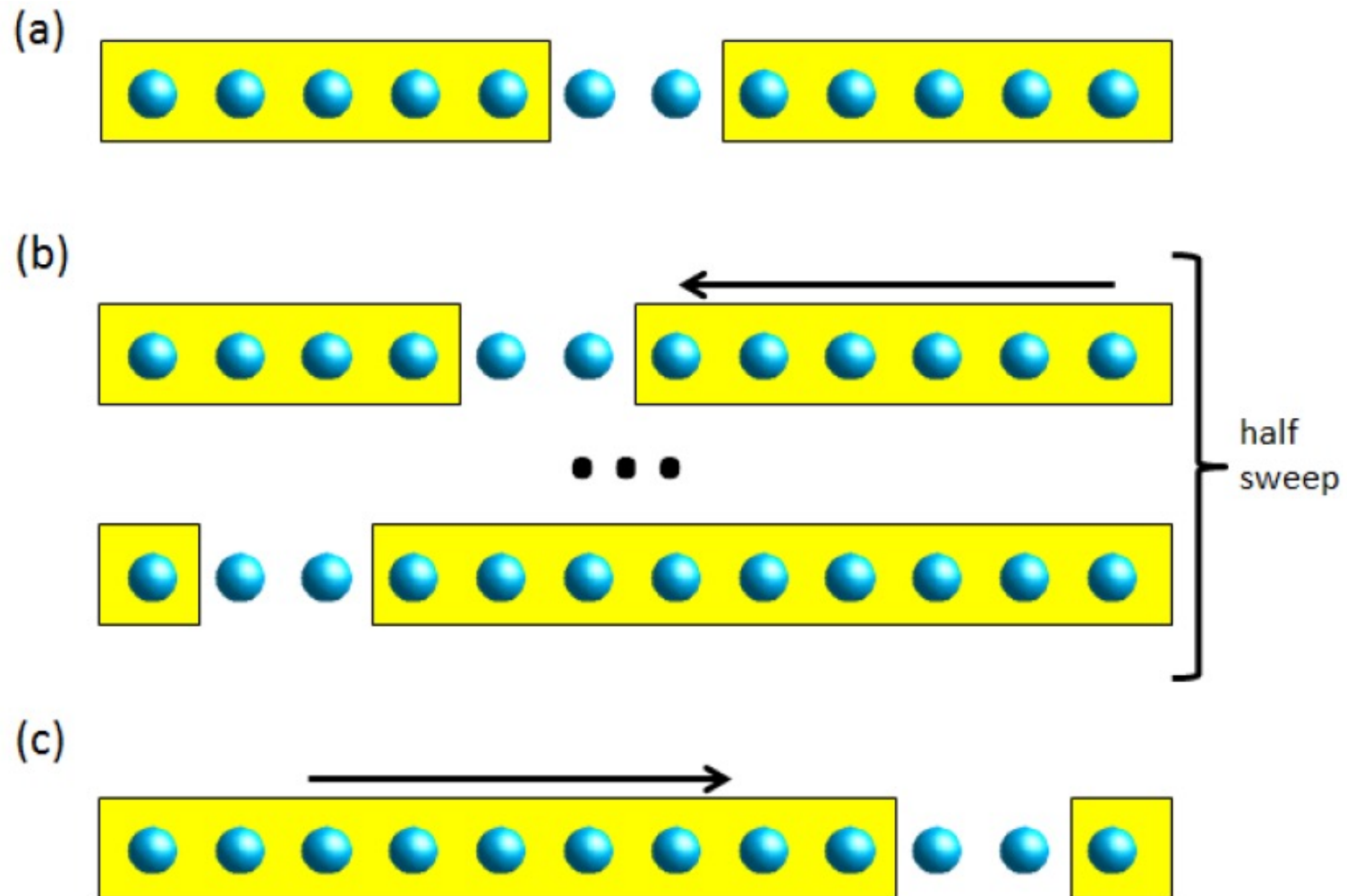**We add one site at a time, until we reach the desired system size**
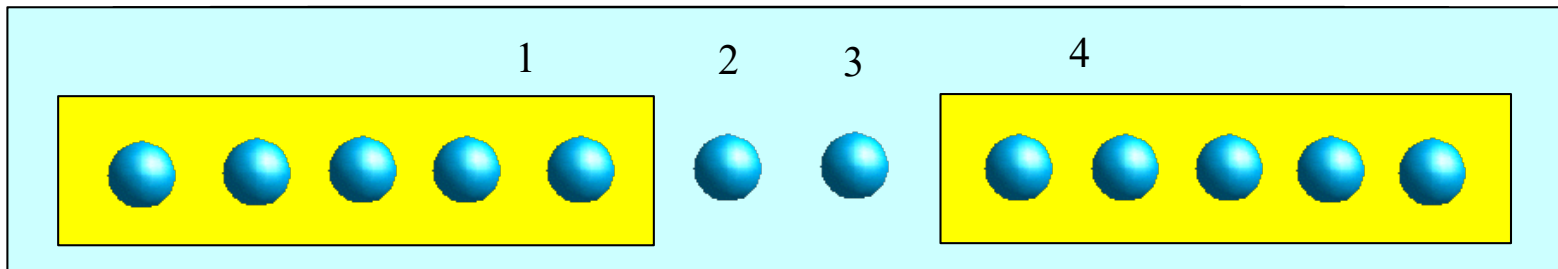
The finite size algorithm

We sweep from right to left

…Until we converge

Finite-size DMRG Flow chart

The discarded weight 1- $\sum^{m}_{\alpha=1}\omega_{\alpha}$ measures the accuracy of the truncation to m states

