Tensor Networks Based DMRG Study on Open Quantum Systems

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Motivation

- The Quantum Many-Body Problem
- Large number of interacting particles

Containing Chaos - Michel Lang, 2015

- Quantum framework

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- In order to store every possible state of a quantum system

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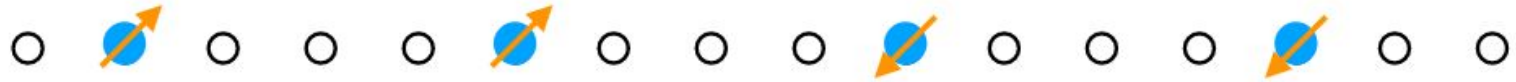

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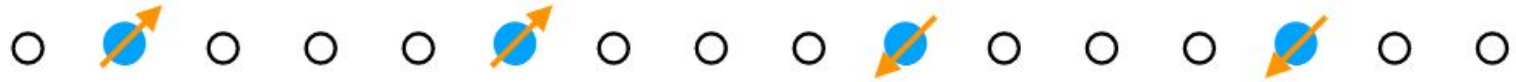

“Highly Non-Trivial” - Simulation would need to store 2^N possible configurations

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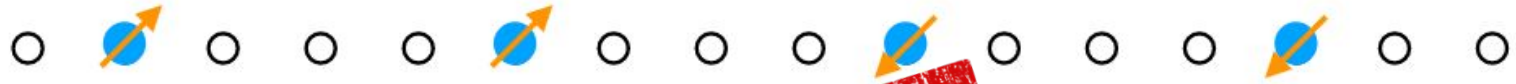

"Highly Non-Trivial" - Simulation would need to store 2^N possible configurations

Solution: Tensors ?

- High Order Data ➡ High Dimensionality ➡ High Computational Cost
  - Tensors store big branches of information and are relatively easy and inexpensive to be used

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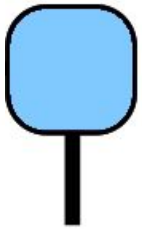
A^{x_1} ➡ 

Ulrich Schollwöck - The density-matrix renormalization group in the age of matrix product states - arxiv:1008.3477

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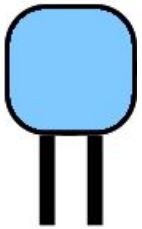
$$A^{x_1 x_2}$$ ➡ 

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Tensor Networks ?

- Tensor with index-oriented structures
  - Shall be used as approximations for our states and operators

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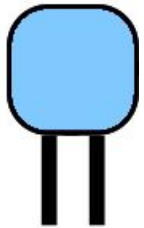
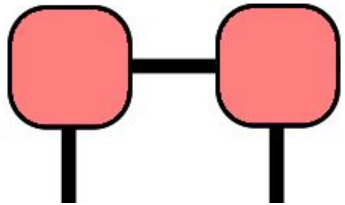


$$A^{x_1 x_2} = \sum_{y_1} B^{x_1}_{y_1} B^{x_2}_{y_1}$$



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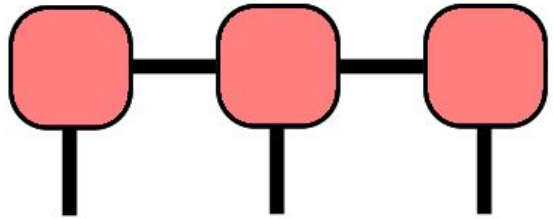

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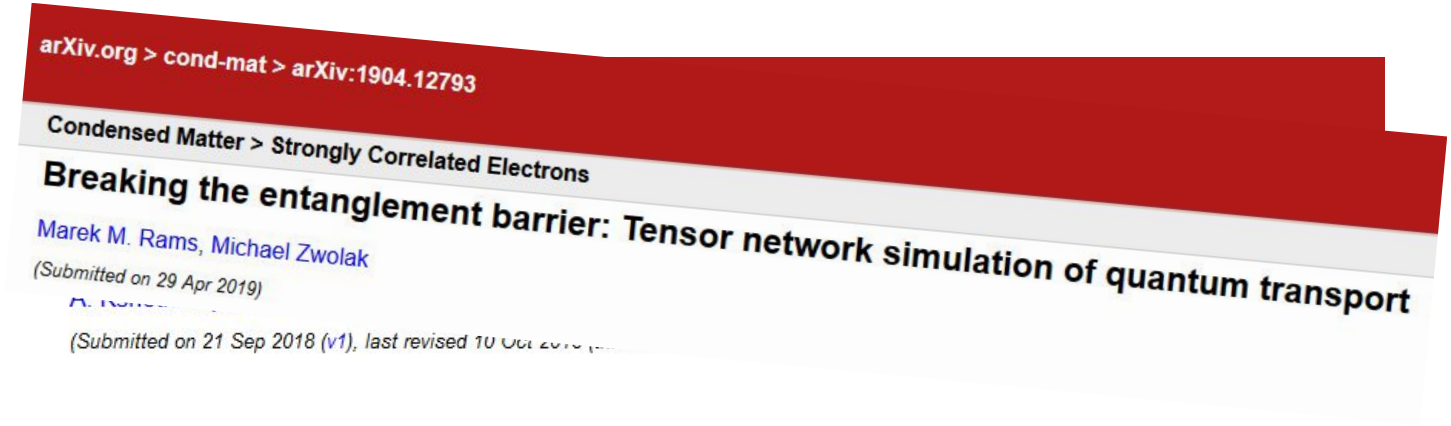

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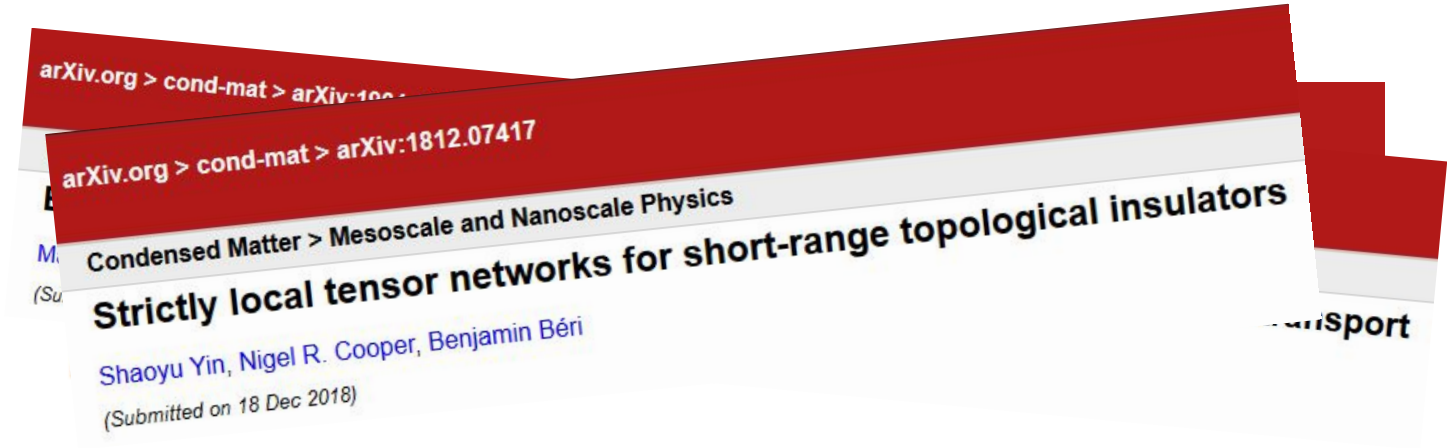

