



MASTER ENGINEERING PHYSICS

Year 2020-2021

MASTER DESERTATOIN

THESIS TENSOR NETWORKS

October 2020

David Devoogdt

Academic supervisor: prof.

Contents

1	Introduction	1
2	Models	1
2.1	Ising model	1
2.1.1	Classical Ising	1
2.1.2	Quantum Ising	1
2.2	Heisenberg	1
2.3	Random	2
3	Criticality	2
4	tensor networks	2
4.1	MPS	2
4.2	graphical notation	3
4.3	MPO	3
4.4	PEPO	4
5	Statistical mechanics	4
5.1	introduction	4
6	MPO Calculations	4
6.1	decomposition	5
6.2	inverse	5
6.2.1	inverse MPO	6
6.3	virtual levels and matrisation	7
6.4	cononical form	7
6.5	compression	7
6.6	Expectation values	7
7	contruction MPO	8
7.1	Time evolution methods	8
7.2	Cluster expansion	9
7.2.1	Type A	10
7.2.2	Type B	11
7.2.3	Type C	15
7.2.4	Type D	15
7.3	Implementation details	17
7.3.1	Sourse code structure	17
7.3.2	internal representation	17
7.3.3	normalisation factor	17
7.3.4	buffering results	17

8	Benchmarking	17
8.1	dioganalsation	17
8.1.1	norms	17
8.1.2	Ising	20
8.1.3	Heisenberg	21
8.1.4	Random	23
8.2	analytical results	26

Todo list

write this	1
in basis: hermitian H	2
(.	2
Figure: make this in graphical notation	2
connect trace and hide legs at M	3
explain https://nl.mathworks.com/help/matlab/ref/mldivide.html	6
fix this	6
explain	7
berken exact en maak tabletje voor de verschillende types	7
...	7
https://tensornetwork.org/mps/algorithms/timeevo/	8
implementeren en testen.	10
implement this!	14
meer uitleg gsvd https://nl.mathworks.com/help/matlab/ref/gsvd.html .	15
primed virtual levels	15
quantify	15
other things could be tried here, WIP	16
fix this	16
time complexity algoritms	17
trace norm, Schatten p norm,	17
make version for cyclic	17
calculate complexity	18
larger orders need reimplementatation (non matrix based)	20
run with $M=11$	23
blabla	23
nog niet klaar	26

1 Introduction

write this

To deal with these strongly correlated systems, a class of methods called tensor networks were introduced.

2 Models

2.1 Ising model

2.1.1 Classical Ising

The classical ising model is given by the following hamiltonian:

$$H = -J \left(\sum_{\langle ij \rangle} \sigma_i \sigma_j + g \sum_i \sigma_i \right) \quad (1)$$

where $\langle ij \rangle$ runs over all neighbouring lattice sites. Classical refers to the fact that all the operators in the hamiltonian commute with each other. The values of σ depends on the spin dimension. For spin 1/2 lattices $\sigma \in -1, +1$.

2.1.1.1 1D Phase Diagram

2.1.1.2 2D Phase Diagram

2.1.2 Quantum Ising

In the quantum Ising model, the operators no longer commute with each other. An example is the transversal ising model given by:

$$\hat{H} = -J \left(\sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x + g \sum_i \sigma_i^z \right) \quad (2)$$

2.1.2.1 1D Phase Diagram

2.1.2.2 2D Phase Diagram

2.2 Heisenberg

The heisenberg model is given by:

$$\hat{H} = - \left(\sum_{\langle ij \rangle} J_x \sigma_i^x \sigma_j^x + J_y \sigma_i^y \sigma_j^y + J_z \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^z \right) \quad (3)$$

These models have different names depending on the values of J_α with $\alpha = x, y, z$. $J_x = J_y \neq J_z = \Delta$ is called the XXZ model.



Figure 1: Caption

2.3 Random

It's also possible to construct random hamiltonians.

in basis:
hermitian
H

3 Criticality

scale invariancem, critical points, universality,critical exponents)

(

4 tensor networks

4.1 MPS

A general quantum state with n sites can be described in a given basis $|i\rangle$ as

$$|\Psi\rangle = \sum_{i_1 i_2 \dots i_n} C^{i_1 i_2 \dots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_n\rangle \quad (4)$$

This requires an exponential number d^n of coefficients C where d is the dimensions of basis $|i\rangle$.

