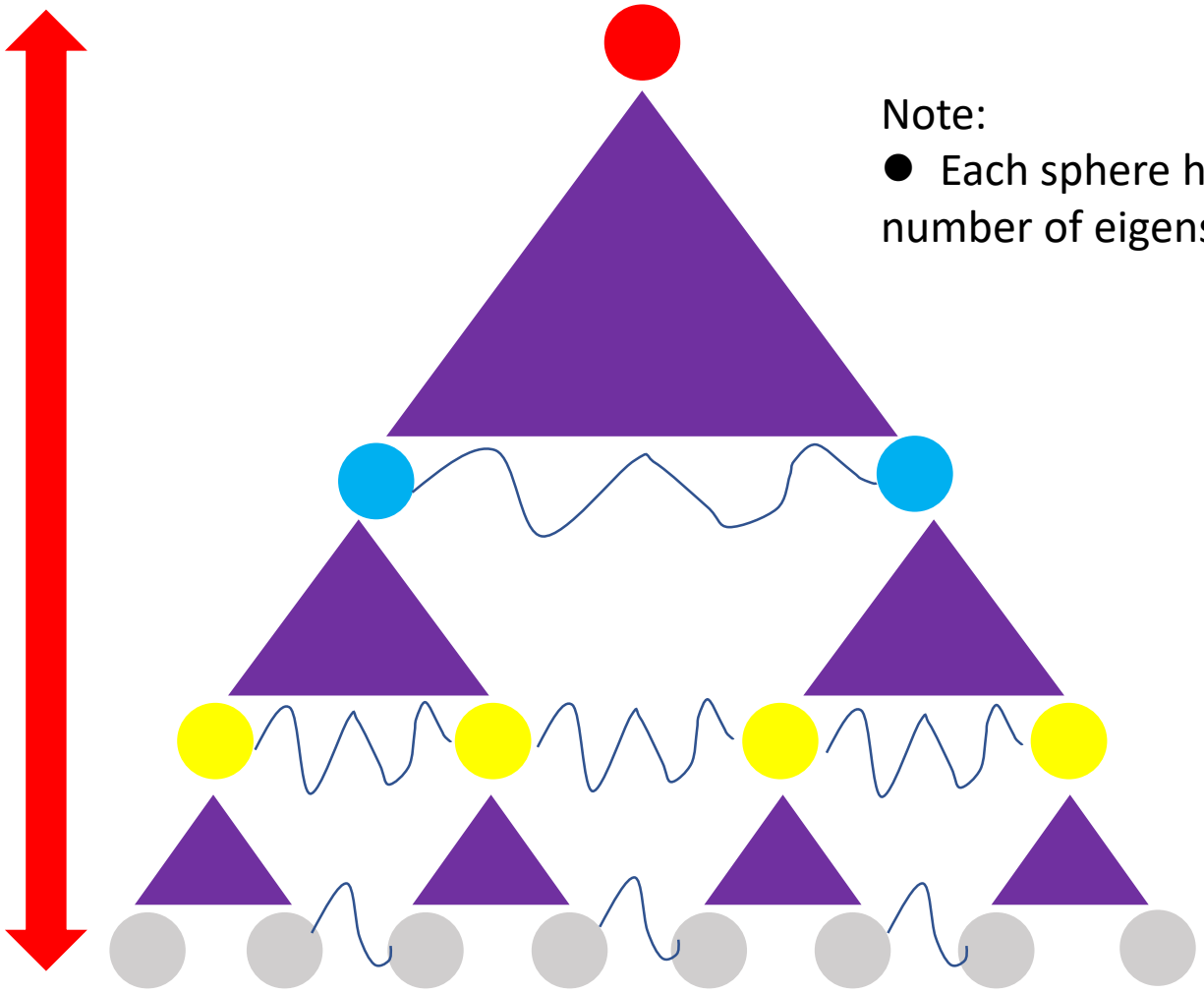
Review of real-space RG

Macroscopic quantum phenomena (fixed point)



Microscopic quantum interaction

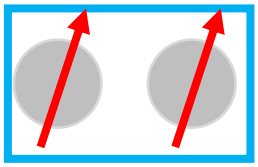
Note:

- Each sphere has the same number of eigenstates;

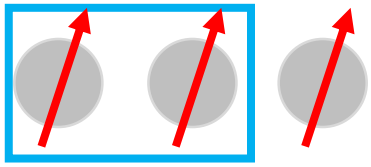
DMRG

The original algorithm, developed to describe systems with nearest neighbor interaction at the thermodynamic limit is composed of the following building blocks:

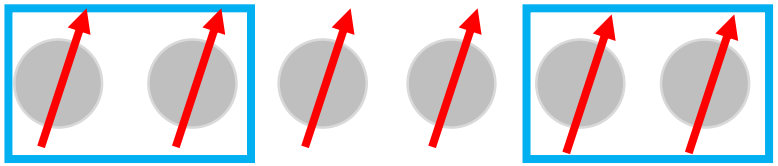
A single site represents an isolated site of the lattice, it could be, for example, a single spin, when you have a chain of spins.
The d.o.f. of single site is d.



A block is a contiguous segment of the lattice. It is a chain of several connected sites. A block could contain just a single site, but it can't be empty. The d.o.f. is D^M, D is the physical d.o.f., M is the site #.