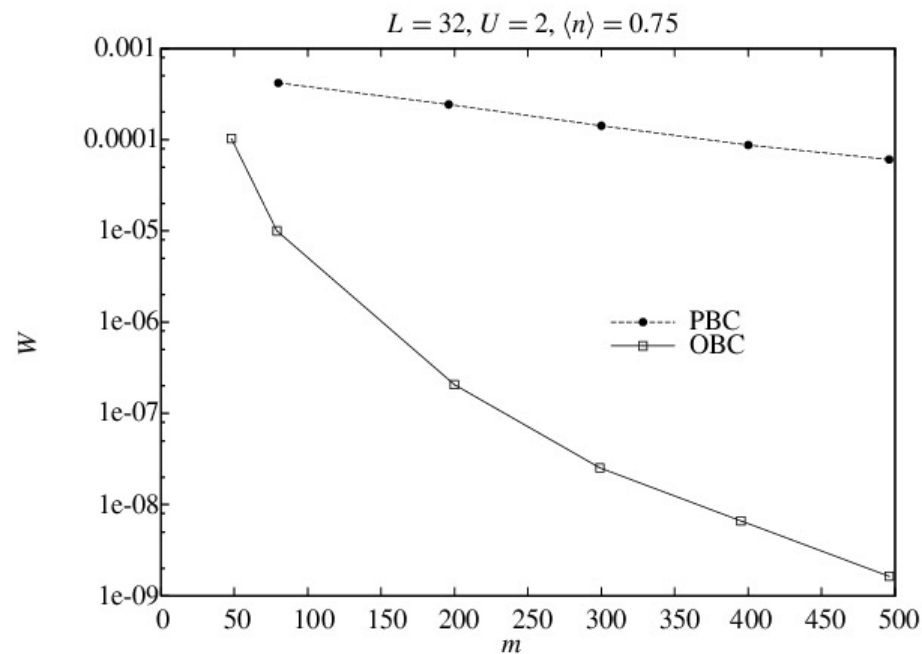Figure 1.4: Sum of the discarded weight of the density matrix eigenvalues for the finite system DMRG algorithm, as a function of the number of states kept m.

Observations

- Sweeping is essential to achieve convergence
- Run the finite-size DMRG and extrapolate to the thermodynamic limit.
- For each system size, extrapolate the results with the number of states m, or fix the truncation error below certain tolerance.

Density Matrix Renormalization Group

A variational method without a-priori assumptions about the physics.

- *Similar capabilities as exact diagonalization.*

- *Can calculate properties of very large systems (1D and quasi-2D) with unprecedented accuracy.*

- *Results are variational, but "quasi-exact": Accuracy is finite, but under control.*

Advantages of the DMRG

- DMRG is very versatile, and easy to adapt to complex geometries and Hamiltonians.

- Can be used to study models of spins, bosons, or fermions.

- General and reusable code: A single program can be used to run arbitrary models without changing a single line (e.g. ALPS DMRG)

- Symmetries are easy to implement.

Limitations of the DMRG

- DMRG is the method of choice in 1d and quasi-1d systems, but it is less efficient in higher dimensions.

- Problems with (i) critical systems, (ii) long range interactions, and (iii) periodic boundary conditions.

- These limitations are due to:
  - The structure of the variational wave function used by the DMRG (the MPS ansatz).
  - Entanglement entropy follows area law.

Technicalities…
Adding a single site to the block
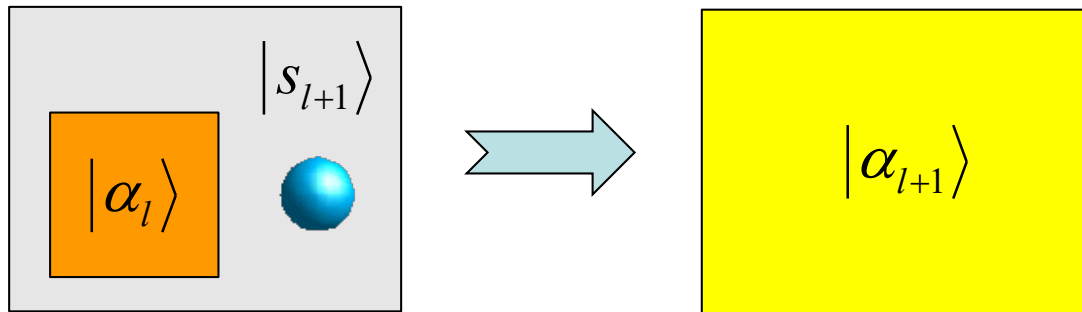
Before truncating we build the new basis as:
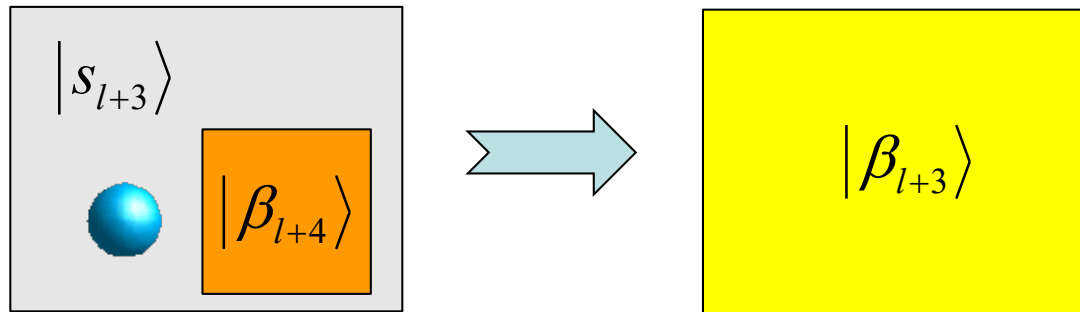
$$\left| \alpha_{l+1} \right\rangle = \left| \alpha_l \right\rangle \otimes \left| s_{l+1} \right\rangle$$