In order to make the problem tractable, the following form is proposed as wavefunction:



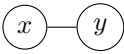
$$C^{i_1 i_2 \dots i_n} = C_{\alpha_1}^{1 i_1} C_{\alpha_1 \alpha_2}^{2 i_2} \dots C_{\alpha_{n-1}}^{n i_n} \quad (5)$$

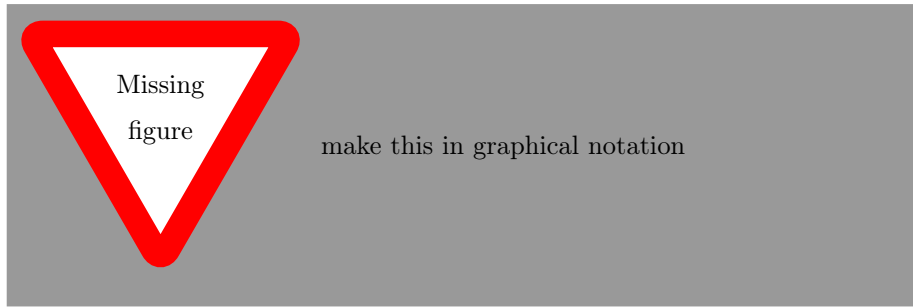
Where summation over shared indices is implied. It is always possible to find such an representation by means of matrix decomposition. The summation over α_i are called virtual bond and their dimension is denoted by χ .

Explicit translational invariance is given by tensor $C_{\alpha\beta}^i$ that don't depend on the location. The chain is closed by setting $\alpha_n = \alpha_0$. We can now write this as a Trace over matrix products:

$$|\Psi\rangle = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n}) |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_n\rangle \quad (6)$$

Table 1: Caption

conventional	Einstein	tensor notation
\vec{x}	x_α	
M	$M_{\alpha\beta}$	
$\vec{x} \cdot \vec{y}$	$x_\alpha y_\alpha$	



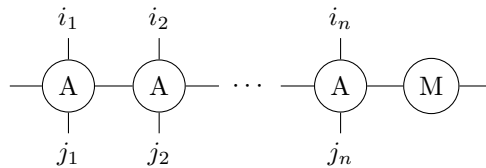
4.2 graphical notation

Tensor networks can be written in a graphical notation. The legs of a tensor denote the number of external indices. The upper Connected legs are summed. Some examples are shown in table 1

4.3 MPO

In a similar fashion, a Matrix Product Operator (MPO) is of the following form:

$$\hat{O} = \sum \text{Tr}(A^{i_1 j_1} A^{i_2 j_2} \dots A^{i_n j_n} M) \times |i_1\rangle \langle j_1| \otimes |i_2\rangle \langle j_2| \otimes \dots \otimes |i_n\rangle \langle j_n| \quad (7)$$



connect
trace and
hide legs at
M

The matrix M contains the boundary conditions of the operator. Many Hamiltonians can be represented by an MPO. For ins

4.4 PEPO

5 Statistical mechanics

5.1 introduction

The physics of a system in thermodynamical equilibrium can be derived from its partition function Z .

$$\begin{aligned} Z &= \sum e^{-\beta E_n} \\ &= \sum_n \langle n | e^{-\beta \hat{H}} | n \rangle \\ &= \text{Tr}(e^{-\beta \hat{H}}) \end{aligned} \tag{8}$$

The first line is the partition function for classical discrete systems. The index n runs over all possible microstates. It is known that the probability to find the system in a given microstate is given by:

$$p_i = \frac{\sum e^{-\beta E_n}}{Z} \tag{9}$$

An useful quantity is the density matrix ρ .

$$\begin{aligned} \rho &= \sum_j p_j |\Psi_j\rangle \langle \Psi_j| \\ &= \sum_j \frac{e^{-\beta \hat{H}}}{Z} |\Psi_j\rangle \langle \Psi_j| \end{aligned} \tag{10}$$

With this notation

$$\begin{aligned} Z &= \text{Tr}(\rho) \\ \langle X \rangle &= \text{Tr}(\rho \hat{X}) \end{aligned} \tag{11}$$

6 MPO Calculations

The manipulations of MPO's is done by manipulating the tensor into a matrix, performing some matrix calculations and casting it back into its original form. This section gives some examples how these manipulations are done in practice:

6.1 decomposition

$$\begin{aligned}
\text{u} \text{---} \boxed{O^{uv,vw}} \text{---} \text{w} &= O_{\alpha_u \gamma_w}^{i_1 i_2 j_1 j_2} \\
&\cong O_{(\alpha_u i_1 j_1)(\gamma_w i_2 j_2)}^{uw} \\
&= O_{(\alpha_u i_1 j_1)\beta_v}^{uv} O_{\beta_v(\gamma_w i_2 j_2)}^{vw} \\
&\cong \text{u} \text{---} \bigcirc \text{---} \bigcirc \text{---} \text{w}
\end{aligned} \tag{12}$$

Step 2 reshapes and groups the indices to one index. The dimension of this index is the sum of the separate dimensions. Step 3 decomposes the matrix into a product of 2 matrices. The exact nature of this decomposition is discussed further. The last step transforms the indices back to separate legs.

For an exact representation, the bond dimension of virtual level v is:

$$\dim v = \min(\dim u, \dim w) + 2 \dim i \tag{13}$$

6.2 inverse

Suppose we want to find a MPO O for given tensors A and B such that the following holds:

$$\text{u} \text{---} \boxed{A} \text{---} \bigcirc \text{---} \text{v} = \text{u} \text{---} \boxed{B} \text{---} \text{v} \tag{14}$$

Again, the indices can be taken together in the following way: $\alpha = (ui_1 i_2 j_1 j_2)$ and $\beta = (i_3 j_3 v)$:

$$A_{\alpha\gamma} O_{\gamma\beta} = B_{\alpha\beta} \tag{15}$$

This will be denoted by

$$\begin{aligned}
\begin{array}{c} i_3 \\ | \\ \text{w} \text{---} \bigcirc \text{---} \text{v} \\ | \\ j_3 \end{array} &= \left[\begin{array}{c} \text{---} \boxed{A} \text{---} \text{w} \\ | \quad | \\ | \quad | \end{array} \right]^{-1} \begin{array}{c} i_3 \\ | \\ \text{---} \boxed{B} \text{---} \text{v} \\ | \quad | \\ | \quad | \end{array} \\
&= \left[\begin{array}{c} \text{w} \text{---} \boxed{A^{-1}} \text{---} \\ | \quad | \\ | \quad | \end{array} \right] \begin{array}{c} i_3 \\ | \\ \text{---} \boxed{B} \text{---} \text{v} \\ | \quad | \\ | \quad | \end{array} \\
&= \begin{array}{c} i_3 \\ | \\ \text{u} \text{---} \boxed{A^{-1}B} \text{---} \text{v} \\ | \\ j_3 \end{array}
\end{aligned} \tag{16}$$

For the first equation the unmarked legs on similar positions need to be connected to each other. The second line the mirrored positions are connected.

This can now be computed with linear algebra packages. Note that it is not necessary to calculate A^{-1} to obtain the solution.

explain
<https://nl.mathworks.com/>

6.2.1 inverse MPO

fix this

Take has to be taken with the indices to apply the inverse.

$$\begin{aligned}
U_{(\alpha ij)\beta}^n A_{\beta\gamma} &= B_{\alpha ij\gamma} \\
A_{\delta\gamma} &= U_{\delta(\alpha ij)}^{n\dagger} B_{\alpha ij\gamma}
\end{aligned} \tag{17}$$

If we now define the MPO O_n^{-1} equal to $U^{n\dagger}$ with the second index split and permuted:

$$\begin{array}{c} i \\ | \\ \delta \text{---} \bigcirc \text{---} \alpha \\ | \\ j \end{array} O_n^{-1} \cong U_{\delta ij\alpha}^{n\dagger} \tag{18}$$

With the notation from eq. (16) we have:

$$\begin{array}{c} \alpha \end{array} \begin{array}{c} | \\ | \\ | \end{array} \begin{array}{c} \cdots \\ | \\ | \end{array} \begin{array}{c} L_n^{-1} \end{array} \begin{array}{c} | \\ | \\ | \end{array} \begin{array}{c} 0 \end{array} = \begin{array}{c} \alpha \end{array} \begin{array}{c} | \\ | \\ | \end{array} \begin{array}{c} O_n^{-1} \end{array} \begin{array}{c} | \\ | \\ | \end{array} \begin{array}{c} O_m^{-1} \end{array} \begin{array}{c} | \\ | \\ | \end{array} \cdots \begin{array}{c} | \\ | \\ | \end{array} \begin{array}{c} O_1^{-1} \end{array} \begin{array}{c} | \\ | \\ | \end{array} \begin{array}{c} 0 \end{array}$$

(19)

The inverse can be applied sequentially.