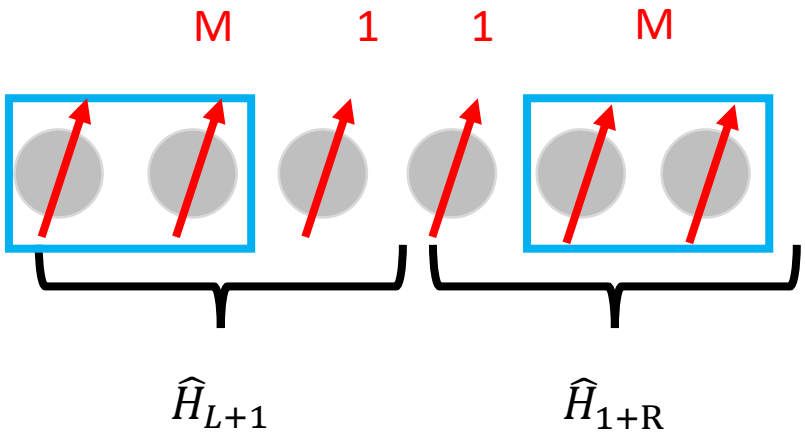
An enlarged block is formed by connecting a block to single additional site. The d.o.f. is dD^M.



A superblock is constructed by connecting two enlarged blocks to each other.

Infinite size DMRG

1. consider the biggest system size N that can be diagonalized exactly with reasonable resources and regroup the N sites in two single sites in the middle and others in two groups of M sites as shown below:



The system's Hamiltonian can be written as

$$H_N = H_{L+1} + H_{\mathrm{int}} + H_{1+R}$$

where $\hat{H}_{L+1}$ and $\hat{H}_{R+1}$ in the literature are referred at as the left and right enlarged blocks, and $\hat{H}_{\mathrm{int}}$ is the interaction among them.
The dimension of the Hilbert space of the system is (dm)^2, where d is the single site physical dimension and m=d^M the dimension of the M grouped sites.

The diagonalization of $\hat{H}_N$ returns the ground state expressed in the basis

$$\left|E_0^N\right\rangle = \sum_{\beta_L \beta_R} \psi_{\beta_L \beta_R} \left|\beta_L \beta_R\right\rangle$$

where $|\beta_{\mathrm{i}}\rangle$ spans the basis of the left and right half sites β_{i}=1,…,d^{M+1}

2. compute the density matrix of the ground state

$$\rho_0^N = \left|E_0^N\right\rangle\left\langle E_0^N\right| = \sum_{\beta_L\beta_R}\sum_{\beta_L^{'}\beta_R^{'}} \psi_{\beta_L\beta_R}\psi^{*}_{\beta_R^{'}\beta_L^{'}} \left|\beta_L\beta_R\right\rangle\left\langle\beta_R^{'}\beta_L^{'}\right|$$

and the reduced density matrix of one half of the system

$$\rho_L = tr_R(\rho_0^N) = \sum_{\beta_R^{''}}\left\langle\beta_R^{''}\right|\Big(\sum_{\beta_L\beta_R}\sum_{\beta_L^{'}\beta_R^{'}} \psi_{\beta_L\beta_R}\psi^{*}_{\beta_R^{'}\beta_L^{'}} \left|\beta_L\beta_R\right\rangle\left\langle\beta_R^{'}\beta_L^{'}\right|\Big)\left|\beta_R^{''}\right\rangle$$

$$= \sum_{\beta_L\beta_L^{'}}\Big(\sum_{\beta_R}\psi_{\beta_L\beta_R}\psi^{*}_{\beta_R\beta_L^{'}}\Big)\left|\beta_L\right\rangle\left\langle\beta_L^{'}\right| = \sum_{\beta_L\beta_L^{'}}(\psi\psi^{*})_{\beta_L\beta_L^{'}}\left|\beta_L\right\rangle\left\langle\beta_L^{'}\right|$$

3, diagonalize ρ_L

$$\rho_L = \sum_{i=1}^{md}\omega_i\left|\omega_i\right\rangle\left\langle\omega_i\right|$$

