DMRG Tutorial

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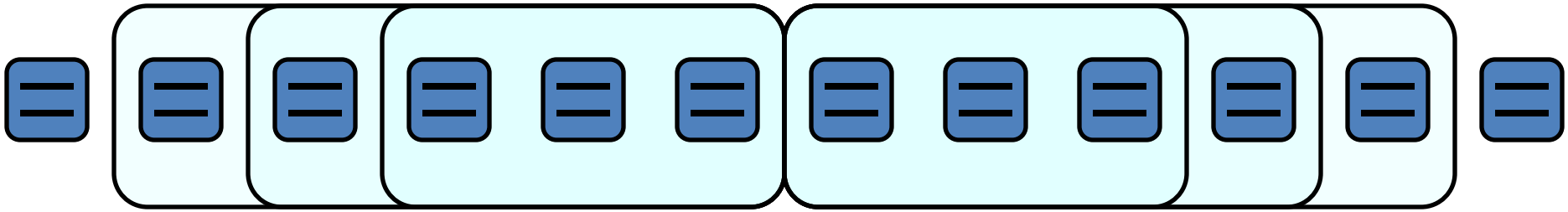

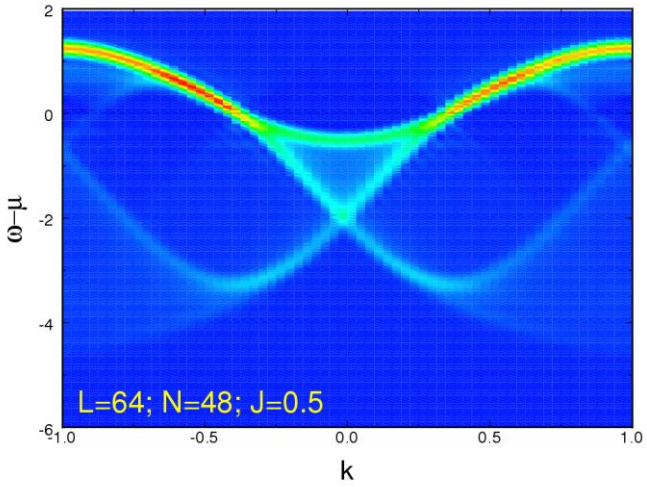

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Let's consider the 1d Heisenberg model

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

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/DMRG

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

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

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

This recursion will generate a 2^lx2^l Hamiltonian matrix that we can easily diagonalize

Another way to put it…

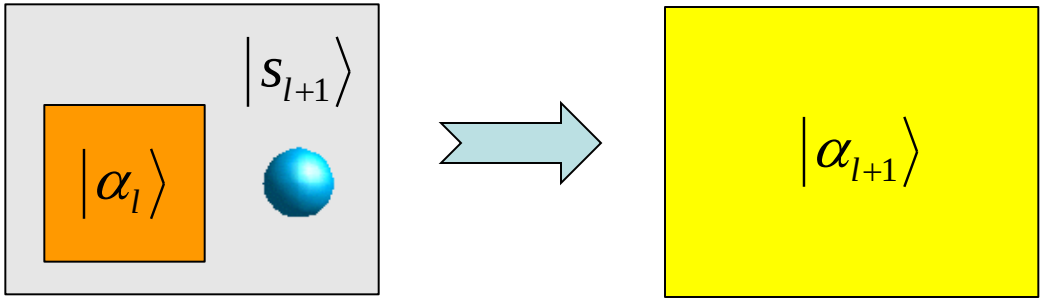
$$H_l = H_{l-1} \otimes I_1 + I_{l-2} \otimes \left[S_0^z \otimes S_0^z + \frac{1}{2} S_0^+ \otimes S_0^- + \frac{1}{2} S_0^- \otimes S_0^+ \right]$$

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

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

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

Adding a single site to the block



Before truncating we build the new basis as:

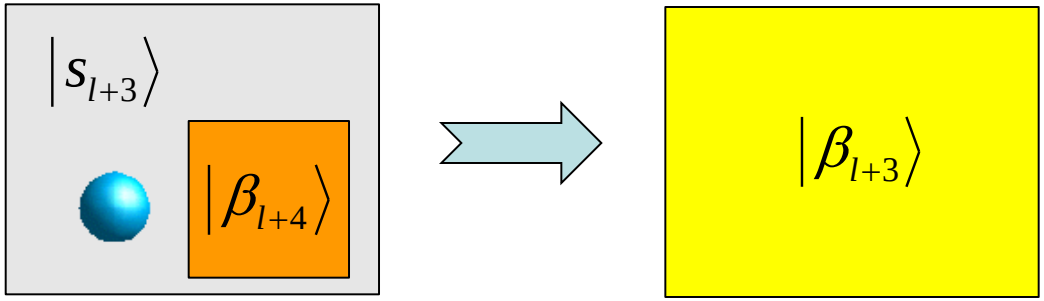
$$|\alpha_{l+1}\rangle = |\alpha_l\rangle \otimes |s_{l+1}\rangle$$

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

.. and for the right block



Before truncating we build the new basis as:

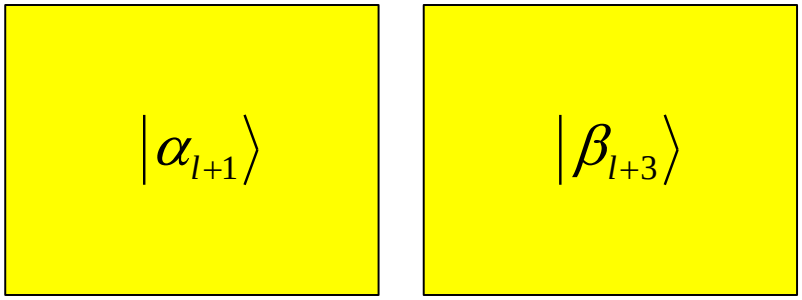
$$|\beta_{l+3}\rangle = |s_{l+3}\rangle \otimes |\beta_{l+4}\rangle$$

And the Hamiltonian for the new block as

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

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

Putting everything together to build the Hamiltonian…

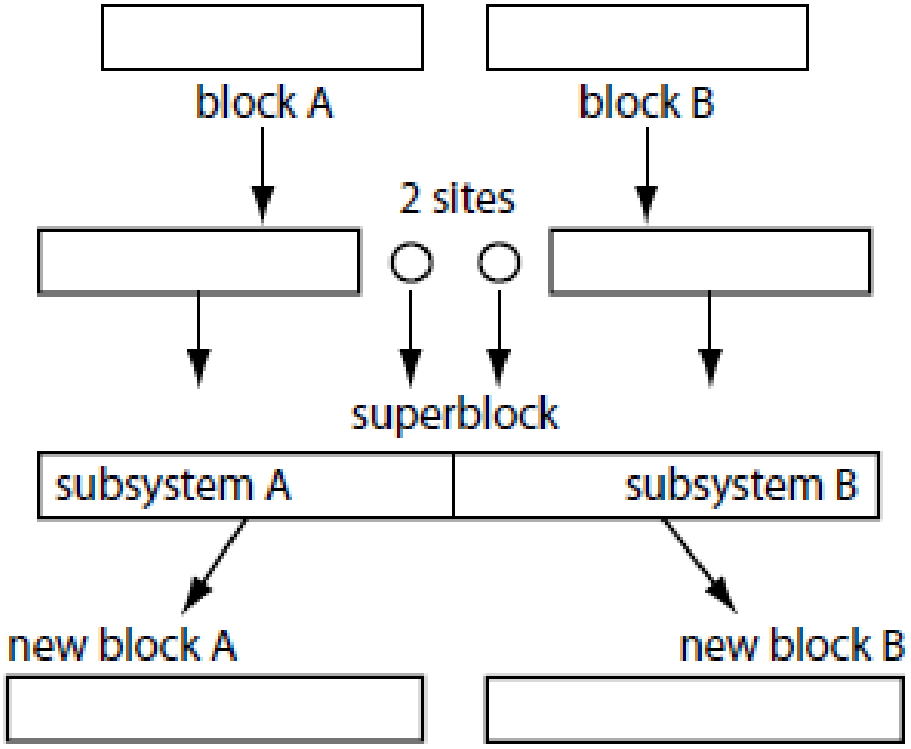


$$H = H_{L,l+1} \otimes I_{R,l+3} + I_{L,l+1} \otimes H_{R,l+3}$$
$$+ O_{L,l+1} \otimes O'_{R,l+3} + \ldots$$