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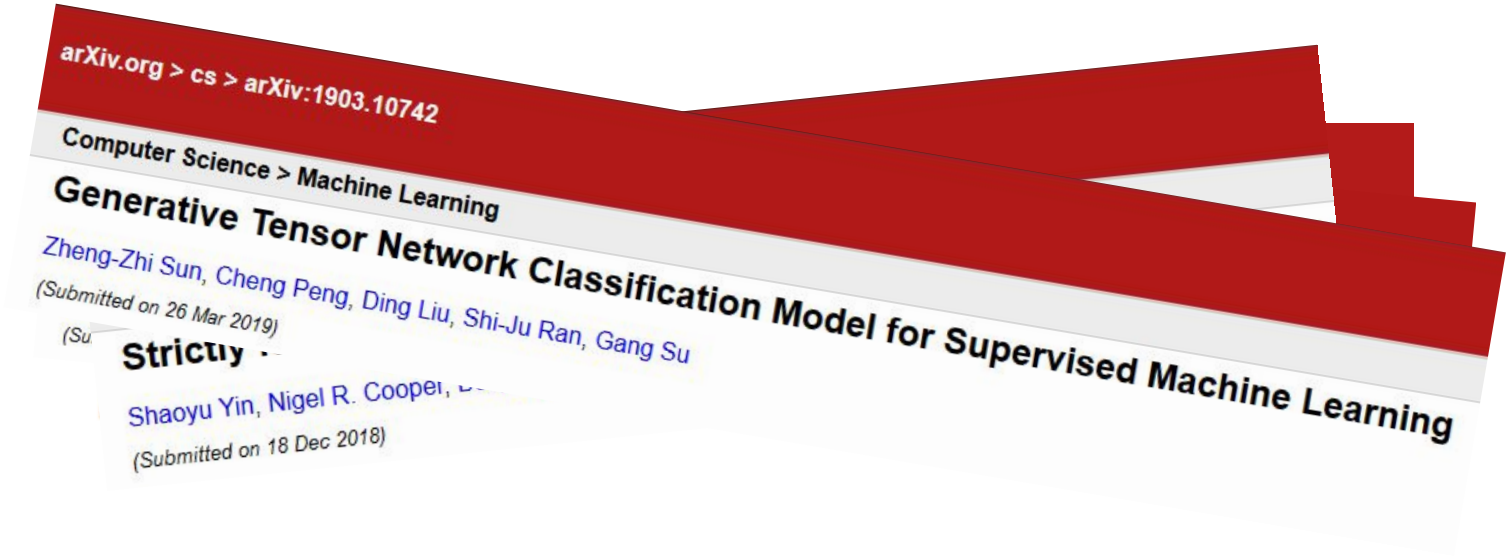

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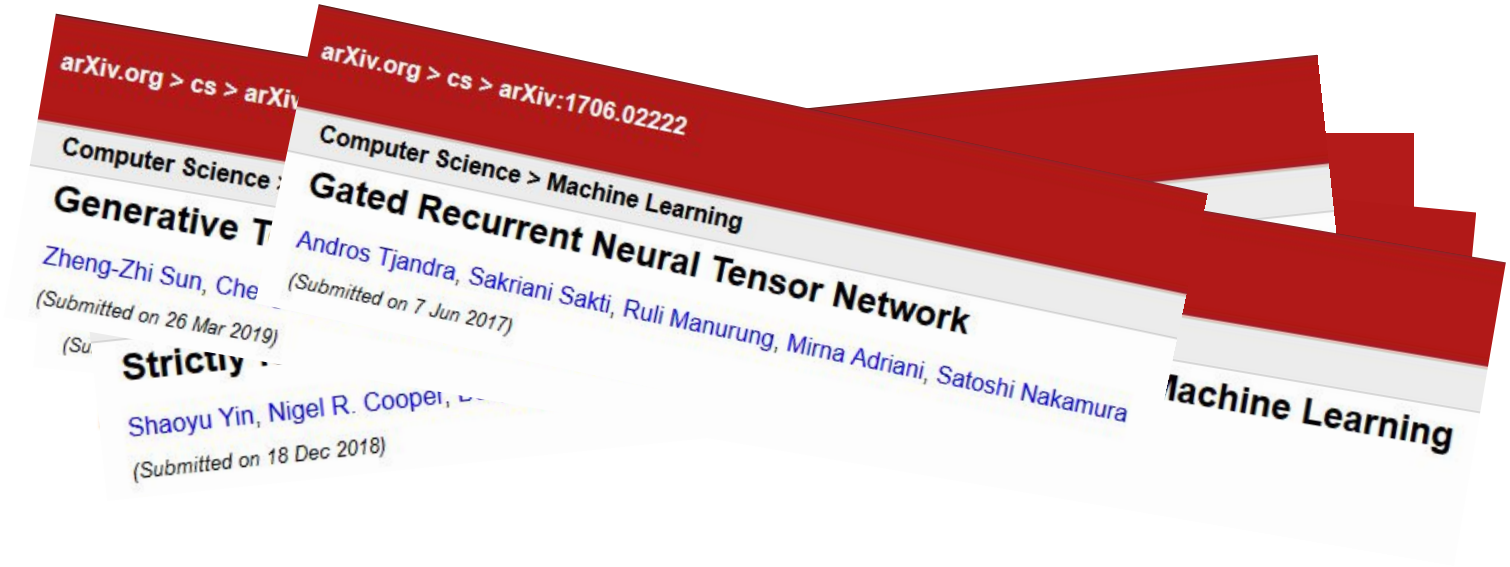

Spin Chains

- Many-body wavefunction as a superposition of basis states

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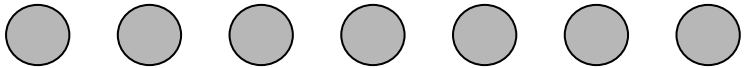

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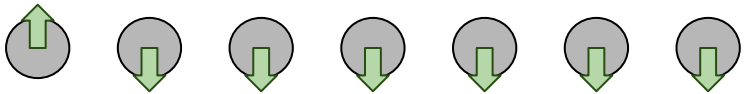

$$|\Psi\rangle = \Psi^{0000000}|0000000\rangle + \Psi^{1000000}|1000000\rangle +$$

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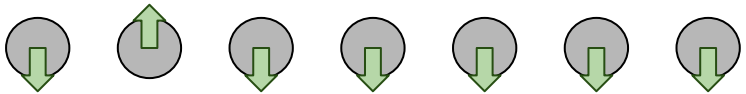

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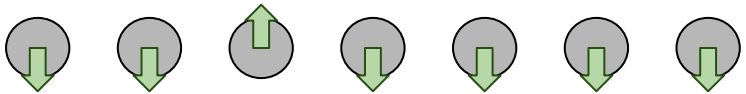