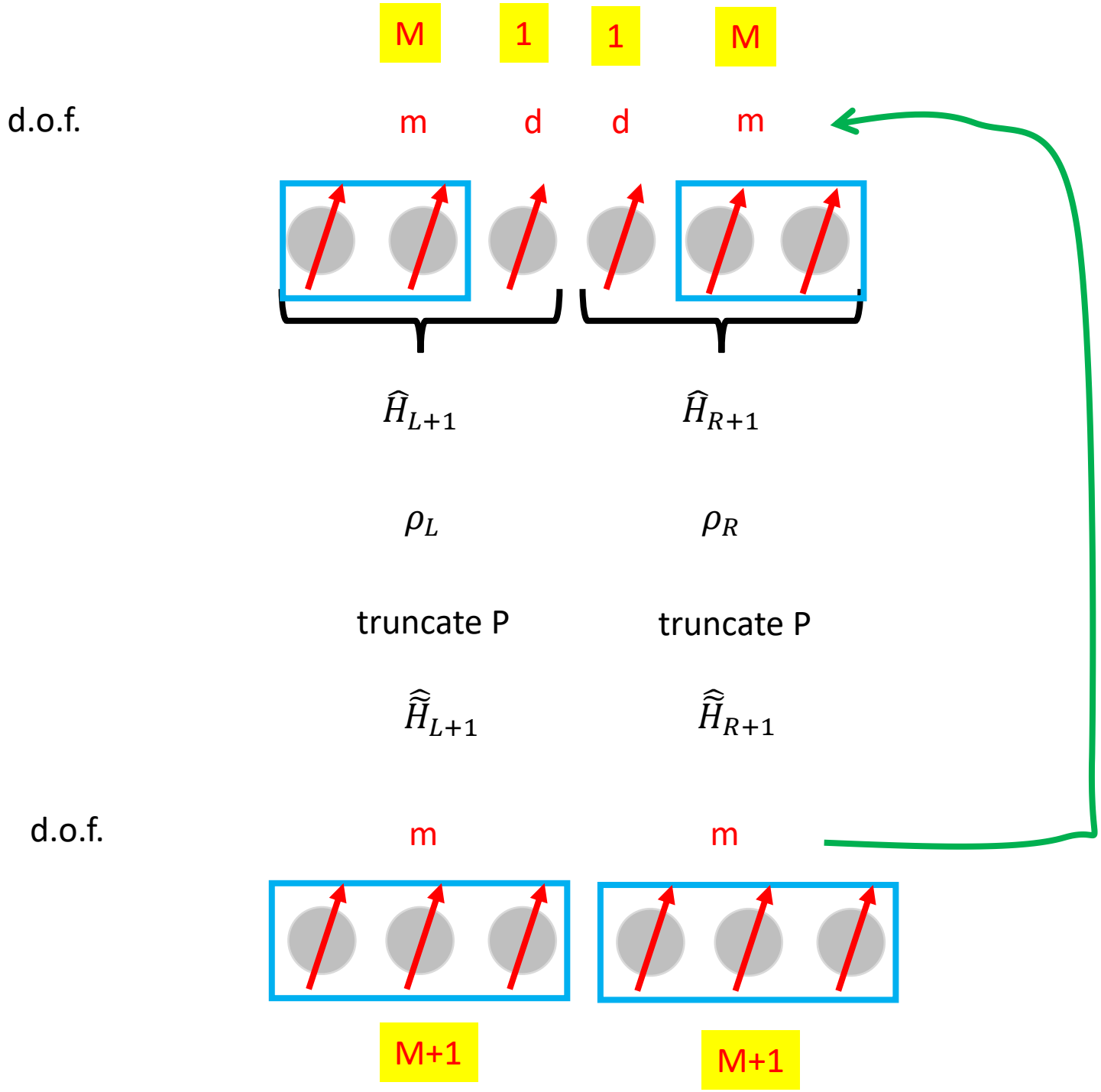
and order the eigenvalues ω_i in descending order. If we assume the system to be left-right symmetric, we also have that $\rho_L = \rho_R$. Define the projector

$$P = \sum_{i=1}^{m}\left|\omega_i\right\rangle\left\langle\omega_i\right|$$

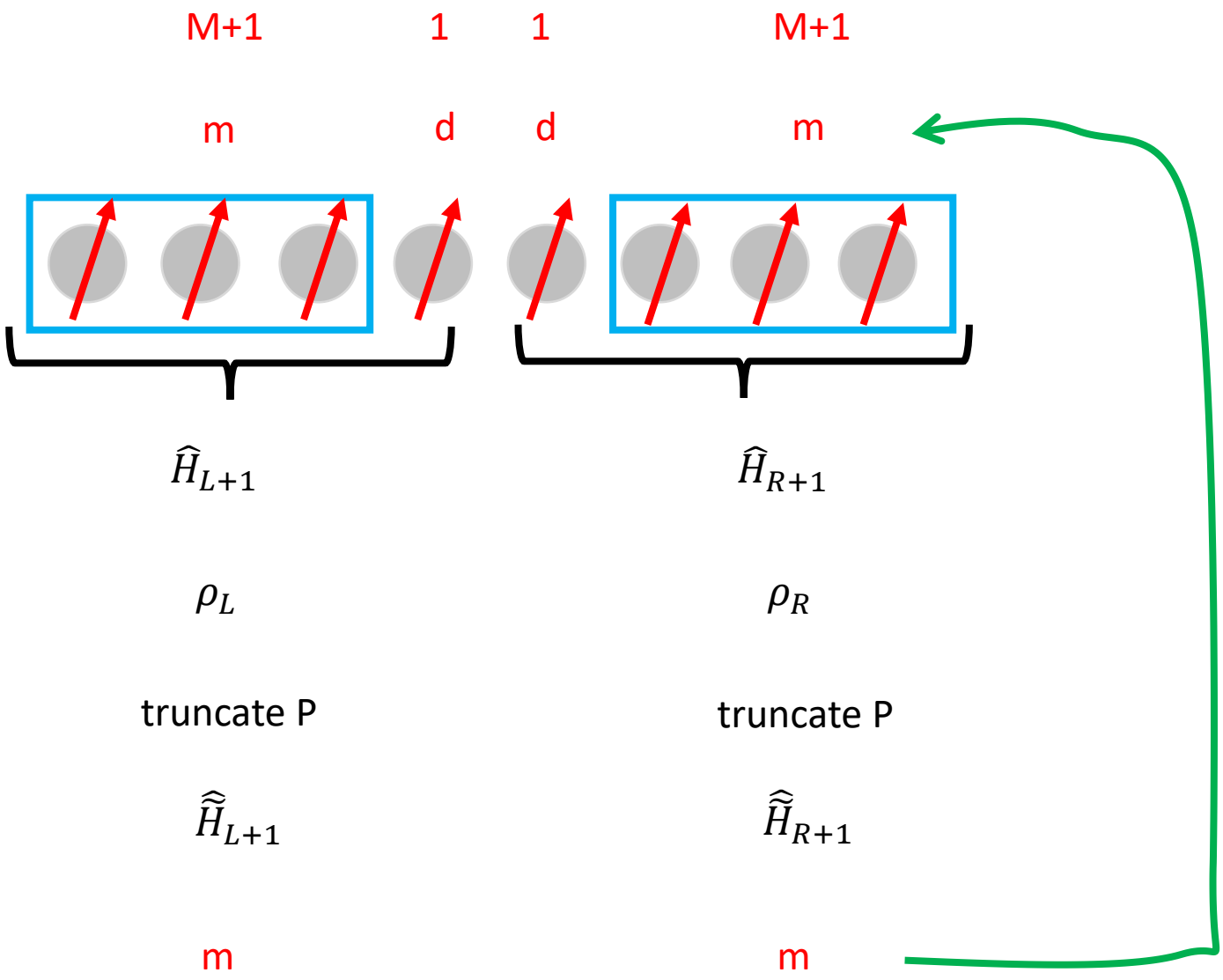
composed by only the first m eigenvalues of ρ_L