6.3 virtual levels and matrisation

The

explain

From the construction with svd we can see that the dimension of virtual bond $\dim n = d^{2n}$ with d the dimension of $|i\rangle$. The virtual levels can be joined into a $\chi \times d \times d \times \chi$ dimensional tensor O . This tensor is given by a tridiagonal block matrix :

$$O_{\alpha\beta}^{ij} = \begin{bmatrix} O^{00,ij} & O^{01,ij} & & \\ O^{10,ij} & O^{11,ij} & O^{12,ij} & \\ & O^{21,ij} & O^{22,ij} & \ddots \\ & & \ddots & \ddots \end{bmatrix}$$

(20)

The boundary conditions (leftmost and rightmost virtual level are zero) correspond to vectors:

$$\begin{aligned} l &= [1 \quad 0 \quad \cdots] \\ r &= l^T \end{aligned}$$

(21)

The total dimension is the sum of dimensions of the virtual level. In this case the

berken exact en maak tabletje voor de verschillende types

6.4 cononical form

6.5 compression

6.6 Expectation values

Suppose that there is an MPO representation of $e^{-\beta \hat{H}}$. A and that the mpo representation for $X Y$ is localised over n sites, then the expectation value is given by:

...

$$\langle X \rangle = \frac{\begin{array}{c} \cdots \text{---} \text{A} \text{---} \text{A} \text{---} \cdots \\ \text{X} \text{---} \text{X} \text{---} \cdots \\ \text{A} \text{---} \text{A} \text{---} \cdots \end{array}}{\begin{array}{c} \cdots \text{---} \text{A} \text{---} \text{A} \text{---} \cdots \\ \text{A} \text{---} \text{A} \text{---} \cdots \end{array}} \quad (22)$$

In the thermodynamic limit there are an infinity number of A to the left and the right. This can be simulated by taking the left and right fixed points of the traced MPO A corresponding to the largest eigenvector λ .

$$G_l \text{---} \text{A} = \lambda G_l \text{---} \quad (23)$$

$$\text{---} \text{A} G_r = \lambda \text{---} G_l \quad (24)$$

Equation eq. (22) can now be easily caclulated:

$$\langle X \rangle = \frac{\begin{array}{c} \text{X} \text{---} \cdots \text{---} \text{X} \\ G_l \text{---} \text{A} \text{---} \cdots \text{---} \text{A} \text{---} G_r \end{array}}{\lambda^n G_r \text{---} G_r} \quad (25)$$

7 contraction MPO

7.1 Time evolution methods

7.2 Cluster expansion

This thesis builds on the cluster expansions introduced in [1]. The idea is to create tensor network with a number of virtual levels. The representation is exact up to M connected sites, where M is the order. Different variations are possible. A Hamiltonian of the following form is assumed

$$\hat{H}_n = \sum_{i=1}^{n-1} \hat{h}_{i,i+1} + \sum_{i=1}^n \hat{h}'_i \quad (26)$$

Virtual level zero is defined as follows:

$$\begin{array}{c} | \\ 0 \text{---} \bigcirc \text{---} 0 \\ | \end{array} = \boxed{e^{-\beta \hat{H}_1}} \quad (27)$$

Similarly, the contraction of elements O_{01} and O_{10} are defined as follows:

$$\begin{array}{c} | \\ 0 \text{---} \bigcirc \text{---} 1 \text{---} \bigcirc \text{---} 0 \\ | \end{array} = \boxed{e^{-\beta \hat{H}_2}} - \begin{array}{c} | \\ 0 \text{---} \bigcirc \text{---} \bigcirc \text{---} 0 \\ | \end{array} \quad (28)$$

Some notation will be introduced that will be used later on. The rensor L_n is the contraction of n MPO's where the virtual index increases between each bond. R_n is similar but the virtual bond starts from n and decreases. The tensor is defined in graphical notation by:

$$\begin{array}{c} | \quad \quad \quad | \quad \quad \quad \dots \quad \quad \quad | \\ 0 \text{---} \boxed{L_n} \text{---} n \\ | \quad \quad \quad | \quad \quad \quad \dots \quad \quad \quad | \end{array} = \begin{array}{c} | \\ 0 \text{---} \bigcirc \text{---} 1 \text{---} \bigcirc \text{---} \dots \text{---} m \text{---} \bigcirc \text{---} n \\ | \end{array} \quad (29)$$