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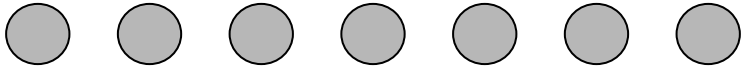

$$|\Psi\rangle = \sum_{s} \Psi^{s_1 s_2 s_3 \ldots s_N} |s_1 s_2 s_3 \ldots s_N\rangle$$

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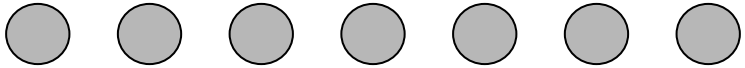

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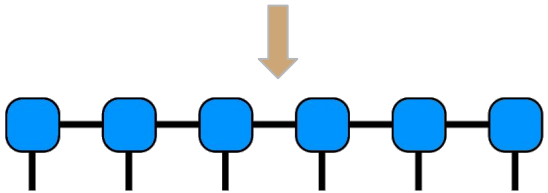
$$\sum_{x_1, x_2, \ldots x_{N-1}} A^{\sigma_1}_{x_1} A^{\sigma_2}_{x_1, x_2} \ldots A^{\sigma_N}_{x_{N-1}}$$



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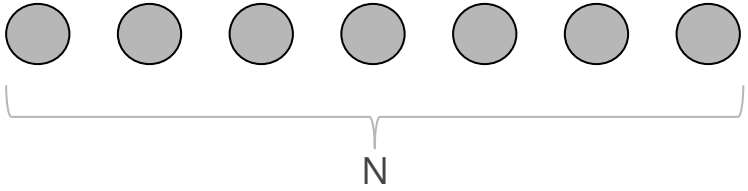
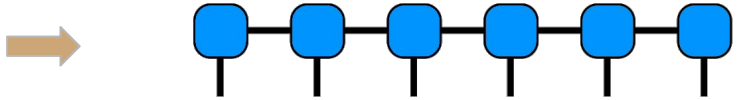


- Matrix Product State Ansatz

$$|\Psi\rangle = \sum_{\substack{\sigma_1,\sigma_2,\ldots\sigma_N \\ x_1,x_2,\ldots,x_{N-1}}} A^{\sigma_1}_{x_1} A^{\sigma_2}_{x_1,x_2} \ldots A^{\sigma_N}_{x_{N-1}} |\sigma_1\sigma_2\ldots\sigma_N\rangle$$



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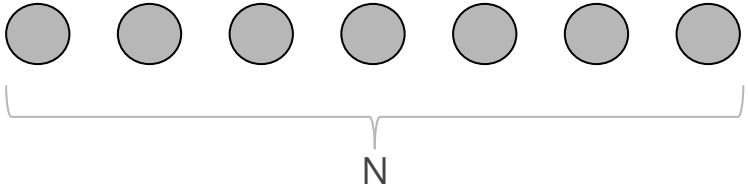

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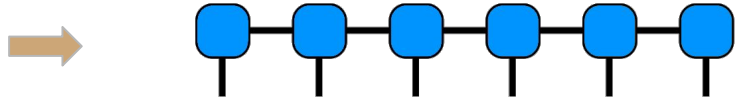
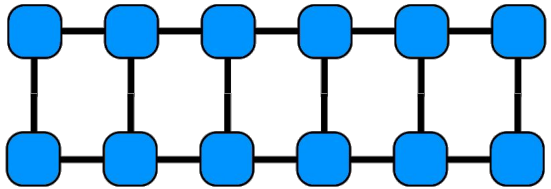


- Computing norm of a MPS

$$\langle\Psi|\Psi\rangle$$

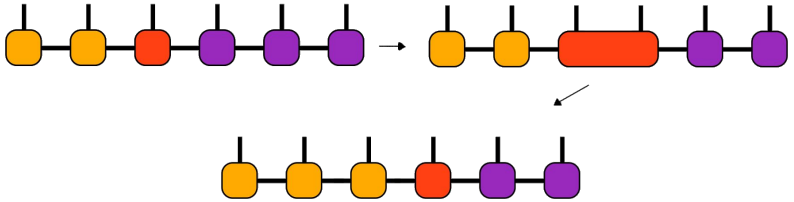


DMRG?

- Variational method to search for the Ground State of a system

$$H|\Psi\rangle = E|\Psi\rangle$$

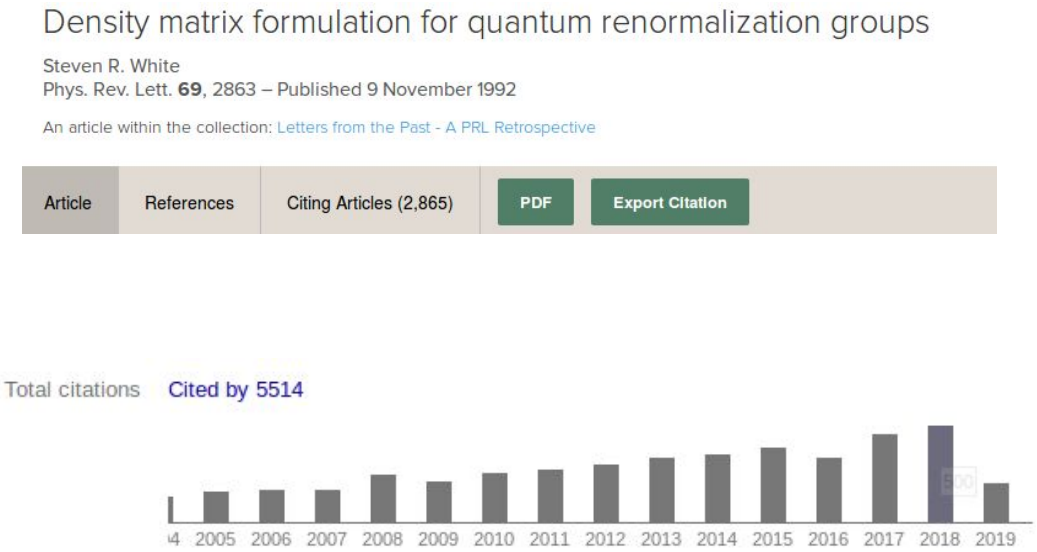
- *Sweeps* over 1D chain



- Minimize parameters in order to reach GS configuration

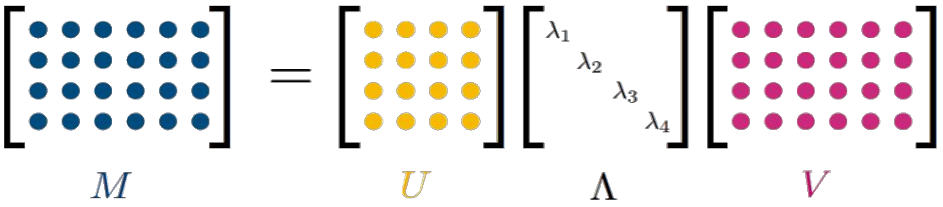
DMRG?

- Density Matrix Renormalization Group



How?