4. the projector P defines a truncation of the Hilbert space from md to states that can be used to compute the effective Hamiltonian of the system and all necessary operators in the reduced space, $\widehat{\widehat{H}}_{L+1} = \hat{P}^{\dagger}\hat{H}_{L+1}\hat{P}$ and given that $\widehat{\widehat{H}}_{\text{int}} = \sum_k c_k A_L^k \otimes B_R^k$ the interaction term in the projected space can be computed applying the projector on the left and right separately. We thus obtain an effective matrix describing the Hamiltonian for the system of N sites of dimension m instead of md.

5. the algorithm is iterated starting again from step 1 provided that the Hamiltonian of the left and right block are replaced with the effective Hamiltonians computed in the previous step. The net effect is that one can describe a system of N+2 sites with a Hamiltonian of size (md)2. At every step, the size of the described system is incremented by two sites while keeping the computational resources constant.

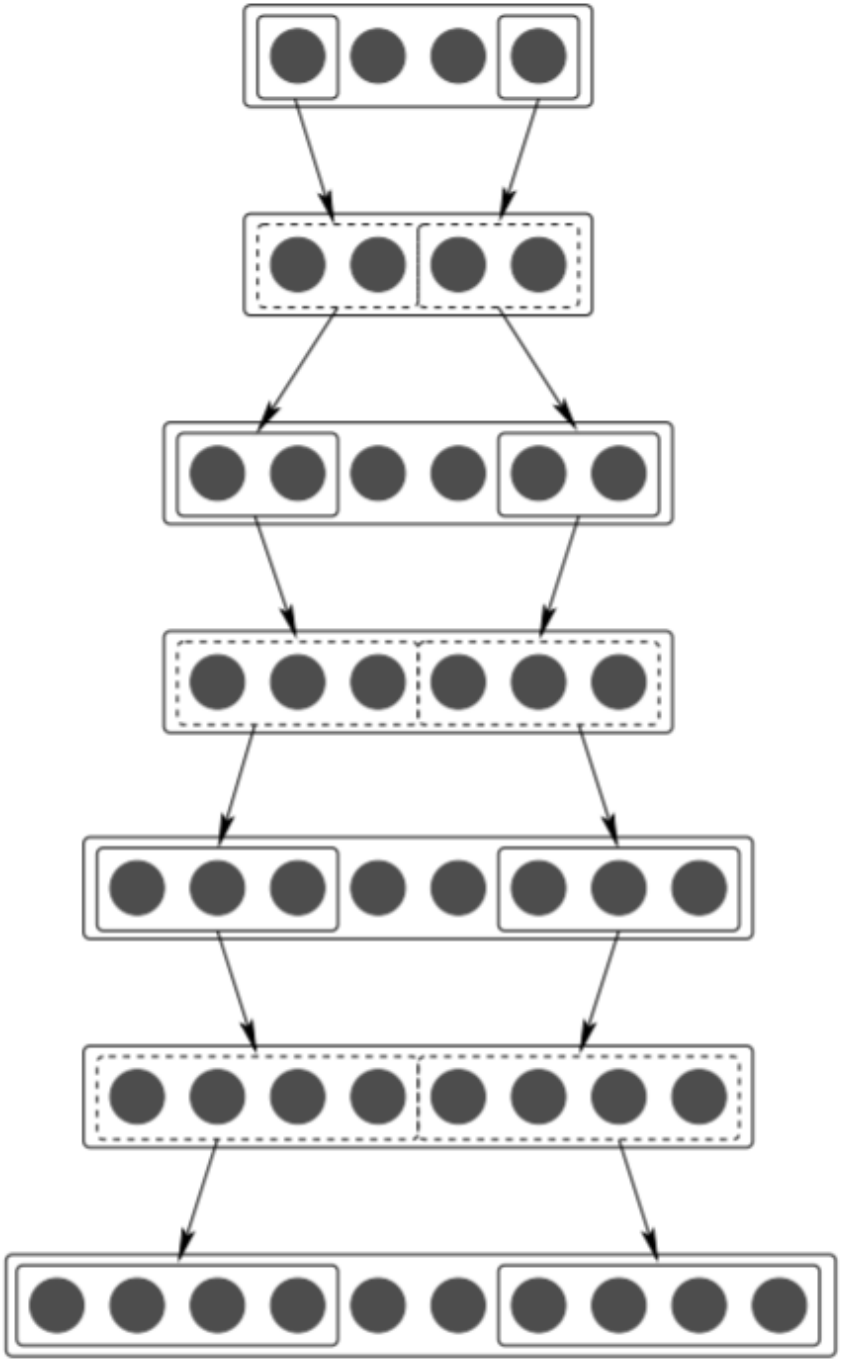

M
1
1
M
d.o.f.
m
d
d
m
$\widehat{H}_{L+1}$
$\widehat{H}_{R+1}$
ρ_L
ρ_R
truncate P
truncate P
$\widehat{\widetilde{H}}_{L+1}$
$\widehat{\widetilde{H}}_{R+1}$
d.o.f.
m
m
M+1
M+1

Now we insert two more sites between left and right superblock



Each step, the size of enlarged block is increased by 1.

