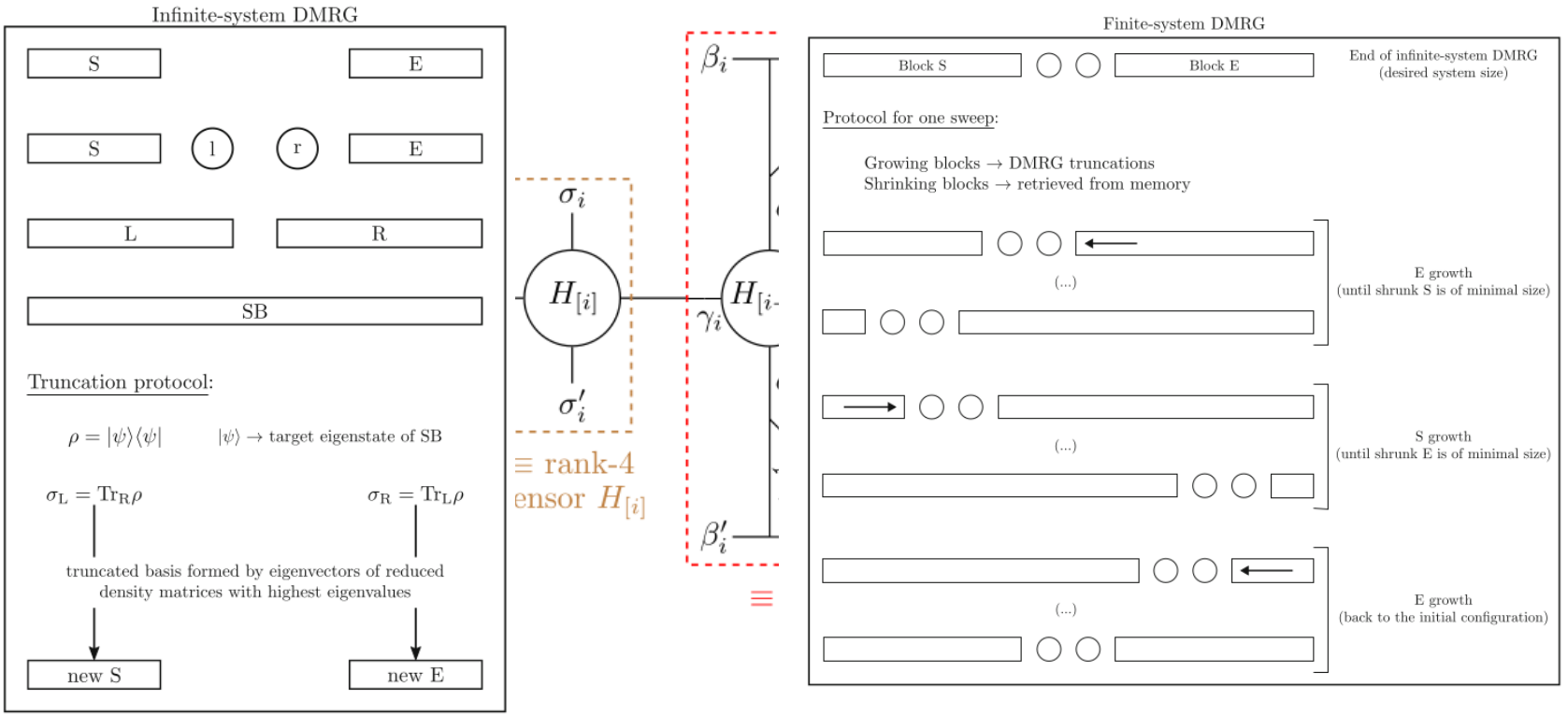
DMRG

Goal: find Groundstate and GS-Energy



Parallelization

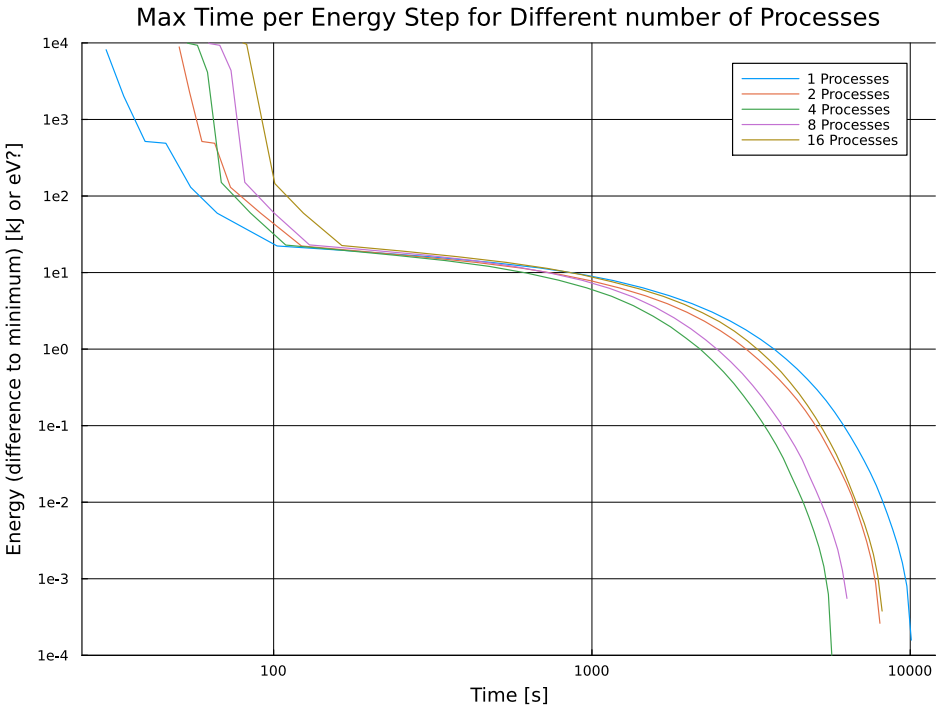
- H: MPO, make use of different sites
- Before build of MPO, we can use so called SumTerms (datastructure in ITensor library)
- Distribute the SumTerms evenly between processors and use preimplemented MPISumTerm to make results coherent
- Add of own implementation for excited states, similar to preexisting sourcecode of the library
- Distribute all information from rank 0 to all ranks

Speedup

$$H = J \cdot \sum_{i=1}^{N} S_i S_{i+1}$$