And the Hamiltonian for the new block as

$$H_{L,l+1} = H_{L,l} \otimes I_1 + I_l \otimes H_0 + O_{L,l} \otimes O'_0 + \ldots$$

with $\qquad O_{L,l} = I_{l-1} \otimes O_0$

.. and for the right block

Before truncating we build the new basis as:

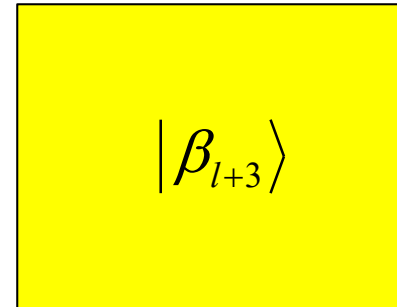$$\left|\beta_{l+3}\right\rangle = \left|s_{l+3}\right\rangle \otimes \left|\beta_{l+4}\right\rangle$$

And the Hamiltonian for the new block as

$$H_{R,l+3} = I_1 \otimes H_{R,l+4} + H_0 \otimes I_{L-(l+4)} + O_0 \otimes O'_{R,l+4} + ...$$

with $\quad O_{R,l} = O_0 \otimes I_{L-(l+1)}$

Putting everything together to build the Hamiltonian...

$$\left|\alpha_{l+1}\right\rangle \qquad \left|\beta_{l+3}\right\rangle$$
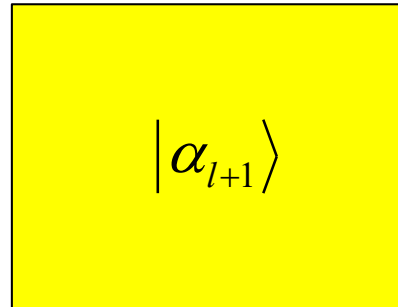
$$H = H_{L,l+1} \otimes I_{R,l+3} + I_{L,l+1} \otimes H_{R,l+3}$$

$$+ O_{L,l+1} \otimes O'_{R,l+3} + ...$$

Truncation

When we add a site to the left block we represent the new basis states as:
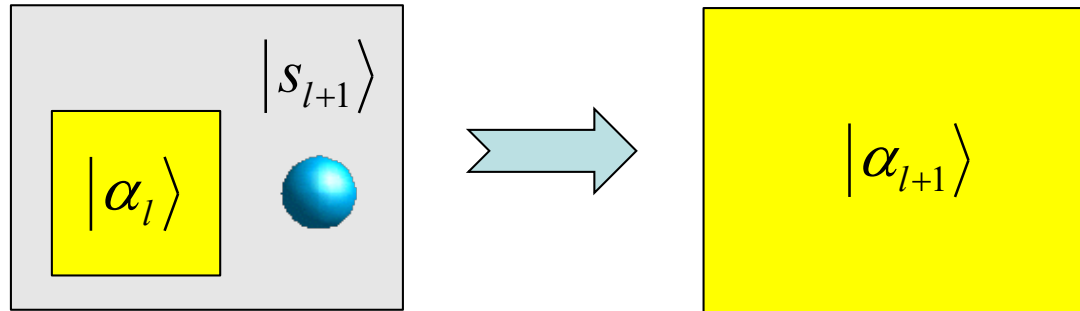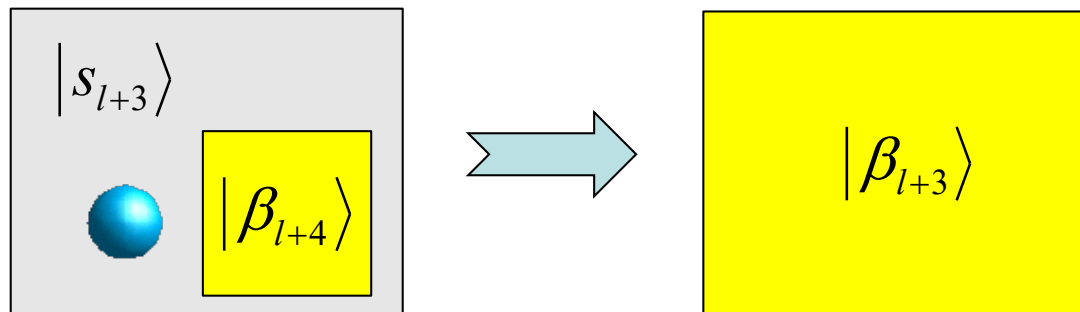

$$|\alpha_{l+1}\rangle = \sum_{s_{l+1},\alpha_l} \langle \alpha_l s_{l+1} | \alpha_{l+1} \rangle | \alpha_l \rangle \otimes | s_{l+1} \rangle = \sum_{s_{l+1},\alpha_l} \left(U_L^{l+1} \right)_{\alpha_l s_{l+1},\alpha_{l+1}} | \alpha_l \rangle \otimes | s_{l+1} \rangle$$

Similarly for the right block:

$$|\beta_{l+3}\rangle = \sum_{s_{l+3},\beta_{l+4}} \langle s_{l+3}\beta_{l+4} | \beta_{l+3} \rangle | s_{l+3} \rangle \otimes | \beta_{l+4} \rangle = \sum_{s_{l+3},\beta_{l+4}} \left(U_R^{l+3} \right)_{s_{l+3}\beta_{l+4},\beta_{l+3}} | s_{l+3} \rangle \otimes | \beta_{l+4} \rangle$$