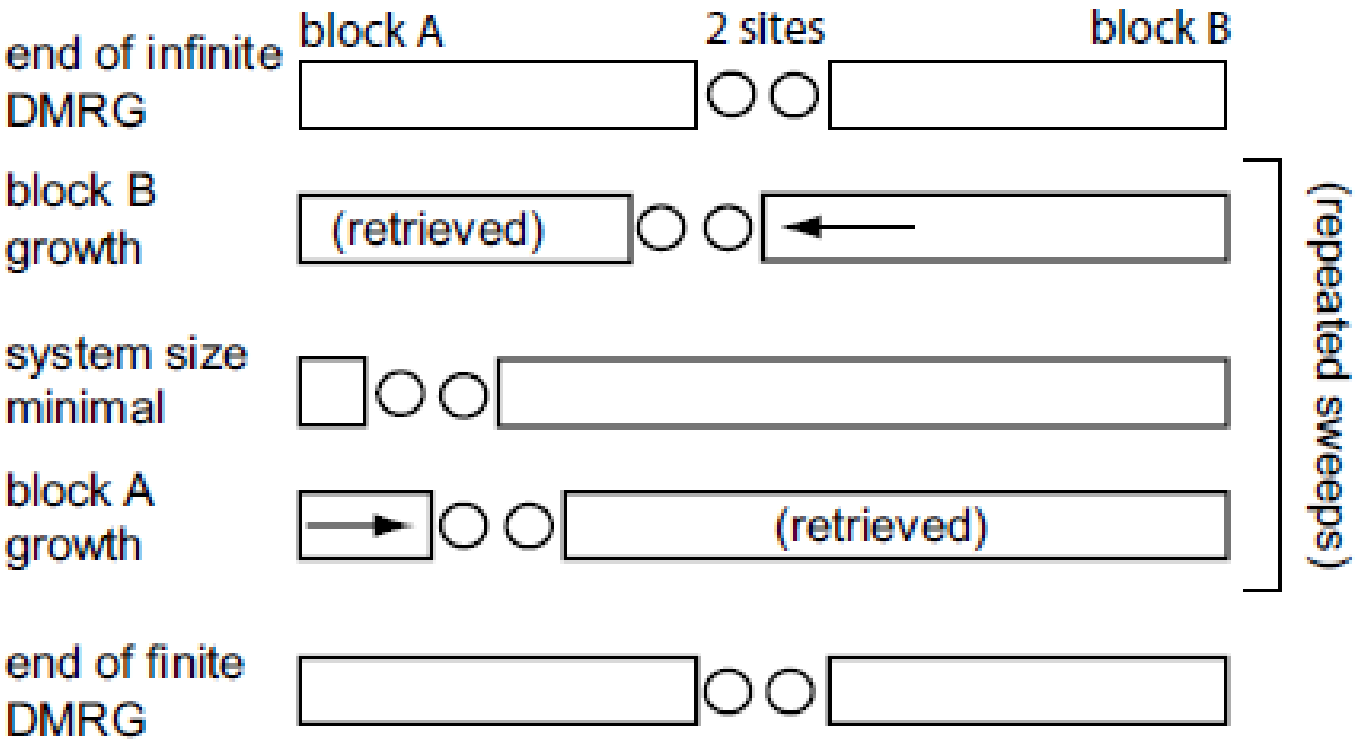
DMRG: The Algorithm

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

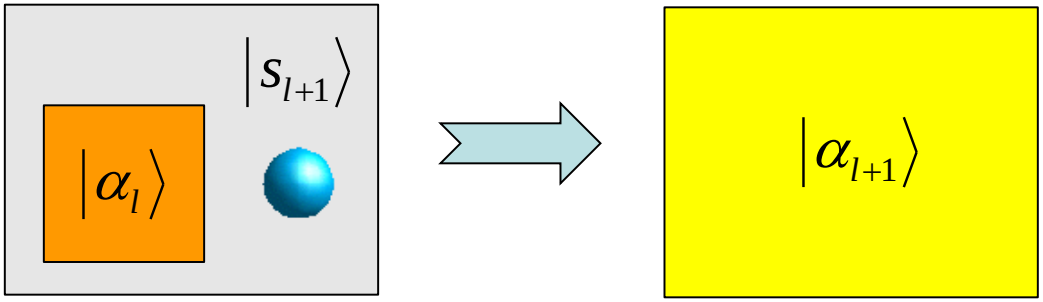


Finite-size DMRG Flow chart



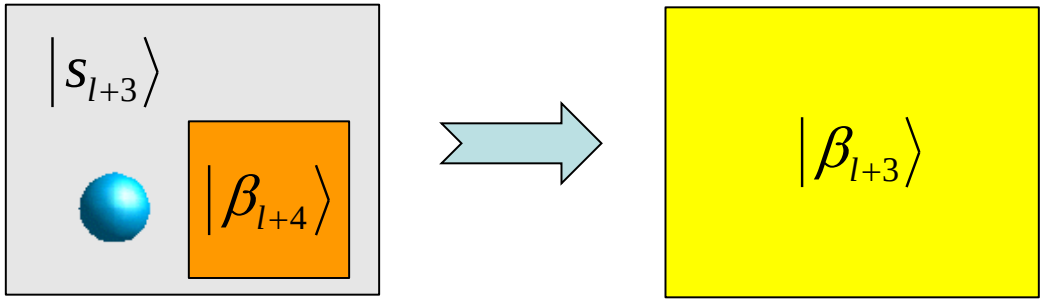
Truncation

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