- Recall Singular Value Decomposition (SVD) operation



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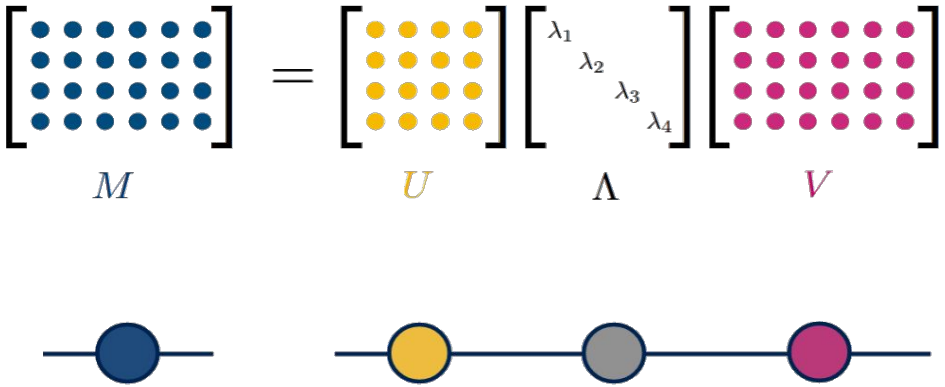


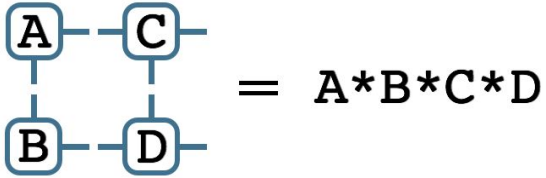
- Upon truncating over the Singular Values one can reduce dimensionality to reach a controlled approximation of the system Steady State

ITensor Library

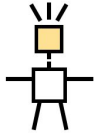
- C++ library

- Intuitive tensor contraction

and index management



- Built-in (super easy to use) DMRG routine, MPS norm calculation, expected operator values, etc.



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//Define Hilbert space of N spin-one sites
int N = 100;
auto sites = SpinOne(N);
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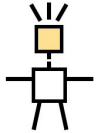

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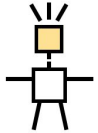

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//Perform 5 sweeps of DMRG
auto sweeps = Sweeps(5);
//Specify max number of states kept each sweep
sweeps.maxm() = 50, 50, 100, 100, 200;
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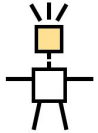