Measuring observables

Suppose we have a chain and we want to
measure a correlation between sites i and j

$$O_i \qquad\qquad O'_j$$

$$i \qquad\qquad j$$
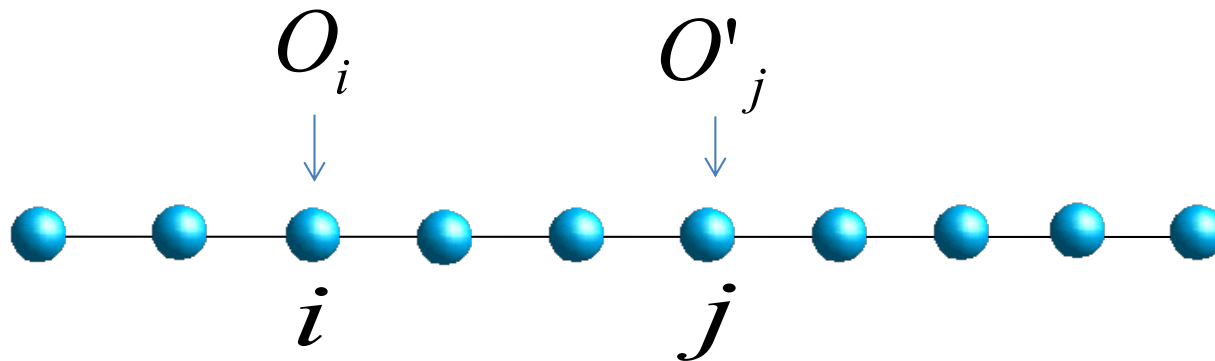
We have two options:
1. Measure the correlation by storing the composite operator in a block
2. Measure when the two operators are on separate blocks

We shall go for option (2) for the moment: simpler and more efficient

Operators on separate blocks
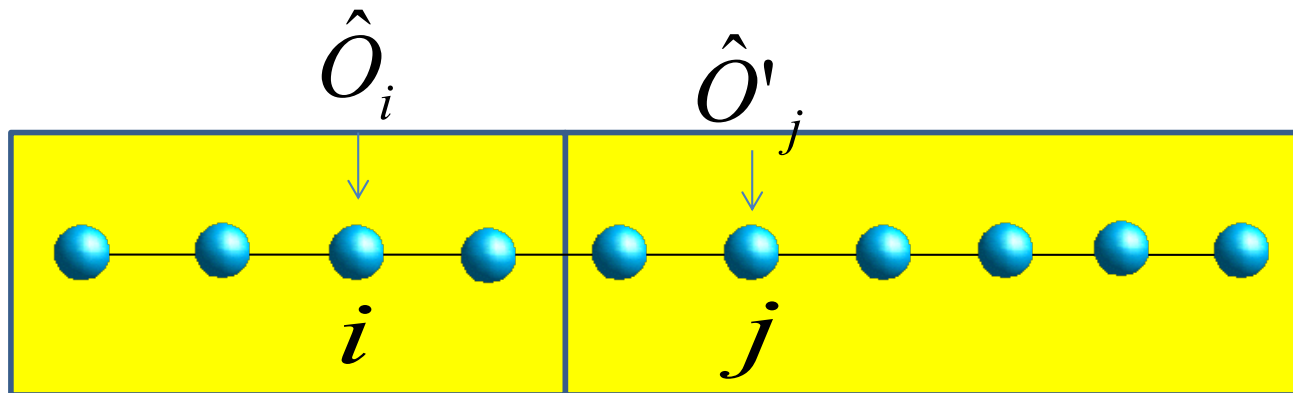
We only measure when we have the following situation:

Then, it is easy to see that:

$$\left\langle O_i O'_j \right\rangle = \left\langle \psi \left| O_i O'_j \right| \psi \right\rangle =$$

$$= \sum_{\alpha\beta, \alpha'\beta'} \psi^*_{\alpha'\beta'} \psi_{\alpha\beta} \left\langle \alpha' \beta' \left| O_i O'_j \right| \alpha\beta \right\rangle$$

$$= \sum_{\alpha\beta, \alpha'\beta'} \psi^*_{\alpha'\beta'} \psi_{\alpha\beta} \left\langle \alpha' \left| O_i \right| \alpha \right\rangle \left\langle \beta' \left| O'_j \right| \beta \right\rangle$$

We cannot do this if the two operators are in the same block!!!

Operators on the same block
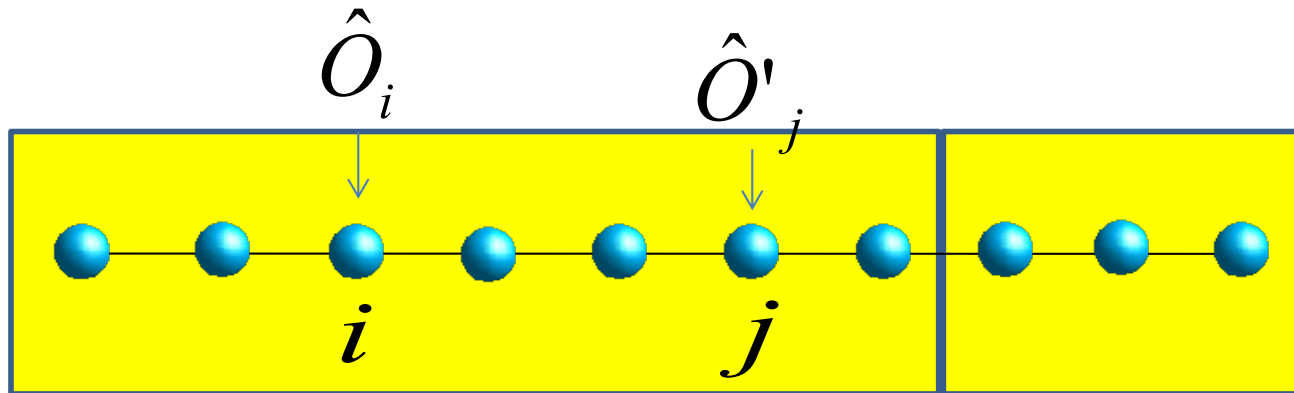
Do never do this:

$$\langle O_i O'_j \rangle = \langle \psi | O_i O'_j | \psi \rangle \neq$$

$$= \sum_{\alpha\beta,\alpha'} \psi^*_{\alpha'\beta} \psi_{\alpha\beta} \langle \alpha' | O_i | \alpha \rangle \langle \alpha' | O'_j | \alpha \rangle$$

We need to propagate the product operator into the block, the same way as we do for the Hamiltonian

Targeting states in DMRG

Our DMRG basis is only guaranteed to represent targeted states, and those only after enough sweeps!

$$\rho = \sum_t w_t |\psi_t\rangle\langle\psi_t|$$

If we target the ground state only, we cannot expect to have a good representation of excited states (dynamics).

If the error is strictly controlled by the DMRG truncation error, we say that the algorithm is "quasiexact".

Non quasiexact algorithms seem to be the source of almost all DMRG "mistakes". For instance, the infinite system algorithm applied to finite systems is not quasiexact.

Excited states

a) If we use quantum numbers, we can calculate the ground states in different sectors, for instance S=0, and S=1, to obtain the spin gap

b) At each step of the DMRG sweep, target the ground state, and the ground state of the modified Hamiltonian:

$$H \rightarrow H' = H + \Lambda |gs\rangle\langle gs|$$

For targeting the two states, we use the density matrix:

$$\rho = \frac{1}{2}|gs\rangle\langle gs| + \frac{1}{2}|1\rangle\langle 1|$$

2D Generalization
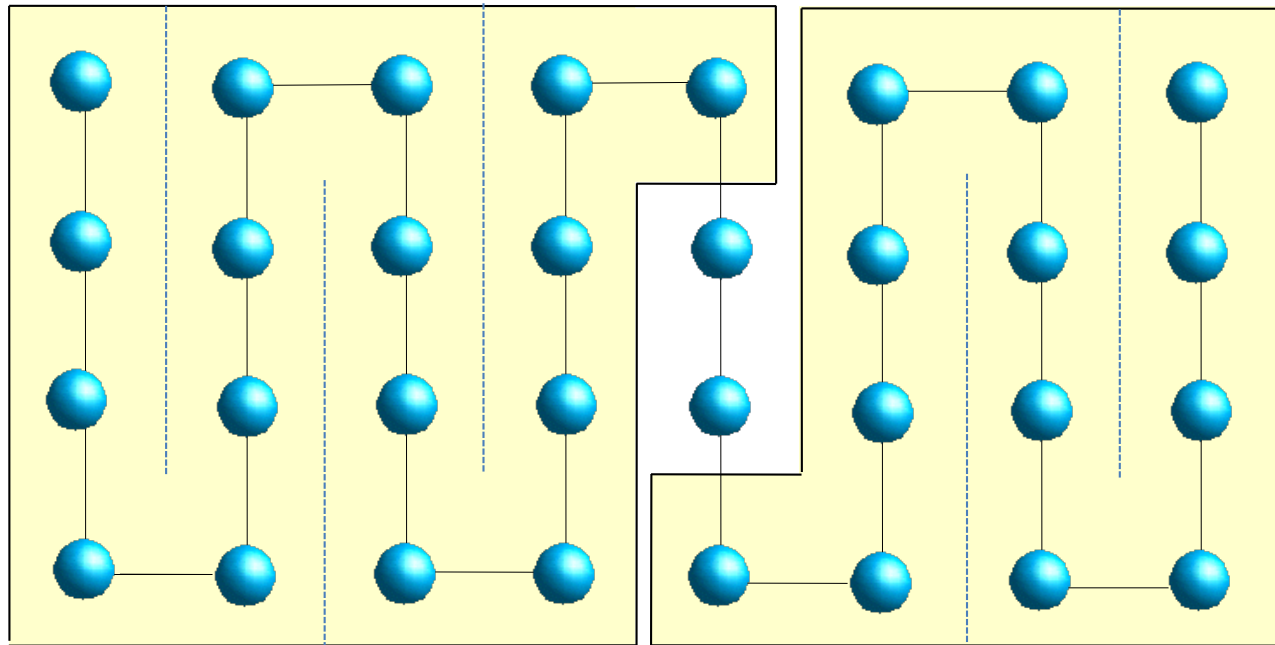
Why does the DMRG work???

ω_α

In other words: what makes the
density matrix eigenvalues
behave so nicely?

good!

bad!