$$|\alpha_{l+1}\rangle = \sum_{s_{l+1},\alpha_l} \langle \alpha_{l+1} | U_L^{l+1} | \alpha_l s_{l+1} \rangle | \alpha_l \rangle \otimes | s_{l+1} \rangle$$

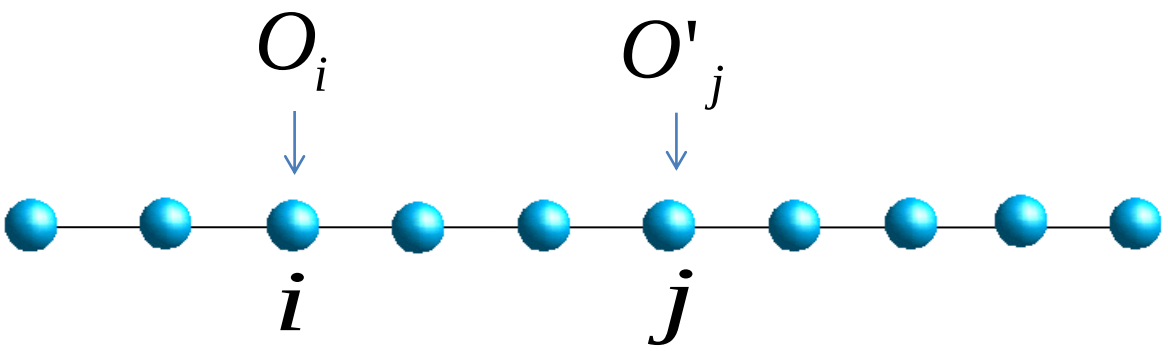
Similarly for the right block:



$$|\beta_{l+3}\rangle = \sum_{s_{l+3},\beta_{l+4}} \langle \beta_{l+3} | U_R^{l+3} | s_{l+3} \beta_{l+4} \rangle | s_{l+3} \rangle \otimes | \beta_{l+4} \rangle$$