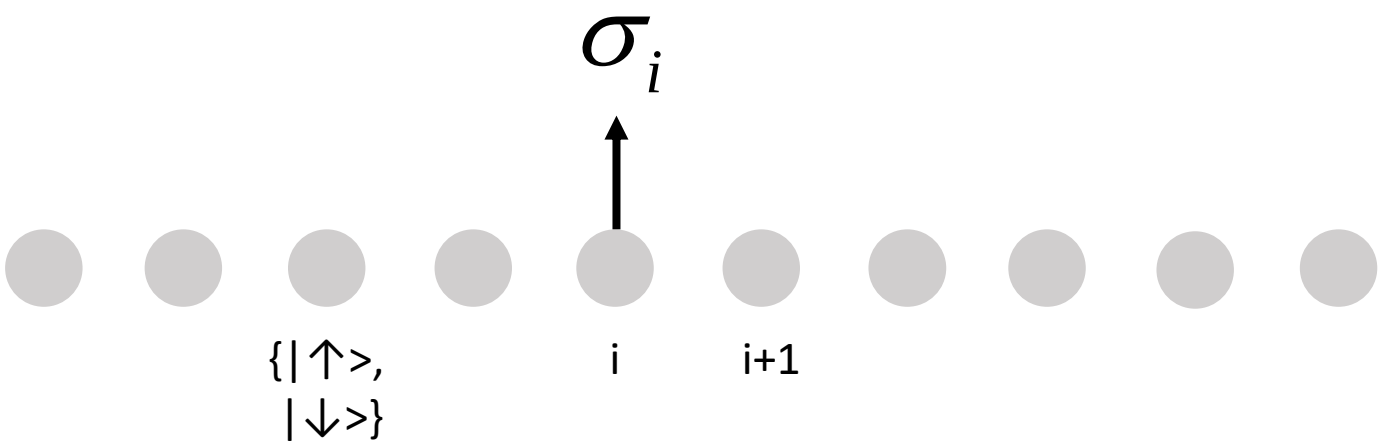
Flow:



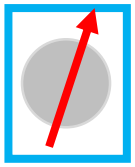
Example:

DMRG treatment of 1D transverse Ising model

$$H = -\sum_i \sigma_i^x \sigma_{i+1}^x - h \sum_i \sigma_i^z$$



Step 1:

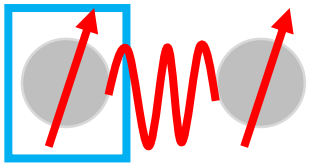


block

$$H_L = -h\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

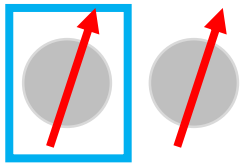
single site

$$H_1 = -h\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



interaction between left block and site

$$H_{\mathrm{L-int-1}} = -\sigma^{x,L} \otimes \sigma^{x,1} = -\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$



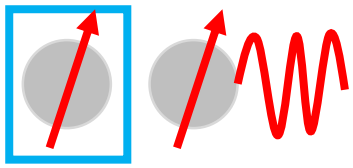
enlarged left block

$$H_{L+1} = H_L \otimes 1^1 + H_{\mathrm{L-int-1}} + 1^L \otimes H_1$$

$$= \begin{pmatrix} -h & \\ & h \end{pmatrix} \otimes 1 + H_{\mathrm{L-int-1}} + 1 \otimes \begin{pmatrix} -h & \\ & h \end{pmatrix}$$

$$= \begin{pmatrix} -h & & & \\ & -h & & \\ & & h & \\ & & & h \end{pmatrix} + H_{\mathrm{L-int-1}} + \begin{pmatrix} -h & & & \\ & h & & \\ & & -h & \\ & & & h \end{pmatrix}$$

$$= \begin{pmatrix} -2h & & & -1 \\ & & -1 & \\ & -1 & & \\ -1 & & & 2h \end{pmatrix}$$



enlarged left block
interaction with others

$$\sigma^{x,L+1} = 1^L \otimes \sigma^{x,1} = \begin{pmatrix} & 1 & & \\ 1 & & & \\ & & & 1 \\ & & 1 & \end{pmatrix}$$