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//Run the DMRG algorithm
dmrg(psi,H,sweeps);
```

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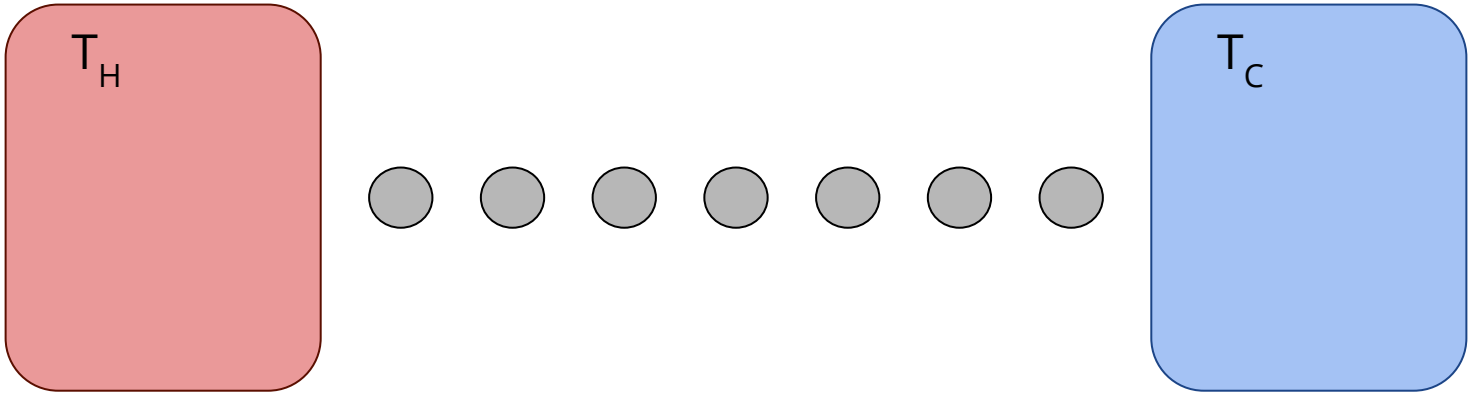
Open Quantum Systems?



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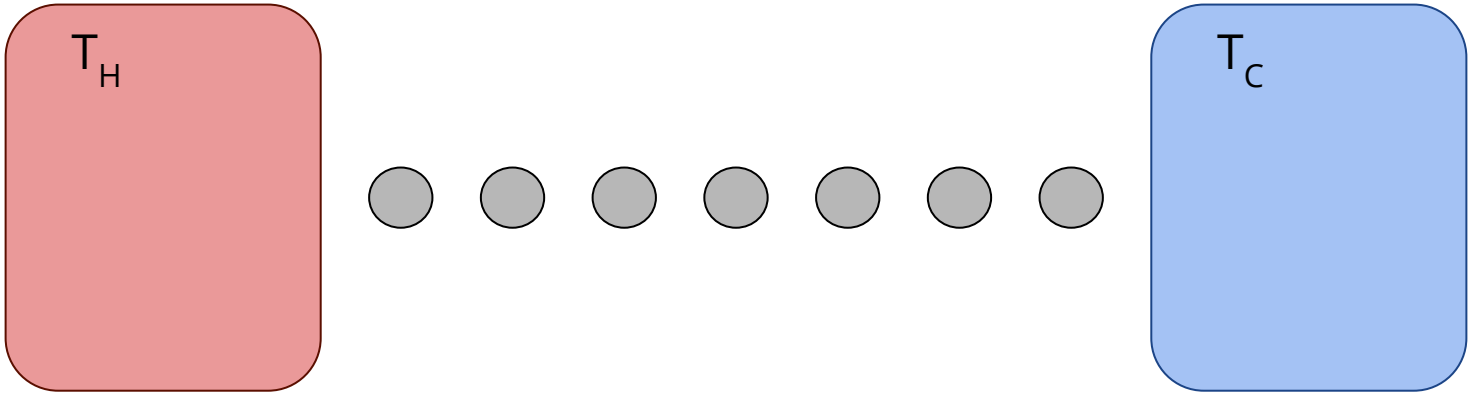
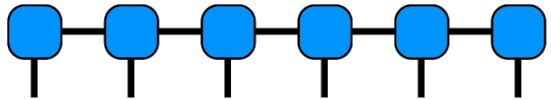


$$\frac{d\rho}{dt} = -i[H,\rho] + D_1(\rho) + D_N(\rho) \equiv \mathscr{L}$$

$$|\Psi\rangle = \sum_{\substack{\sigma_1,\sigma_2,\ldots\sigma_N \\ x_1,x_2,\ldots,x_{N-1}}} A^{\sigma_1}_{x_1} A^{\sigma_2}_{x_1,x_2} \ldots A^{\sigma_N}_{x_{N-1}} |\sigma_1\sigma_2\ldots\sigma_N\rangle$$



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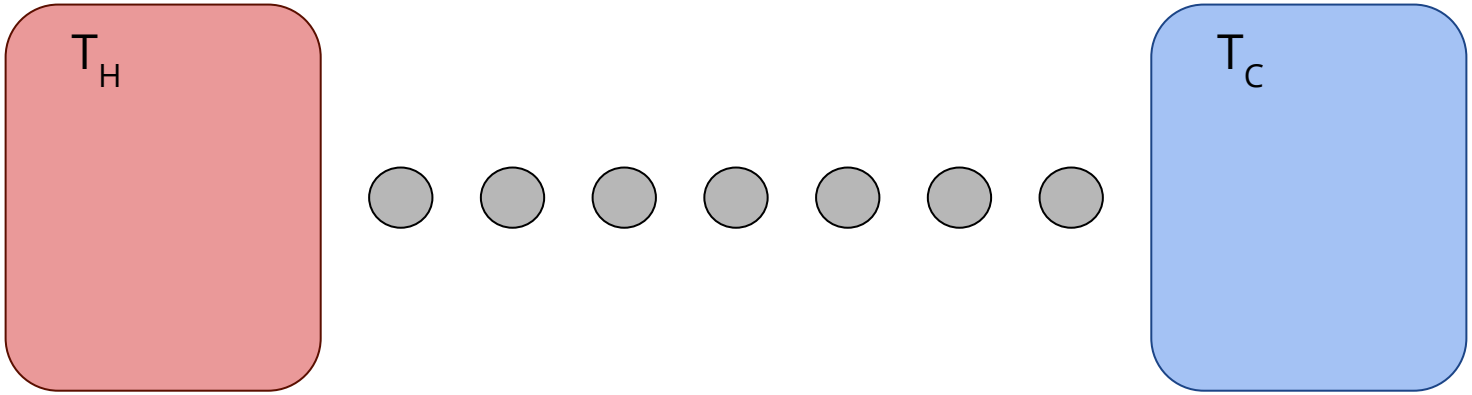

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PLAUSIBLE

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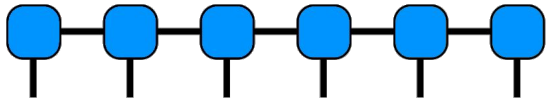

Open Quantum Systems?

- XXZ Heisenberg Spin Chain

$$H = \sum_i \left\{ \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z \right\}$$

- Dissipators

$$D_i(\rho) = \gamma f_i \left[\sigma_i^- \rho \sigma_i^+ - \frac{1}{2} \sigma_i^+ \sigma_i^+ \rho - \frac{1}{2} \rho \sigma_i^+ \sigma_i^- \right] +$$