α

Entanglement

We say that a two quantum systems A and B are "entangled" when we cannot describe the wave function as a product state of a wave function for system A, and a wave function for a system B
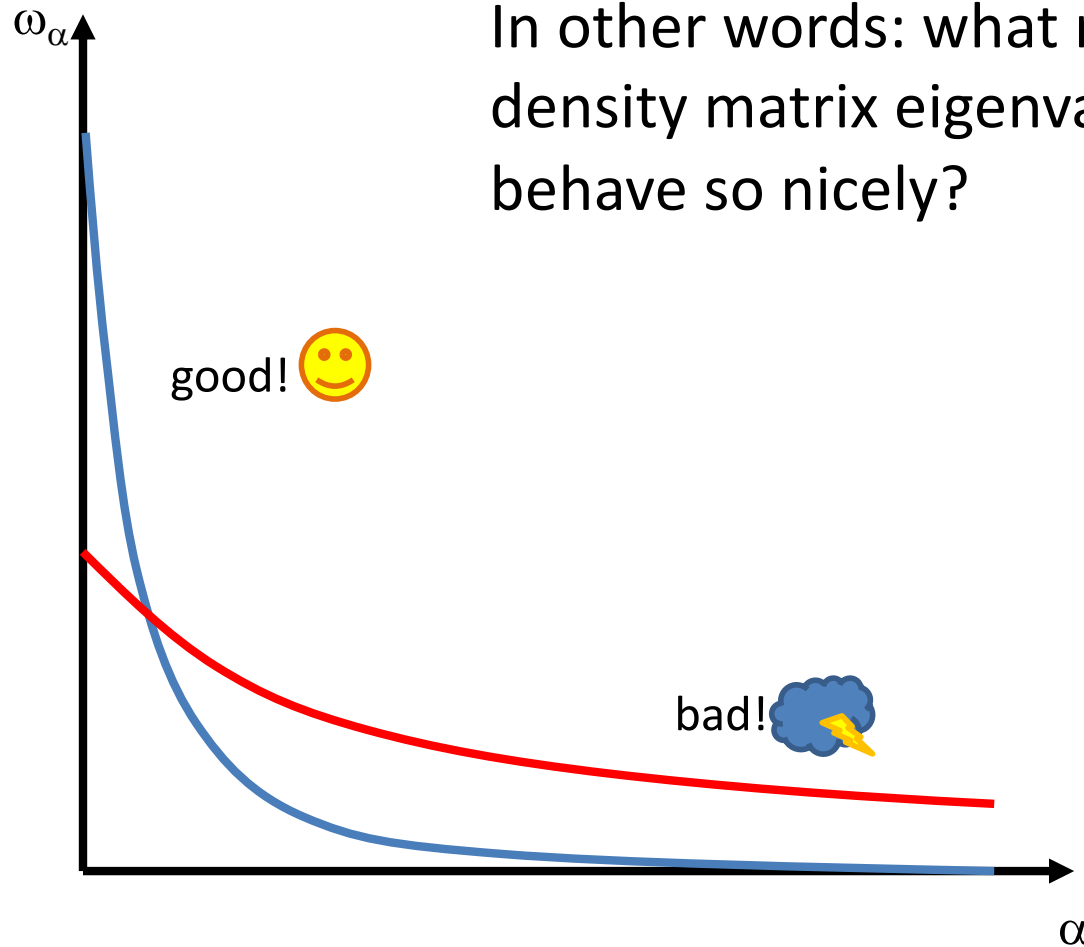
For instance, let us assume we have two spins, and write a state such as:

$$|\psi\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$$

We can readily see that this is equivalent to:

$$|\psi\rangle = (|\uparrow\rangle + |\downarrow\rangle) \otimes (|\uparrow\rangle + |\downarrow\rangle) = |\uparrow\rangle_x \otimes |\downarrow\rangle_x$$
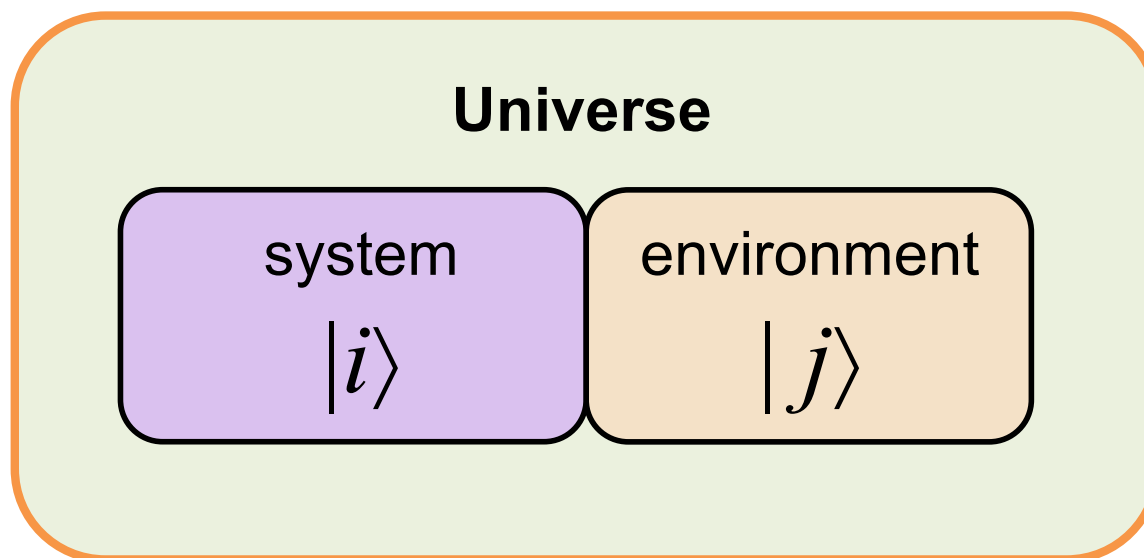
-> The two spins are not entangled! The two subsystems carry information independently

Instead, this state:

$$|\psi\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$$

is "maximally entangled". The state of subsystem A has ALL the information about the state of subsystem B

The Schmidt decomposition

$$|\psi\rangle_{AB} = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B$$

We assume the basis for the left subsystem has dimension $\dim_A$, and the right, $\dim_B$. That means that we have $\dim_A$ x $\dim_B$ coefficients.
We go back to the original DMRG premise: Can we simplify this state by changing to a new basis? (what do we mean with "simplifying", anyway?)