J = 1 meV

N = 100



Custom SiteTypes

- Until now only S=½ and S=1 are implemented in the library
- I added the implementation of a general S using Rational{Int} and function overloading

Dynamical correlator

$$\chi(\omega) = \langle \mathrm{GS} | \hat{A} \delta(\omega \mathcal{I} - \hat{H} + E_{\mathrm{GS}}) \hat{B} | \mathrm{GS} \rangle$$

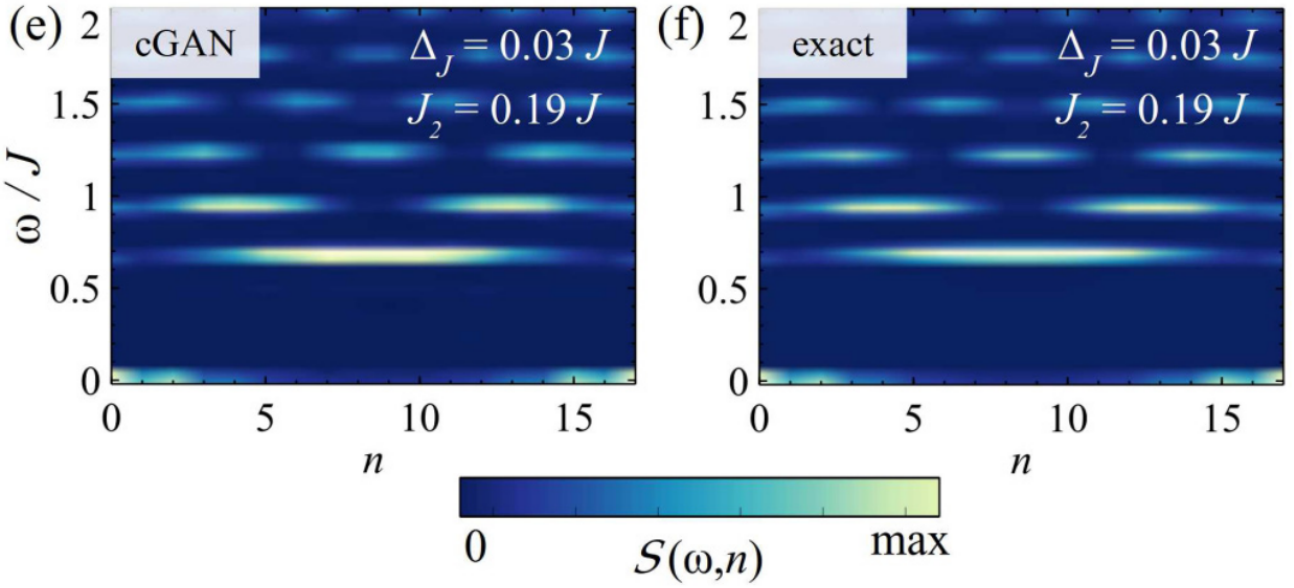
$$H(\Delta_J, J_2) = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} + J_2 \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+2} + \Delta_J \sum_n (-1)^n \mathbf{S}_n \cdot \mathbf{S}_{n+1}$$