M_n is the difference between the exponentiated hamiltonian for n sites and the contraction of the MPO over all the currently assigned combinations of virtual levels.

$$\begin{array}{c}
\begin{array}{|c|c|c|c|c|} \hline \vdots & \vdots & \dots & \vdots & \vdots \\ \hline \end{array} \\
\begin{array}{|c|c|c|c|c|} \hline M_n \\ \hline \end{array} \\
\begin{array}{|c|c|c|c|c|} \hline \vdots & \vdots & \dots & \vdots & \vdots \\ \hline \end{array}
\end{array} = \begin{array}{c}
\begin{array}{|c|c|c|c|c|} \hline \vdots & \vdots & \dots & \vdots & \vdots \\ \hline \end{array} \\
\begin{array}{|c|c|c|c|c|} \hline e^{-\beta \hat{H}_n} \\ \hline \end{array} \\
\begin{array}{|c|c|c|c|c|} \hline \vdots & \vdots & \dots & \vdots & \vdots \\ \hline \end{array}
\end{array}
\quad (30)$$

$$- \begin{array}{c} 0 \\ \vdots \\ \text{O} \end{array} - \begin{array}{c} \vdots \\ \text{O} \end{array} - \dots - \begin{array}{c} \vdots \\ \text{O} \end{array} 0$$

In what follows different constructions will be detailed. Some notes on the practical implementation is given later in this section.

7.2.1 Type A

This type was originally proposed in [1]. The following types of blocks appear in the cluster expansion:

$$\begin{array}{c} \text{n} \\ \vdots \\ \text{O} \end{array} \begin{array}{c} \vdots \\ \text{m} \end{array}, \quad \begin{array}{c} \vdots \\ \text{m} \\ \text{O} \end{array} \begin{array}{c} \vdots \\ \text{n} \end{array} \quad \text{and} \quad \begin{array}{c} \text{n} \\ \vdots \\ \text{O} \end{array} \begin{array}{c} \vdots \\ \text{n} \end{array} \quad \text{with } n \in \mathbb{N}_0 \text{ and } m = n - 1.$$

7.2.1.1 O^{nn} The O^{nn} block is defined by eq. (31)

$$\begin{array}{c} \text{n} \\ \vdots \\ \text{O} \end{array} \begin{array}{c} \vdots \\ \text{n} \end{array} = \begin{array}{c} \text{n} - \begin{array}{|c|c|c|} \hline L_n^{-1} M_{2n+1} R_n^{-1} \\ \hline \end{array} - \text{n} \\ \vdots \end{array} \quad (31)$$

The residual error M is calculated for a chain of size $2n + 1$. The left and right inverses L_n and R_n are applied to M to find the block O^{nn} .

7.2.1.2 O^{mn} and O^{nm} The contraction of O^{nm} and O^{mn} is defined by:

$$\begin{array}{c} \text{n} \\ \vdots \\ \text{O} \end{array} \begin{array}{c} \vdots \\ \text{m} \end{array} \begin{array}{c} \vdots \\ \text{O} \end{array} \begin{array}{c} \vdots \\ \text{n} \end{array} = \begin{array}{c} \text{n} - \begin{array}{|c|c|c|} \hline L_n^{-1} M_{2n+2} R_n^{-1} \\ \hline \end{array} - \text{n} \\ \vdots \end{array} \quad (32)$$

The individual elements O^{mn} and O^{nm} are obtained by doing an svd decomposition as explained in section 6.1. The square root of the singular values is multiplied to the left and right of the decomposition. The operator L_{n+1} and R_{n+1} can be constructed directly.

implementeren
en testen.

During the svd the bond dimension can be lowered by only keeping the rows and columns belonging to $\sigma_i > \sigma_0$. This also helps the invertibility. Increasing σ_0 reduces the precision of the MPO.