The Schmidt decomposition

We have seen that through a SVD decomposition, we can rewire the state as:

$$\left|\psi\right\rangle_{AB} = \sum_{\alpha}^{r} \lambda_{\alpha}\left|\alpha\right\rangle_{A}\left|\alpha\right\rangle_{B}$$

Where

$$r = \min(\dim_{A}, \dim_{B}); \ \ \lambda_{\alpha} \geq 0 \ \text{ and } \left|\alpha\right\rangle_{A}; \left|\alpha\right\rangle_{B} \ \text{ are orthonormal}$$

Notice that if the Schmidt rank *r*=1, then the wave-function reduces to a product state, and we have "disentangled" the two subsystems.

After the Schmidt decomposition, the reduced density matrices for the two subsystems read:

$$\rho_{A/B} = \sum_{\alpha}^{r} \lambda_{\alpha}^{2}\left|\alpha\right\rangle_{A/B} \ _{A/B}\left\langle\alpha\right|$$

The Schmidt decomposition, entanglement and DMRG

It is clear that the efficiency of DMRG will be determined by the spectrum of the density matrices (the "entanglement spectrum"), which are related to the Schmidt coefficients:

- If the coefficients decay very fast (exponentially, for instance), then we introduce very little error by discarding the smaller ones.
- Few coefficients mean less entanglement. In the extreme case of a single non-zero coefficient, the wave function is a product state and it completely disentangled.
- NRG minimizes the energy...DMRG concentrates entanglement in a few states. The trick is to disentangle the quantum many body state!

Quantifying entanglement

In general, we write the state of a bipartite system as:

$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle$$

We saw previously that we can pick and orthonormal basis for "left" and "right" systems such that

$$|\psi\rangle = \sum_{\alpha} \lambda_{\alpha} |\alpha_L\rangle |\alpha_R\rangle$$

We define the "von Neumann entanglement entropy" as:

$$S = -\sum_{\alpha} \lambda_{\alpha}^2 \log \lambda_{\alpha}^2$$

Or, in terms of the reduced density matrix:

$$\rho_L = \sum_{\alpha} \lambda_{\alpha}^2 |\alpha_L\rangle\langle\alpha_L| \rightarrow S = -\text{Tr}(\rho_L \log \rho_L)$$

Entanglement entropy

Let us go back to the state:

$$|\psi\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$$

We obtain the reduced density matrix for the first spin, by tracing over the second spin (and after normalizing):

$$\rho_L = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

We say that the state is "maximally entangled" when the reduced density matrix is proportional to the identity.

$$S = -\frac{1}{2}\log\frac{1}{2} - \frac{1}{2}\log\frac{1}{2} = \log 2$$

Entanglement entropy

- If the state is a product state:

$$|\psi\rangle = |\alpha_L\rangle|\alpha_R\rangle \rightarrow w_\alpha = \{1,0,0,...\} \rightarrow S = 0$$

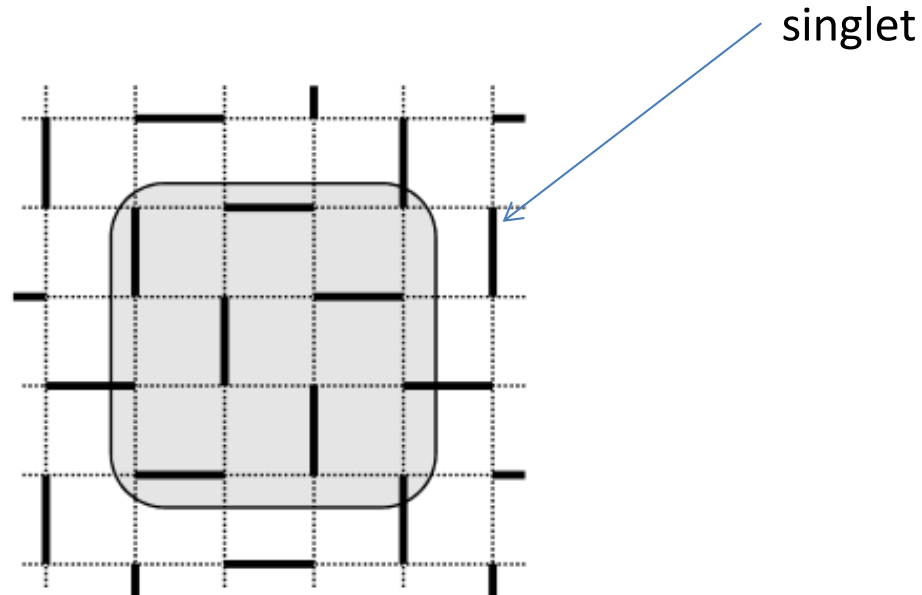- If the state maximally entangled, all the w_α are equal

$$\rightarrow w_\alpha = \{\tfrac{1}{D}, \tfrac{1}{D}, \tfrac{1}{D},...\} \rightarrow S = \log D$$

where D is

$$D = \min\{\dim H_L, \dim H_R\}$$

Area law: Intuitive picture

Consider a valence bond solid in 2D

singlet

$$S = \log 2 \times (\# \text{ of bonds cut}) \approx L \log 2$$

The entanglement entropy is proportional to the area of the boundary separating both regions. This is the prototypical behavior in gapped systems. Notice that this implies that the entropy in 1D is independent of the size of the partition