$$\widehat{A} = S^z$$
$$\widehat{B} = S^z$$
$$\omega \in (0, 2J]$$

E_{GS} and |GS> from DMRG

Goal: Reproduce this

$$H(\Delta_J, J_2) = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} + J_2 \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+2} + \Delta_J \sum_n (-1)^n \mathbf{S}_n \cdot \mathbf{S}_{n+1}$$



Discretization

$$\chi(\omega) = \frac{2W'/W}{\pi\sqrt{1-\omega'^2}}\left[g_0\mu_0 + 2\sum_{n=1}^{N-1} g_n\mu_n T_n(\omega')\right]$$

General Chebyshev expansion:

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), T_0(x) = 1, T_1(x) = x$$

Rescale $\widehat{H}' s.t.\ \lambda_i \in (-1,1) \forall i$

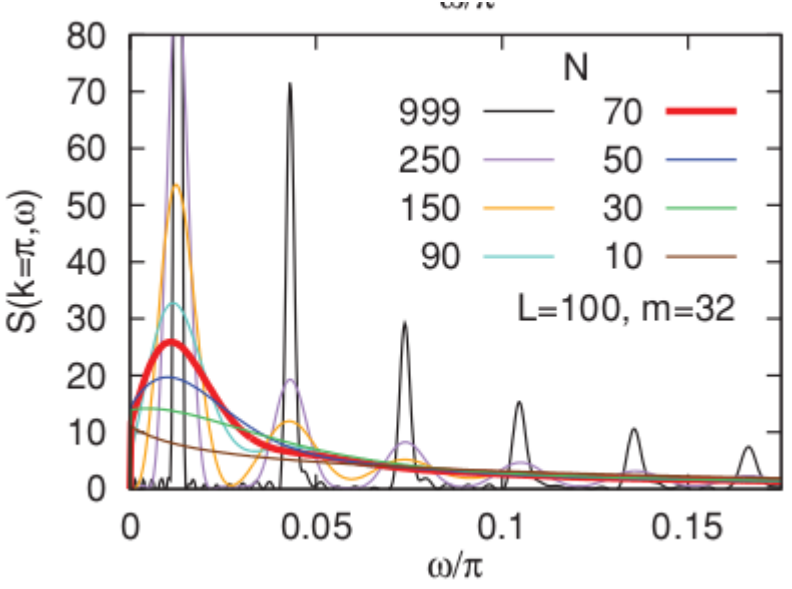
$$\mu_n = \langle GS|\widehat{B}T_n(\widehat{H}')\widehat{C}|GS\rangle$$

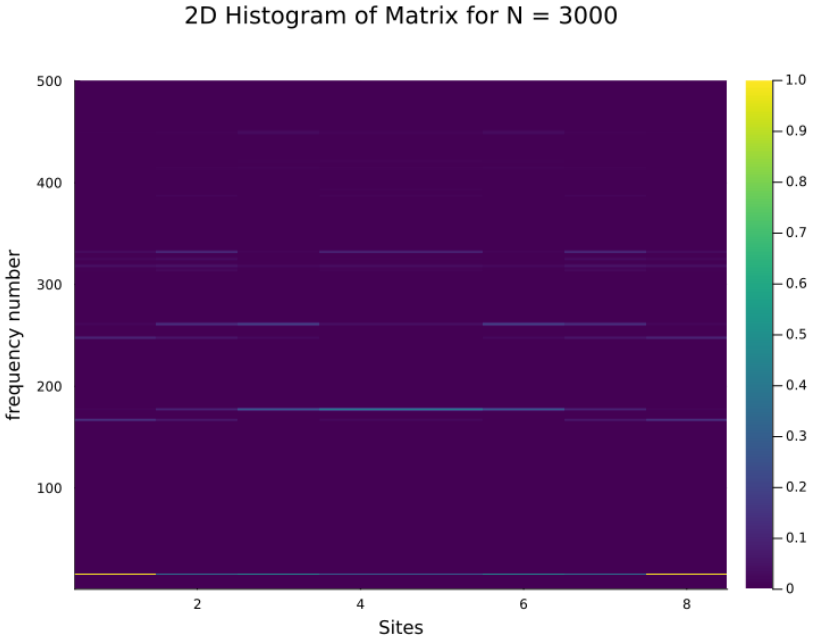
g_n are the Jackson dampening factors to reduce numeric oscillations