$$\gamma (1 - f_i) \left[\sigma_i^+ \rho \sigma_i^- - \frac{1}{2} \sigma_i^- \sigma_i^+ \rho - \frac{1}{2} \rho \sigma_i^- \sigma_i^+ \right]$$

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Open Quantum Systems?

- Usual Lindblad Master Equation, with baths as Dissipators

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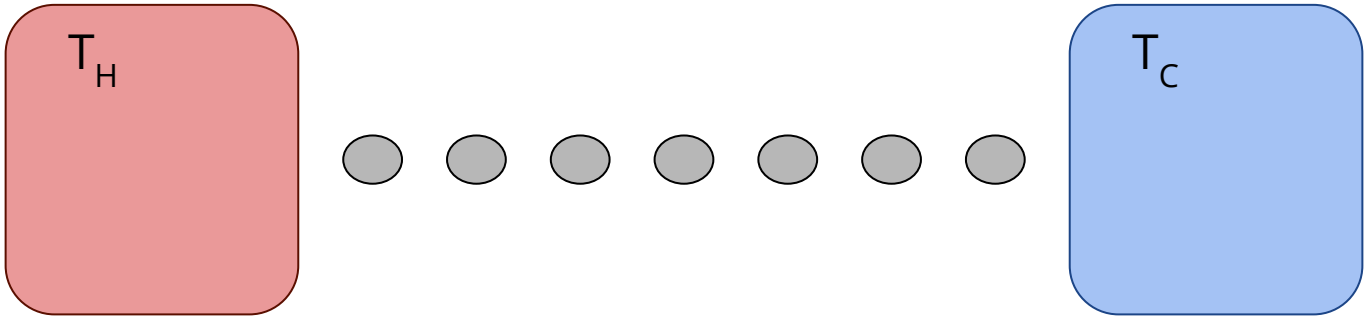
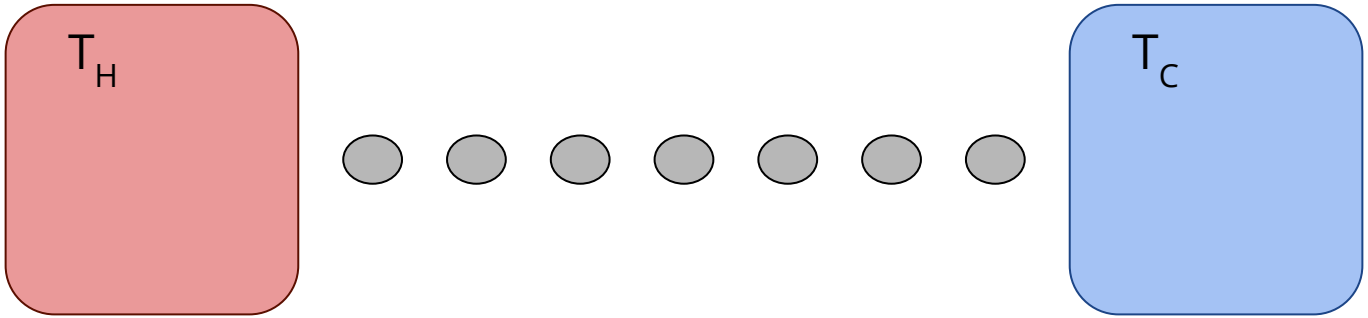


- Use DMRG to reach the non-equilibrium steady state

Open Quantum Systems?

- Usual Lindblad Master Equation, with baths as Dissipators

$$\frac{d\rho}{dt} = -i[H,\rho] + D_1(\rho) + D_N(\rho) \equiv \mathscr{L}$$



- Use DMRG to reach the non-equilibrium steady state
- Our goal is to reach something analogous to $H|\Psi\rangle = E|\Psi\rangle$

Vectorization

- Or Choi's isomorphism: $|\sigma_j\rangle\langle\sigma'_j| \longrightarrow |\sigma_j\sigma'_j\rangle$

$$\mathrm{vec}\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a \\ c \\ b \\ d \end{pmatrix}$$

$$\mathrm{vec}(ABC) = (C^{\mathrm{T}} \otimes A)\mathrm{vec}(B)$$

Jian Cui, J. Cirac, M. C. Bañuls PRL, 10.1103/PhysRevLett.114.220601
G. T. Landi, E. Novaes, M. J. de Oilveira, D. Karevski - PRE 90, 042142 (2014)

Vectorization