Critical systems in 1D

$$S_{PBC} = \frac{c}{3} \log(L),$$

$$S_{OBC} = \frac{c}{6} \log(L),$$

c is the "central charge" of the system, a measure of the number of gapless modes
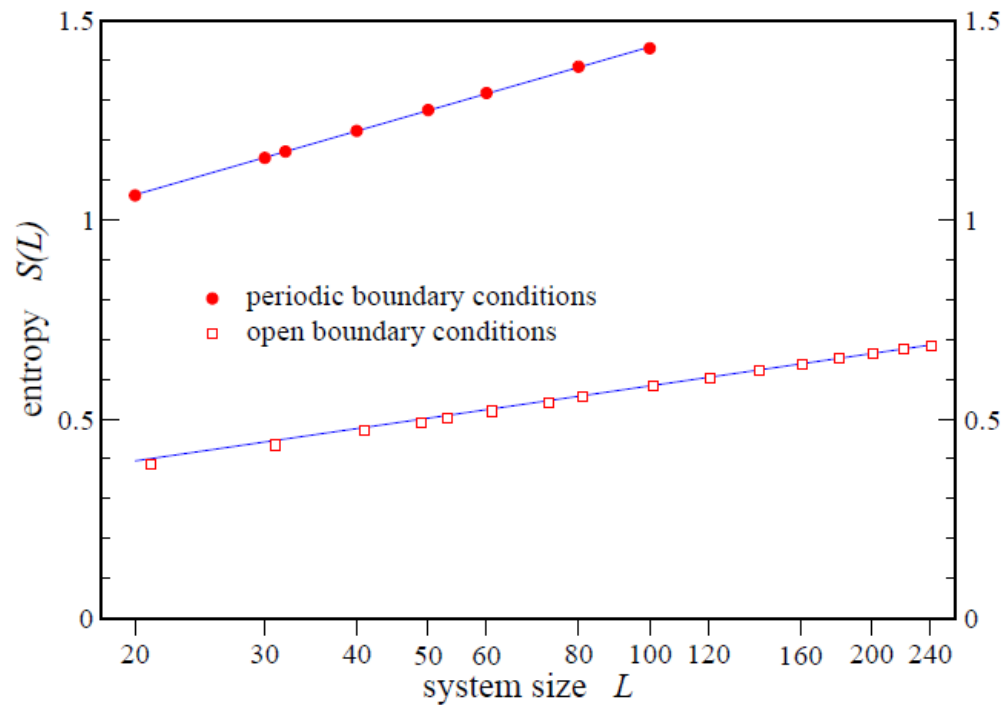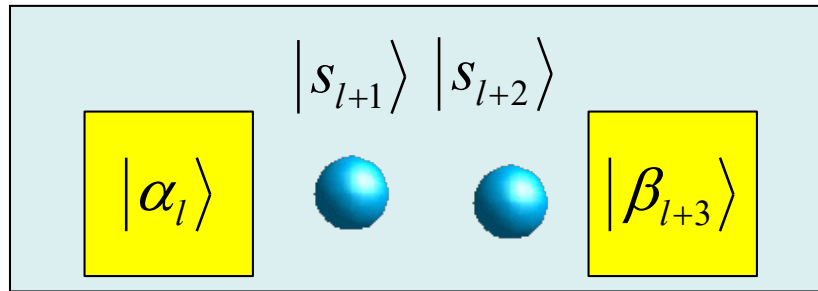
Entropy and DMRG

The number of states that we need to keep is related to the entanglement entropy:

$$m \approx \exp S$$

- Gapped system in 1D: m=const.
- Critical system in 1D: m=L^α
- Gapped system in 2D: m=exp(L)
- In 2D in general, most systems obey the area law (not free fermions, or fermionic systems with a 1D Fermi surface, for instance)…
- Periodic boundary conditions in 1D: twice the area -> m^2

The wave-function transformation

Before the transformation, the superblock state is written as:

$$|\psi\rangle = \sum_{\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3}} \langle \alpha_l s_{l+1} s_{l+2} \beta_{l+3} | \psi \rangle | \alpha_l \rangle \otimes | s_{l+1} \rangle \otimes | s_{l+2} \rangle \otimes | \beta_{l+3} \rangle$$

After the transformation, we add a site to the left block, and we "spit out" one from the right block

$$|\psi\rangle = \sum_{\alpha_{l+1}, s_{l+2}, s_{l+3}, \beta_{l+4}} \langle \alpha_{l+1} s_{l+2} s_{l+3} \beta_{l+4} | \psi \rangle | \alpha_{l+1} \rangle \otimes | s_{l+2} \rangle \otimes | s_{l+3} \rangle \otimes | \beta_{l+4} \rangle$$

After some algebra, and assuming $\sum_{\alpha_l} |\alpha_l\rangle\langle\alpha_l| \approx 1$, one readily obtains:

$$\langle \alpha_{l+1} s_{l+2} s_{l+3} \beta_{l+4} | \psi \rangle \approx \sum_{\alpha_l, s_{l+1}, \beta_{l+3}} \langle \alpha_{l+1} \| \alpha_l s_{l+1} \rangle \langle \alpha_l s_{l+1} s_{l+2} \beta_{l+3} | \psi \rangle \langle s_{l+3} \beta_{l+4} \| \beta_{l+3} \rangle$$

What have we left out?

...Exploiting quantum numbers