Measuring observables

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



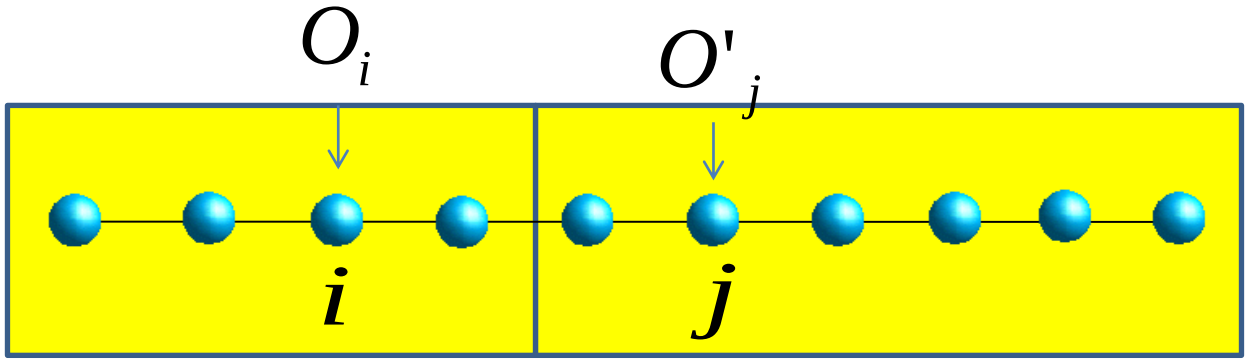
We have two options:

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:

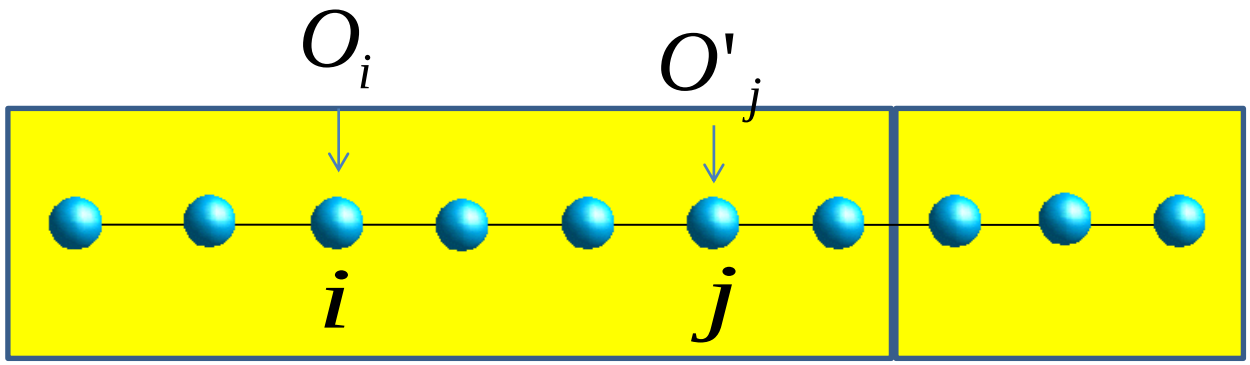
$$\left\langle O_i O'_j \right\rangle = \left\langle \psi \left| O_i O'_j \right| \psi \right\rangle =$$

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

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

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

Operators on the same block



Do never do this:

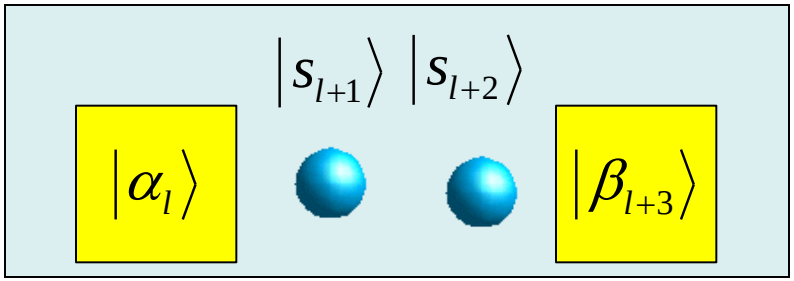
$$\left\langle O_i O'_j \right\rangle = \left\langle \psi \left| O_i O'_j \right| \psi \right\rangle \neq$$

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

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

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 $\sum_{\alpha} |\alpha\rangle\langle\alpha| \approx 1$, one readily obtains:

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

Time evolution using Suzuki-Trotter

1st order Suzuki-Trotter decomposition:

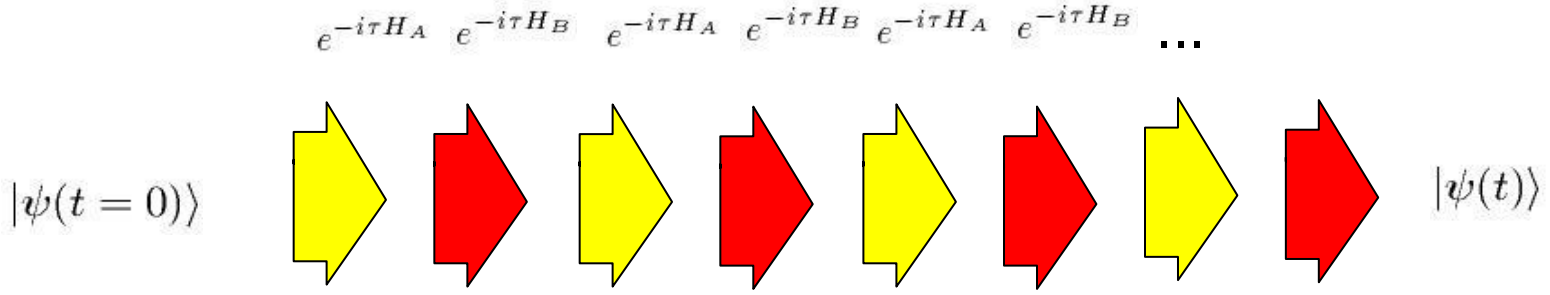
$$e^{-i\tau H} \approx e^{-i\tau H_A} e^{-i\tau H_B}$$

where $H = H_A + H_B$. Here we make A the even bonds and B the odd, 1D only. The individual link-terms $\exp(-i\tau H_j)$ (coupling sites j and $j+1$) within H_A or H_B commute. Thus

$$e^{-i\tau H_B} = e^{-i\tau H_1} e^{-i\tau H_3} e^{-i\tau H_5} \ldots$$

No error introduced!

So the time-evolution operator is a product of individual link terms.
Each link term only involves two-sites interactions => small matrix, easy to calculate!



The two-site evolution operator

Example: Heisenberg model (spins)

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

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 calculate the Hamiltonian matrix:

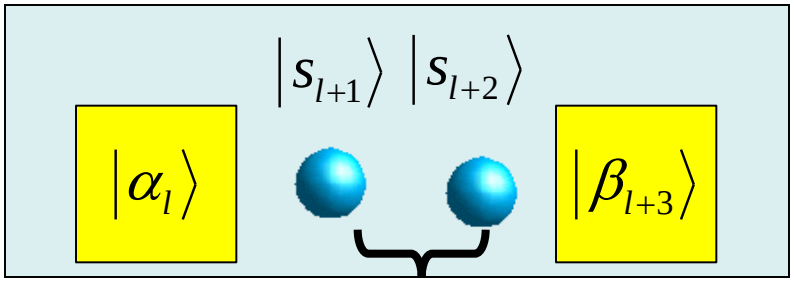
$$H = \begin{pmatrix} 1/4 & & & 0 \\ & -1/4 & 1/2 & \\ & 1/2 & -1/4 & \\ 0 & & & 1/4 \end{pmatrix}$$

Exercise: Exponentiate (by hand) the matrix by following these steps:

1. Diagonalize the matrix and calculate eigenvalues and eigenvectors
2. Calculate the exponential of *H* in the diagonal basis
3. Rotate back to the original basis

Evolving the wave-function

We want to apply the evolution operator between the two central sites:



$e^{-i\tau Hij}$

As we've seen before, the link evolution operator can be written as

$$e^{-itH_{l+1,l+2}} = U^{s_{l+1},s_{l+2}}_{s'_{l+1},s'_{l+2}} \left| s_{l+1} s_{l+2} \right\rangle \left\langle s'_{l+1}\, s'_{l+2} \right|$$