$$W = E_{max} - E_{GS}$$

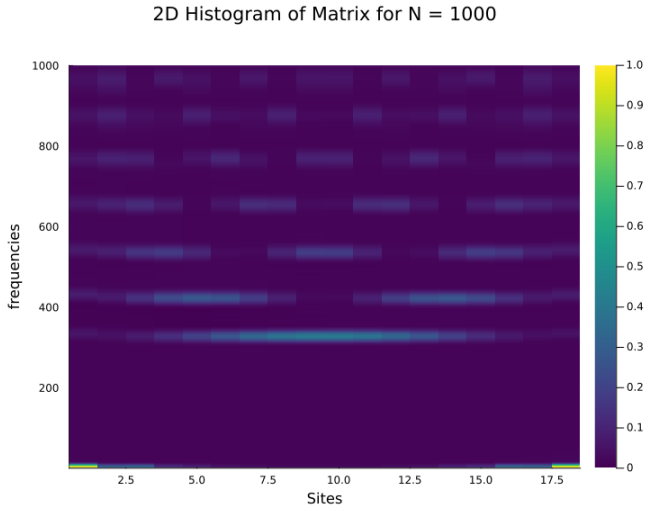
$'$ means rescaled to the array [-1, 1], because of Chebyshev expansion

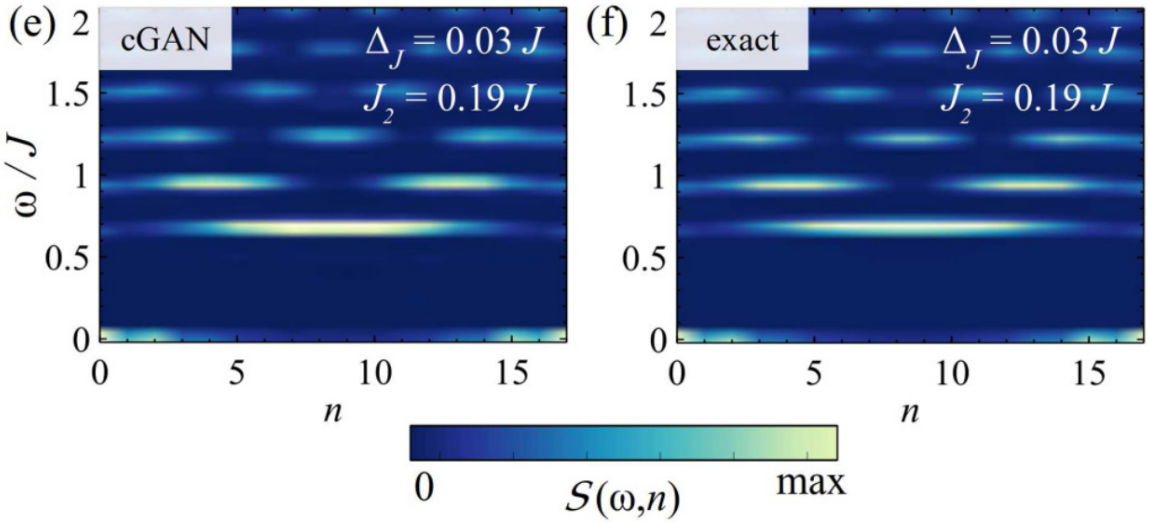
Plots


S(k=π,ω)
ω/π
N
999
250
150
90
70
50
30
10
L=100, m=32
0
10
20
30
40
50
60
70
80
0
0.05
0.1
0.15