- For example:

$$-i[H,\rho] \longrightarrow -i(\mathbf{1}\otimes H - H^T \otimes \mathbf{1})|\rho\rangle$$

- From which we reach the standard variational search setup after doing the same for every other term in the Master Eq.

$$\mathscr{L}^\dagger \mathscr{L}\,|\rho\rangle = 0 \quad \Rightarrow \quad H\,|\Psi\rangle = E\,|\Psi\rangle$$

- Now we reach the same scenario of the usual DMRG implementations

Jian Cui, J. Cirac, M. C. Bañuls PRL, 10.1103/PhysRevLett.114.220601

Study?

- Focused in Magnetization Flux along the chain

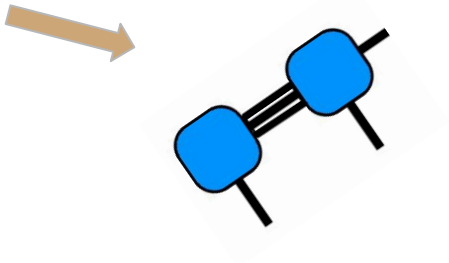
$$J_k = 2\alpha\langle\sigma_k^x\sigma_{k+1}^y - \sigma_k^y\sigma_{k+1}^x\rangle$$

G. T. Landi, E. Novaes, M. J. de Oilveira, D. Karevski - PRE 90, 042142 (2014)

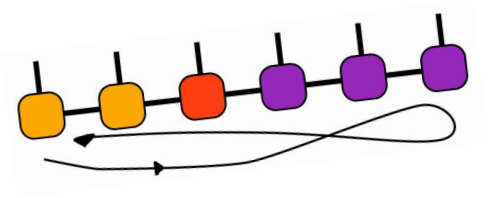
Study?

Technical study of convergence by varying internal code parameters, namely

- Bond Dimension



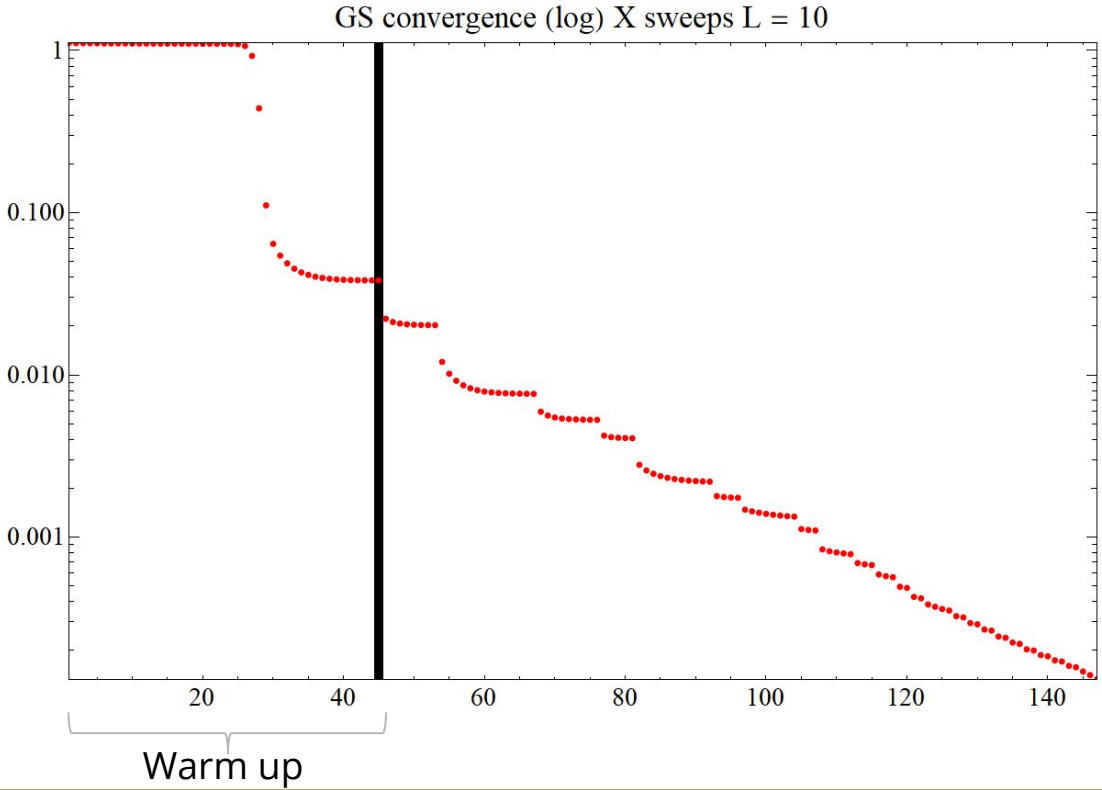
- Sweeps Number



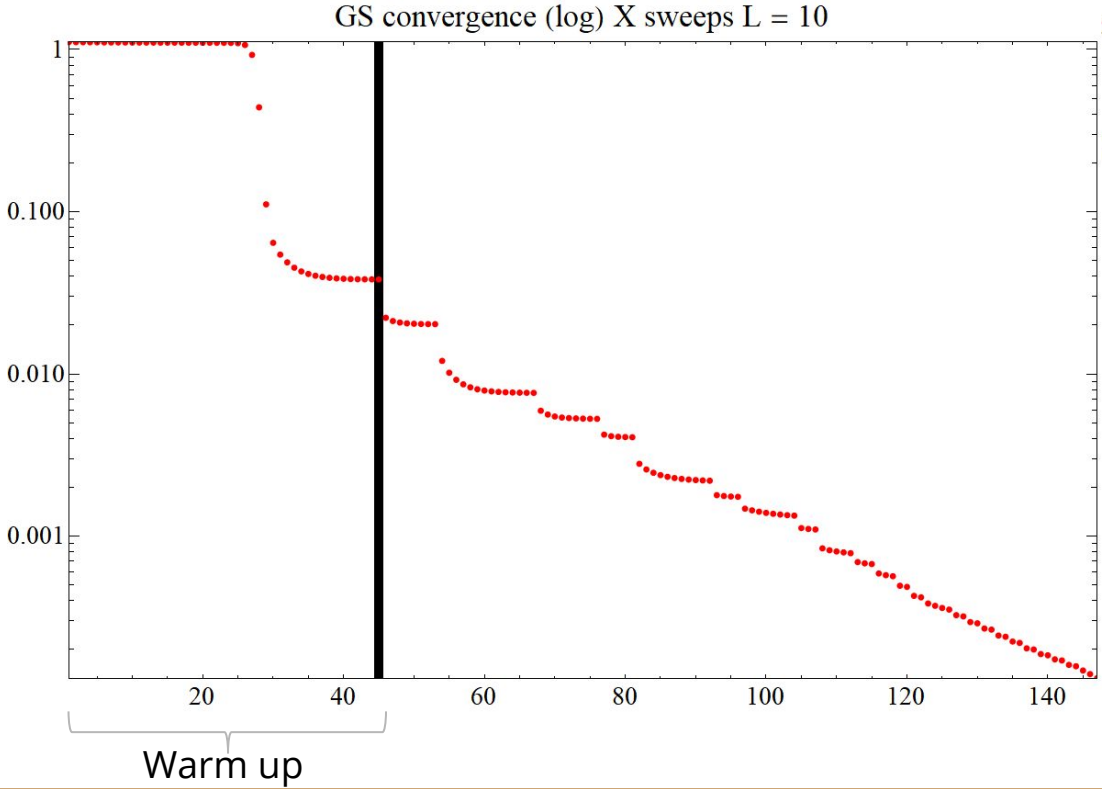
Results

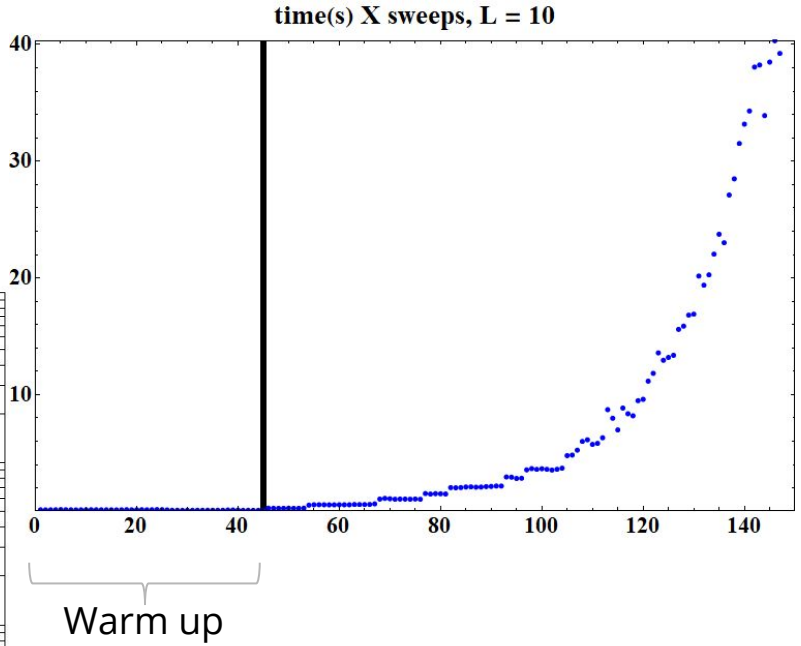
- Since doing sweeps with low bond dimension is computationally not demanding, we implemented a warm round up until an energy threshold is reached

Results

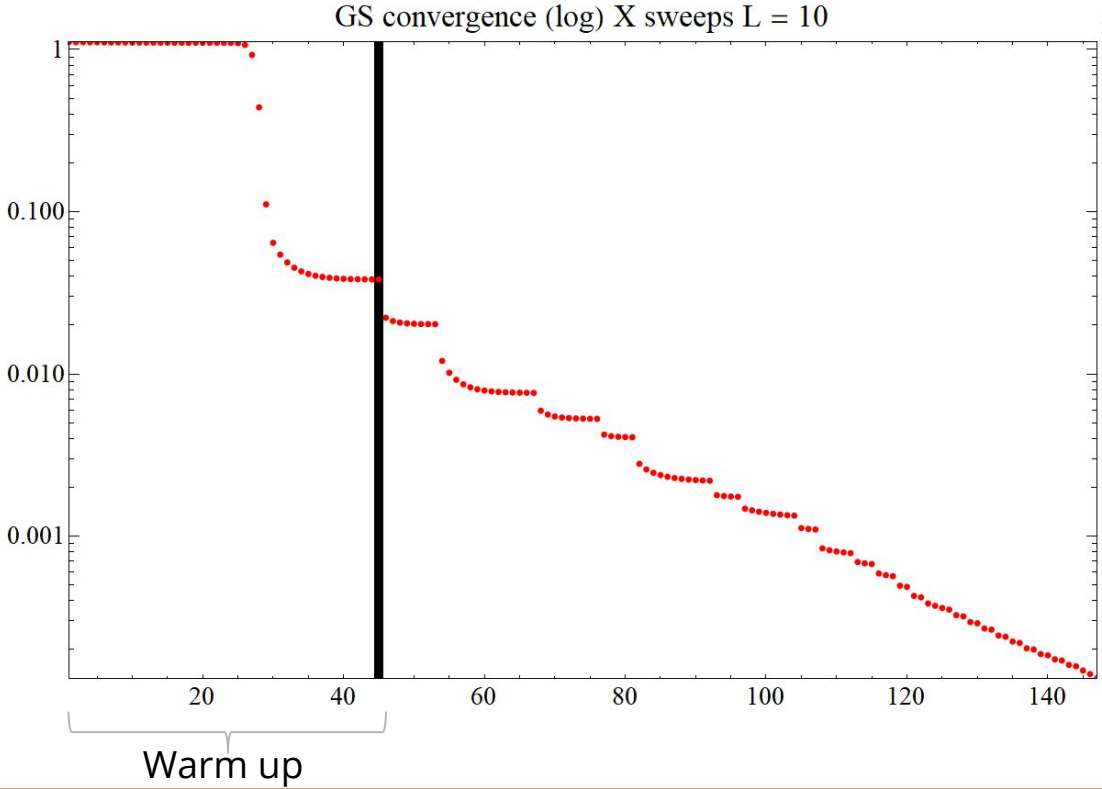