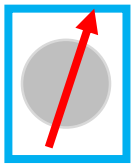
Do the same to the right block

$$H_1 = -h\sigma^z = -h\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

single site

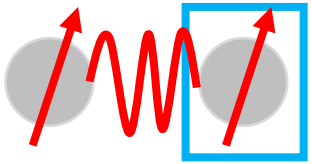
$$H_R = -h\sigma^z = -h\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

block



$$H_{1-\text{int}-\text{R}} = -\sigma^{x,1} \otimes \sigma^{x,R} = -\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

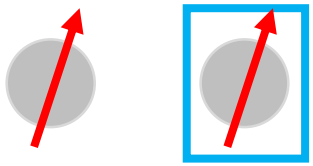
interaction between left block and site



$$H_{1+R} = H_1 \otimes 1^R + H_{1-\text{int}-\text{R}} + 1^1 \otimes H_R$$

$$= 1 \otimes \begin{pmatrix} -h & \\ & h \end{pmatrix} + H_{1-\text{int}-\text{R}} + \begin{pmatrix} -h & \\ & h \end{pmatrix} \otimes 1$$

enlarged right block

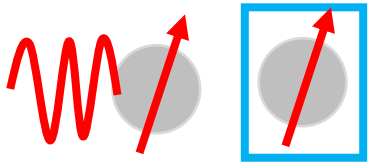


$$= \begin{pmatrix} -h & & & \\ & h & & \\ & & -h & \\ & & & h \end{pmatrix} + H_{1-\text{int}-\text{R}} + \begin{pmatrix} -h & & & \\ & -h & & \\ & & h & \\ & & & h \end{pmatrix}$$

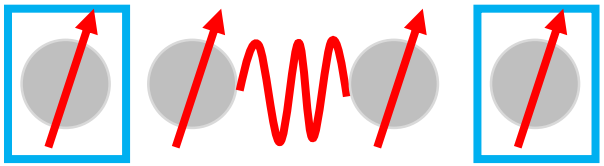
$$= \begin{pmatrix} -2h & & & -1 \\ & & -1 & \\ & -1 & & \\ -1 & & & 2h \end{pmatrix}$$

$$\sigma^{x,1+\text{R}} = \sigma^{x,1} \otimes 1^R = \begin{pmatrix} & 1 & & \\ & & & 1 \\ 1 & & & \\ & 1 & & \end{pmatrix}$$

enlarged right block
interaction with others



Now we need to treat the interaction between the left enlarged block and the right enlarged block:

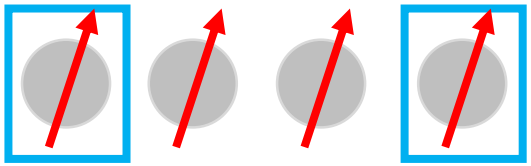


interaction between
left enlarged block
and
right enlarged block

$$H_{\mathrm{L+1-int-1+R}} = -\sigma^{x,\mathrm{L+1}}\sigma^{x,1+\mathrm{R}} = -\begin{pmatrix} & 1 & & \\ 1 & & & \\ & & & 1 \\ & & 1 & \end{pmatrix} \otimes \begin{pmatrix} & & 1 & \\ & & & 1 \\ 1 & & & \\ & 1 & & \end{pmatrix}$$

$$= -\begin{pmatrix} & & & & 0 & 0 & 1 & 0 & & & & \\ & & & & 0 & 0 & 0 & 1 & & & & \\ & & & & 1 & 0 & 0 & 0 & & & & \\ & & & & 0 & 1 & 0 & 0 & & & & \\ 0 & 0 & 1 & 0 & & & & & & & & \\ 0 & 0 & 0 & 1 & & & & & & & & \\ 1 & 0 & 0 & 0 & & & & & & & & \\ 0 & 1 & 0 & 0 & & & & & & & & \\ & & & & & & & & 0 & 0 & 1 & 0 \\ & & & & & & & & 0 & 0 & 0 & 1 \\ & & & & & & & & 1 & 0 & 0 & 0 \\ & & & & & & & & 0 & 1 & 0 & 0 \\ & & & & 0 & 0 & 1 & 0 & & & & \\ & & & & 0 & 0 & 0 & 1 & & & & \\ & & & & 1 & 0 & 0 & 0 & & & & \\ & & & & 0 & 1 & 0 & 0 & & & & \end{pmatrix}$$

Finally we reach the last step in step 1:



$$H_4 = H_{L+1} \otimes 1 + H_{\mathrm{L+1-int-1+R}} + 1 \otimes H_{R+1} = \begin{pmatrix} -2h & & & -1 \\ & & -1 & \\ & -1 & & \\ -1 & & & 2h \end{pmatrix} \otimes 1 + H_{\mathrm{L+1-int-1+R}} + 1 \otimes \begin{pmatrix} -2h & & & -1 \\ & & -1 & \\ & -1 & & \\ -1 & & & 2h \end{pmatrix}$$

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

Step 2: For simplicity, we will now set h=2.