And the wave function after the transformation:

$$e^{-itH_{l+1,l+2}} \left|\psi\right\rangle = \sum_{\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3}} \varphi(\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3}) \left|\alpha_l\right\rangle \otimes \left|s_{l+1}\right\rangle \otimes \left|s_{l+2}\right\rangle \otimes \left|\beta_{l+3}\right\rangle$$

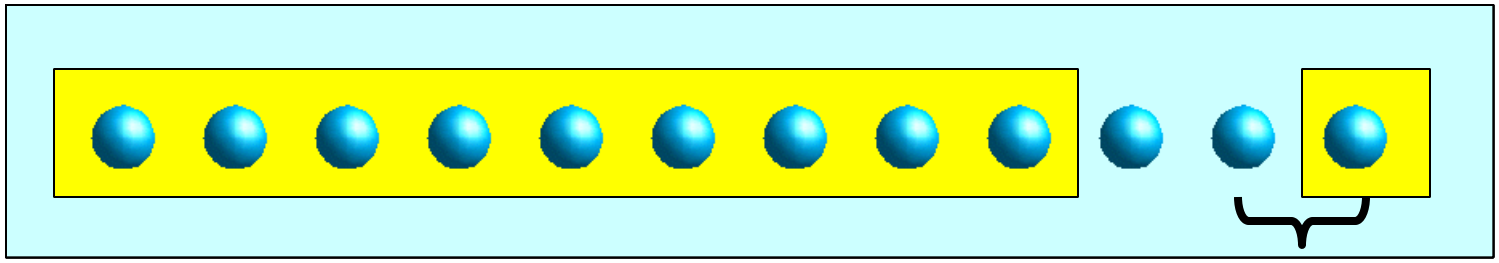
$$\text{with } \varphi(\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3}) = \sum_{s'_{l+1}, s'_{l+2}} U^{s_{l+1},s_{l+2}}_{s'_{l+1},s'_{l+2}} \psi(\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3})$$

tDMRG: The algorithm

S.R.White and A.E. Feiguin, PRL (2004), Daley et al, J. Stat. Mech.: Theor. Exp. (2004)

We turn off the diagonalization and start applying the evolution operator

We move to the end to start time-evolution



$e^{-i\tau Hij}$

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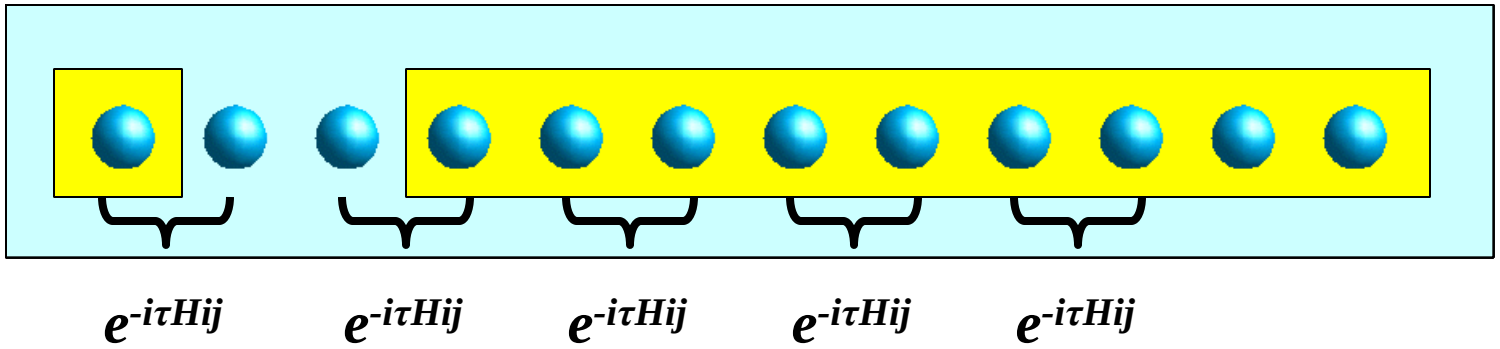

Depending on the S-T break-up, a few sweeps evolve a time step

Each link term only involves two-sites interactions: small matrix, easy to calculate! Much faster than Lanczos!