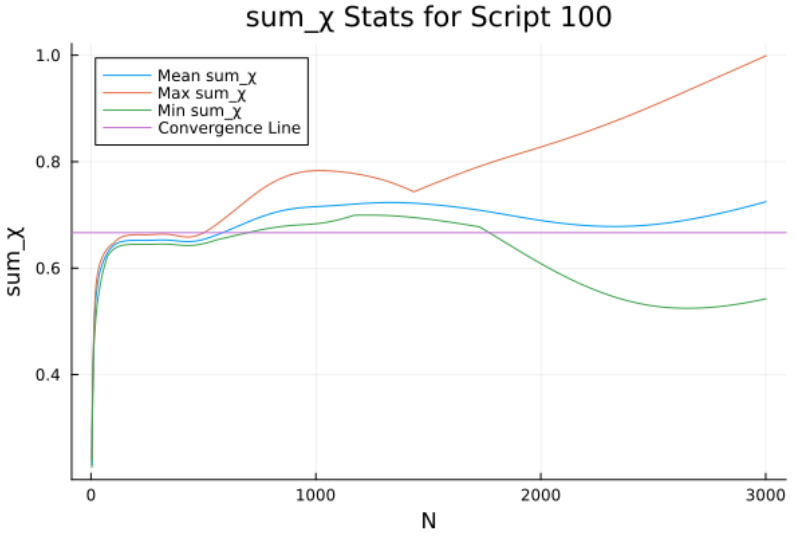

2D Histogram of Matrix for N = 3000
frequency number
Sites
100
200
300
400
500
2
4
6
8
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Plots

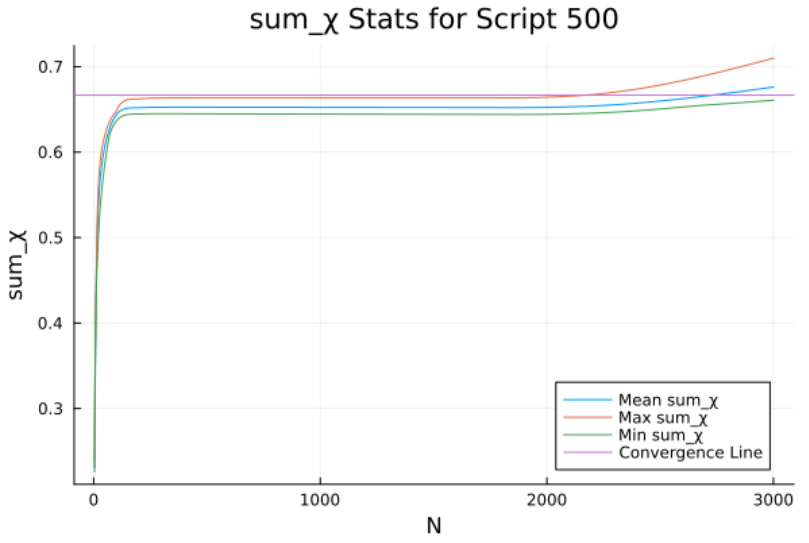

2D Histogram of Matrix for N = 1000
frequencies
Sites
1000
800
600
400
200
2.5
5.0
7.5
10.0
12.5
15.0
17.5
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0


(e)
cGAN
$\Delta_J = 0.03\,J$
$J_2 = 0.19\,J$
(f)
exact
$\Delta_J = 0.03\,J$
$J_2 = 0.19\,J$
ω / J
n
$\mathcal{S}(\omega,n)$
0
max

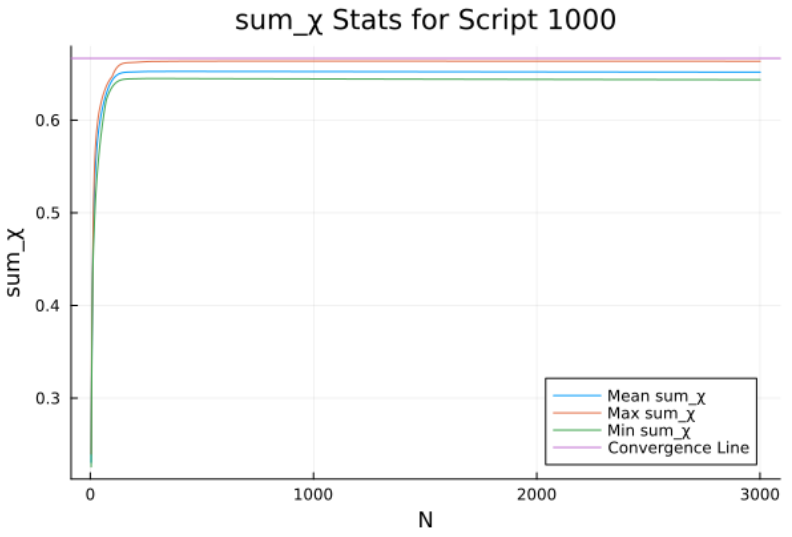
Problem: how many omegas?



Problem: how many omegas?



Problem: how many omegas?



Problem: How many N?