The G.S. is

$$|\psi_0\rangle = \begin{pmatrix} 0.976082 \\ 0. \\ 0. \\ 0.122 \\ 0. \\ 0.0304289 \\ 0.123787 \\ 0. \\ 0. \\ 0.00911006 \\ 0.0304289 \\ 0. \\ 0.122 \\ 0. \\ 0. \\ 0.0154554 \end{pmatrix}, \qquad E_0 = -8.3768$$

And the density matrix of the G.S. is

$$\rho_0^4 = |\psi_0\rangle\langle\psi_0|$$

Step 3: The reduced density matrix is:

$$\rho_L = tr_R(\rho_0^4) = \begin{pmatrix} 0.967619 & 0. & 0. & 0.120967 \\ 0. & 0.0162492 & 0.00404391 & 0. \\ 0. & 0.00404391 & 0.00100891 & 0. \\ 0.120967 & 0. & 0. & 0.0151228 \end{pmatrix}$$

And the eigenvalue and eigenstate of reduced density matrix is

Eigenstates	$\begin{pmatrix} -0.992276 \\ 0. \\ 0. \\ -0.12405 \end{pmatrix}$	$\begin{pmatrix} 0. \\ 0.970392 \\ 0.241536 \\ 0. \end{pmatrix}$	$\begin{pmatrix} 0. \\ 0.241536 \\ -0.970392 \\ 0. \end{pmatrix}$	$\begin{pmatrix} -0.12405 \\ 0. \\ 0. \\ 0.992276 \end{pmatrix}$
Weights	0.982742	0.0172557	2.35975×10^{-6}	4.14343×10^{-8}

Say we want to keep the first and second eigenstates, then we construct the truncation matrix as:

$$P = \begin{pmatrix} -0.992276 & 0 \\ 0. & 0.970392 \\ 0. & 0.241536 \\ -0.12405 & 0. \end{pmatrix}$$

Step 4: recover the left enlarged Hamiltonian:

$$H_{L+1} = P^{\dagger} H_{L+1} P = \begin{pmatrix} -4.12308 & 0 \\ 0 & -0.468768 \end{pmatrix} \qquad \sigma^z, 1$$

And the interaction becomes

$$\sigma^{x,L+1} = P^{\dagger}(\sigma^{x,L+1})P = \begin{pmatrix} 0. & -0.992859 \\ -0.992859 & 0. \end{pmatrix} \qquad \sigma^x$$

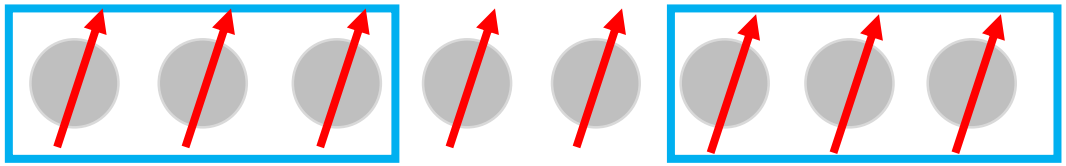
This concludes the renormalization transformation. We constructed an effective interaction $\widehat{\widehat{H}}_{L+1}$ for a block of two spins with only two d.o.f..

$$H_L = \sigma^z \rightarrow H_{L+1} = \sigma^z, 1$$

$$\sigma^{x,L} \rightarrow \sigma^{x,L+1} = \sigma^x$$

It's clear the change of Hamiltonian form is just like that of real space RG.

Step 5: growth



Hint from the above example:
1, the matrix are always sparse matrix
2, the G.S. and E.S. are equivalent

Density Matrix Renormalization Group calculations for the Ising Model with a Transverse Field

Bachelor Thesis

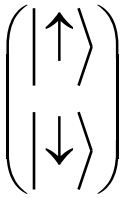
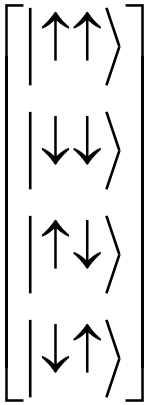
A.H. Kole

Natuur- en Sterrenkunde & Scheikunde

Supervisor:
Dr. L. Fritz
Institute for Theoretical Physics

Matlba Code

See 1D transverse Ising model_1D_infinite

	DMRG	NRG
Basis		
Truncation	density matrix	m lowest exact state
Growth speed	linearly	exponentially