GS convergence (log) X sweeps L = 10
1
0.100
0.010
0.001
20
40
60
80
100
120
140
Warm up

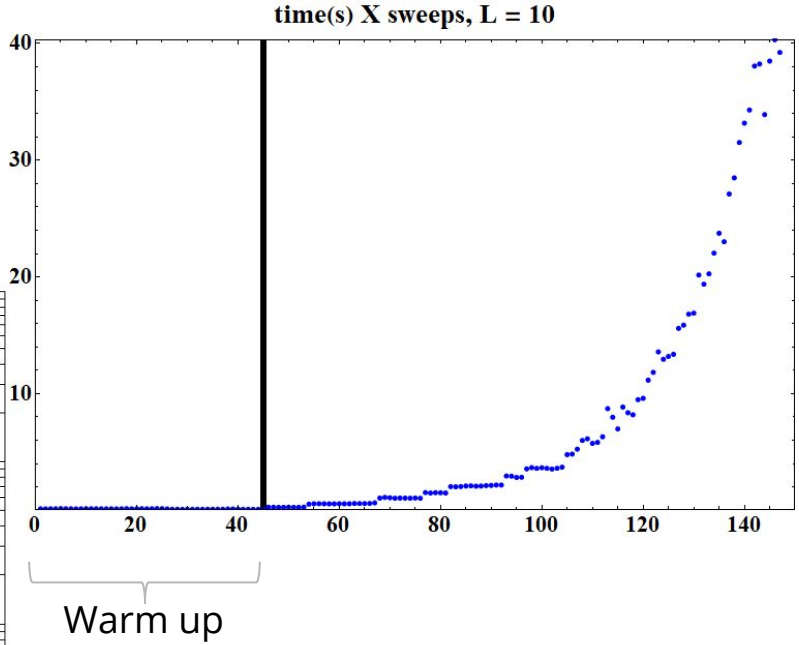
Results


GS convergence (log) X sweeps L = 10
1
0.100
0.010
0.001
20
40
60
80
100
120
140
Warm up


time(s) X sweeps, L = 10
40
30
20
10
0
20
40
60
80
100
120
140
Warm up

Results





Very good!

Results

- For increasing values of L we reach convergence as well

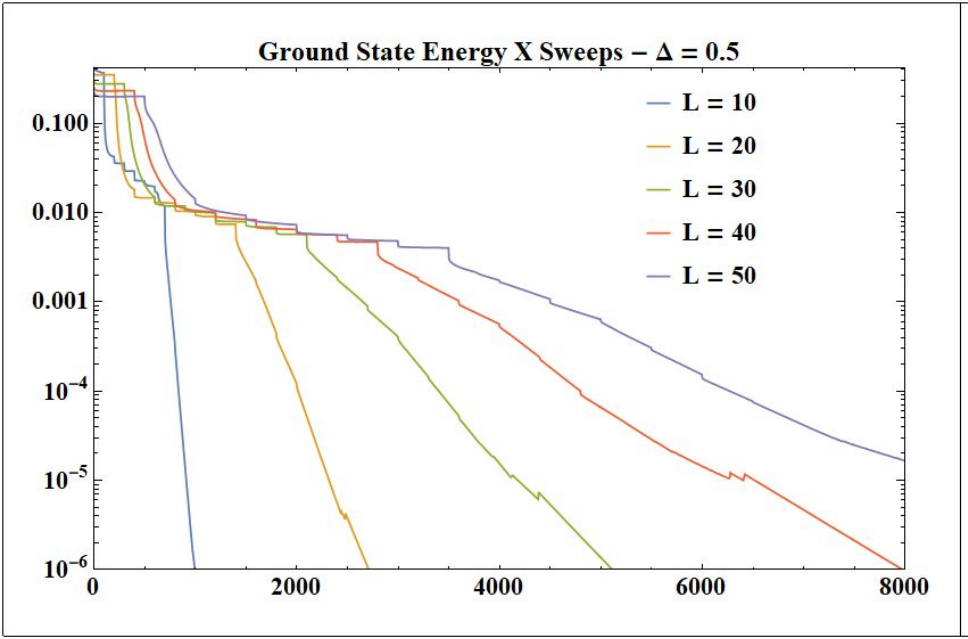
Results

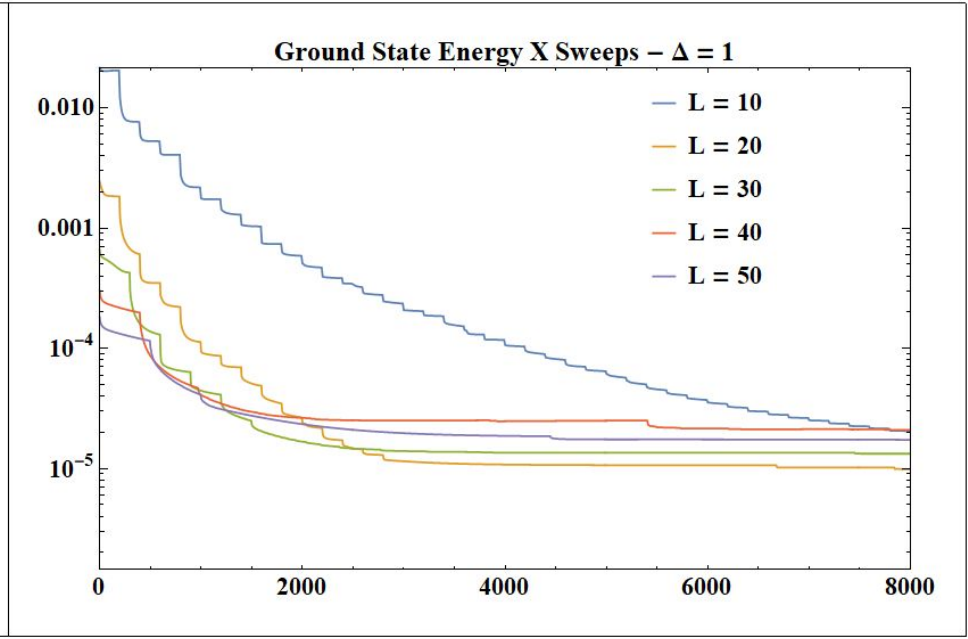
- For increasing values of L we reach convergence as well

- Even though it takes longer, it does not make the simulation unviable

Results

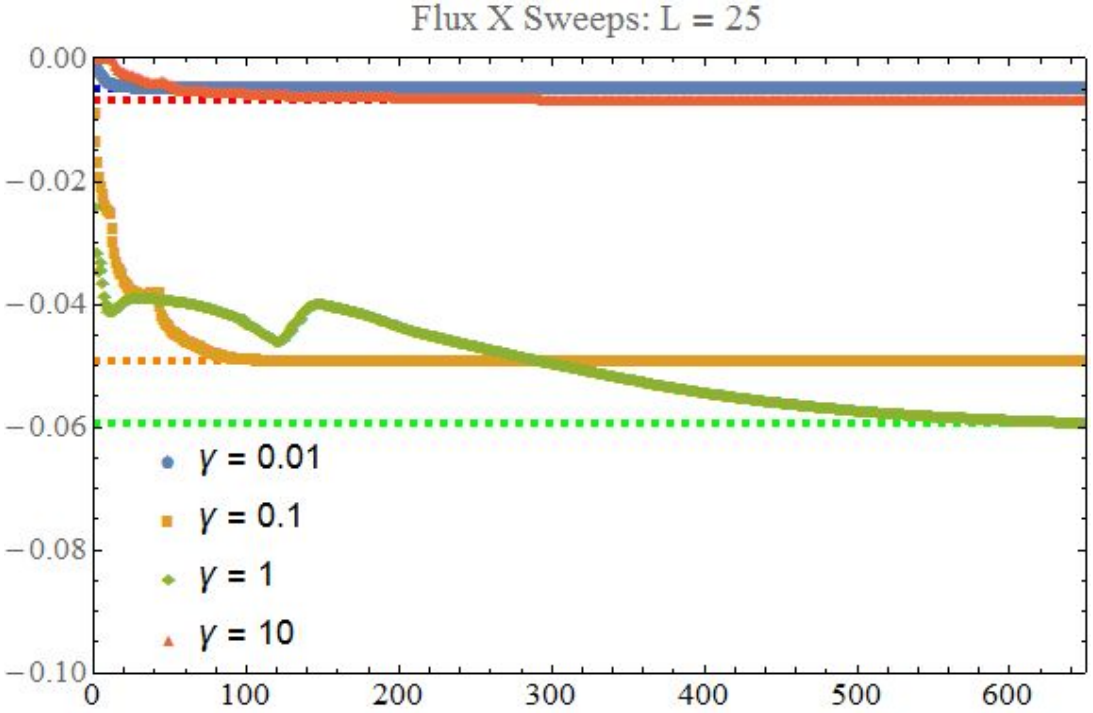
- For different values of Δ





Results

- We can then compare it to the analytical values*



* G. T. Landi, D. Karevski - PRB 91 174422 (2015)

Conclusions

- Reached a viable simulation protocol up to L = 50 easily doable in a simple desktop. This is remarkable

- Assured convergence by warming up and then dynamically changing BD with increasing sweeps
- Starting from physical state usually keeps the system well-behaved

- Code to be uploaded in Git to be used

Thanks!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