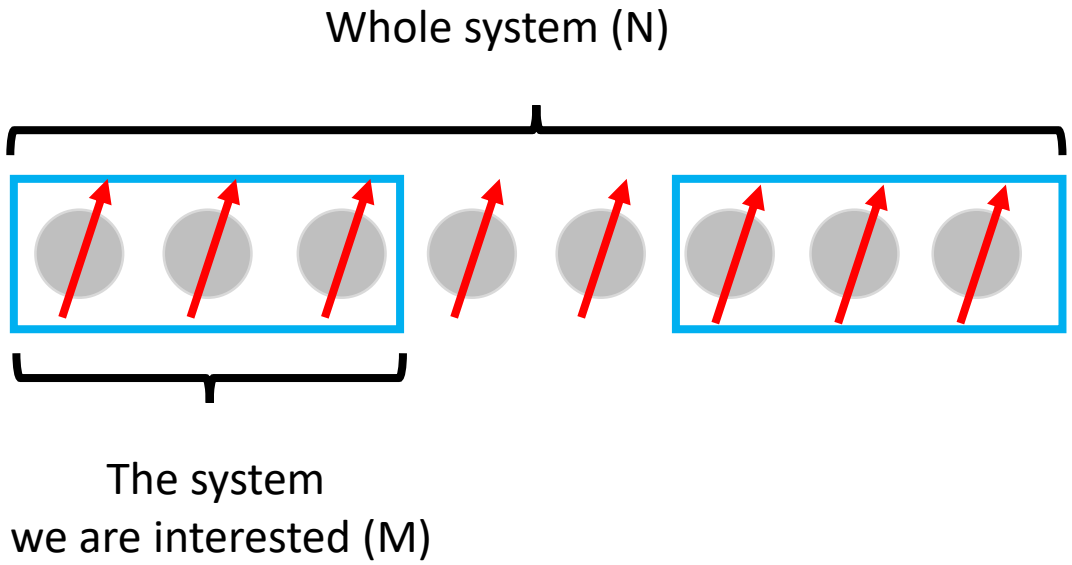
The truncation means the way we choose basis. Density matrix can be thought as mixed basis (contain both the m lowest exact state and other state), which is better to some point.

From infinite system to finite system

The optimization concern only the bipartition of the system in two equal subsystems: it might be possible to have a better approximation of the global many-body states if we could optimize the reduced density matrix of all possible bipartitions of the system. This refinement procedure is provided by the finite DMRG algorithm, which aims to refine the representation of a system composed of N sites. The algorithm is defined as follows:

finite system algorithm= infinite system +additional sweep

1, build the representation of a system composed of N=2M+2 sites using the infinite DMRG algorithm.
Here M is the number of sites we are interested in.
During this process, store all the left and right blocks, with their corresponding operators and basis transformations.

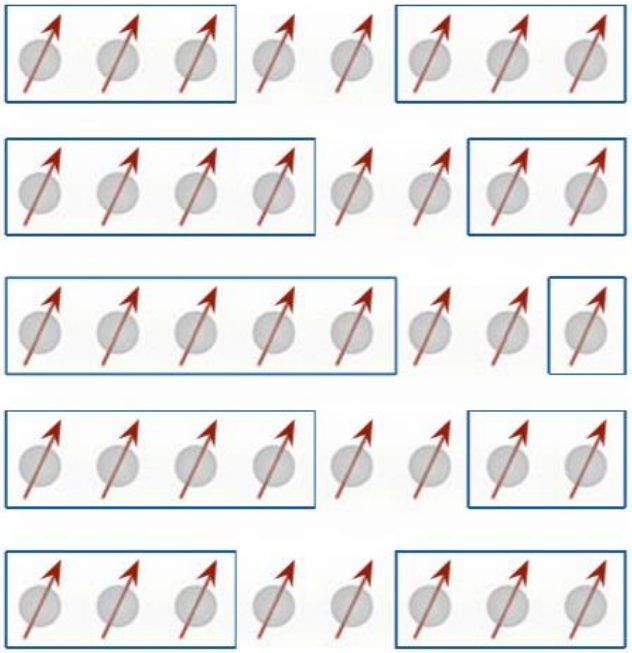


2. start a new DMRG iteration taking care when building the new system Hamiltonian to keep the system size fixed to N. That is:

$$H_N = H_{M+2} + H_{\text{int}} + H_M$$

Notice that the left and right enlarged block now are different and represent a different number of sites. Obtain the truncated representation of the Hamiltonian $\widehat{\widetilde{H}}_{M+2}$.

3. keep on iterating, increasing the size of the left block and decreasing that of the right block, keeping N constant. When the boundary is reached, reverse the process and keep iterating inverting the role of the left and right block.



This sweeping process works in a similar fashion as a self-consistent loop where we iteratively improve the solution. In fact, the DMRG can be formulated as a variational method, in which the variational parameters are continuously improved to minimize an energy functional.

Intuitively a way to see it is by imagining a “demon” probing the environment around the block for the optimal state to improve the basis to represent the ground state. These states are absorbed inside the block by the density matrix and its eigenvectors.

Why DMRG works so well in comparison to NRG?

system and environment

entanglement introduced by density matrix

DMRG: How to do it efficiently enough to do big systems

- Use commuting quantum numbers to keep all matrices and vectors in block form. Store as separate dense blocks, not sparse form. Typically S_z, $N_{particle}$. Spatial symmetries can't be used.
- Translate almost all operations to matrix-matrix multiplies, and make sure these are done use dgemm in an excellent BLAS (MKL, Gotoblas). Shoot for 90-95% of time in BLAS. Make sure no operation is worse than m^3.
- Use extrapolation in the truncation error (energies, local observables)
- Never use fully periodic BCs (cylindrical are great). Like doing a system twice as wide, plus danger of getting stuck.
- Pin the state if there is order or to see if there is order. To measure order, try cylindrical BC/aspect ratio method (White & Chernyshev, PRL 99, 127004 (2007)). Avoid correlation functions.
- To avoid getting stuck, apply initial pinning fields then turn off, and add special noise term to density matrix (White, PRB 72, 180403 (2005))
- Watch your state evolve.