7.2.1.3 Truncation Intoduction of a new block can result in large fluctuating errors. This happens because the inverses are possible ill conditioned. Therefore the construction of the MPO should be stopped at a certain optimal order. Many different criteria can be tought of (and have been tried), but the most reliable method is as follows:

7.2.1.4 O^{nn} The O^{nn} blocks can form long chains. To test whether these chains improve accuracy, the norm (see section 8.1.1) of the residul error is calculated before and after the insertion of the block for a cyclic chain. A closed chain is used with the same number of sites. The closed chain resembles much better an infite chain than the open counterpart.

Only strict improvements are accepted, otherwise the MPO without the newly calculated blocks is returned.

7.2.1.5 O^{mn} and O^{nm} For these the same procedure holds.

7.2.1.6 dimension From the construction is can be seen that the dimension of the new virtual level is at most d^2 times the dimension of the previous level. Depending on σ_0 , the bond dimension is even lower.

7.2.1.7 discussion The only parameter in the construction is σ_0 As can be seen in ??, mainly the construction for small values of β get affected by the choice of σ_0 . This can be seen in fig. 2. A good tradeoff seems to be $\sigma_0 = 10^{-12}$. There is almost no precision loss vor small β , while for intermediate it performs optimal for intermediate β .

In practice, the truncation criterium is not completely optimal in some specific cases.

7.2.2 Type B

Type B only contains blocks of the following form; O^{mn} and O^{n0}

$$\begin{array}{c}
 \begin{array}{ccccc}
 & i_n & & i_{n+1} & \\
 & | & & | & \\
 m & \bigcirc & \text{---} & \bigcirc & 0 \\
 & | & & | & \\
 & j_n & & j_{n+1} &
 \end{array}
 & = &
 \begin{array}{ccc}
 & i_n & i_{n+1} \\
 & | & | \\
 m & \boxed{L_m^{-1} M_{n+1}} & 0 \\
 & | & | \\
 & j_n & j_{n+1}
 \end{array}
 \end{array} \tag{33}$$

$$\begin{aligned}
 &\cong X_{(\alpha_m i_n j_n)(i_{n+1} j_{n+1})} \\
 &= U^n \Sigma V^\dagger
 \end{aligned}$$

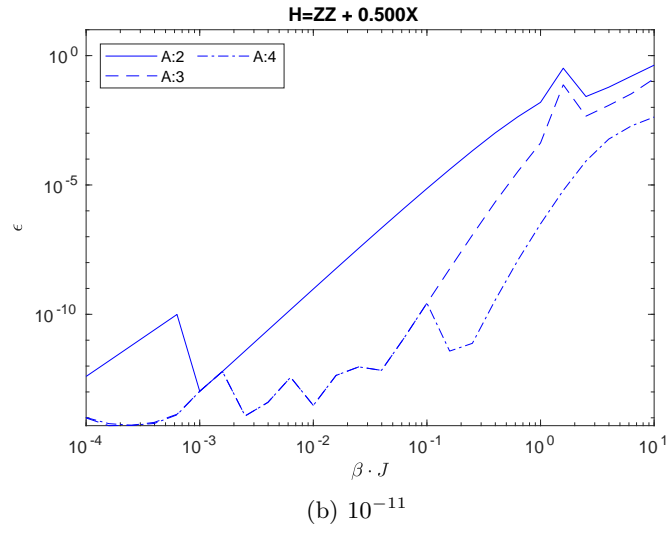
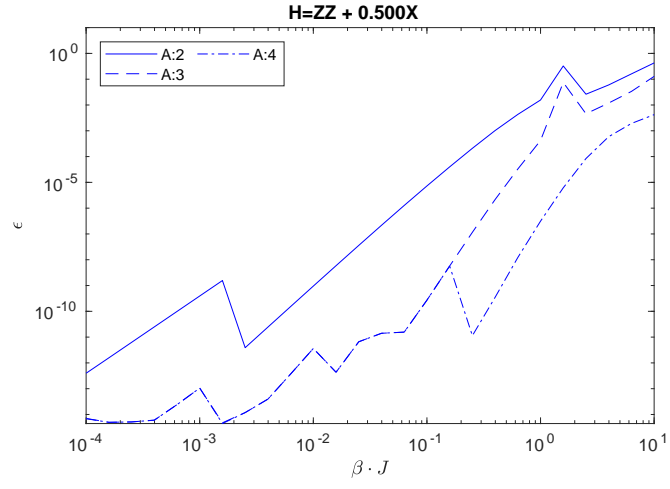
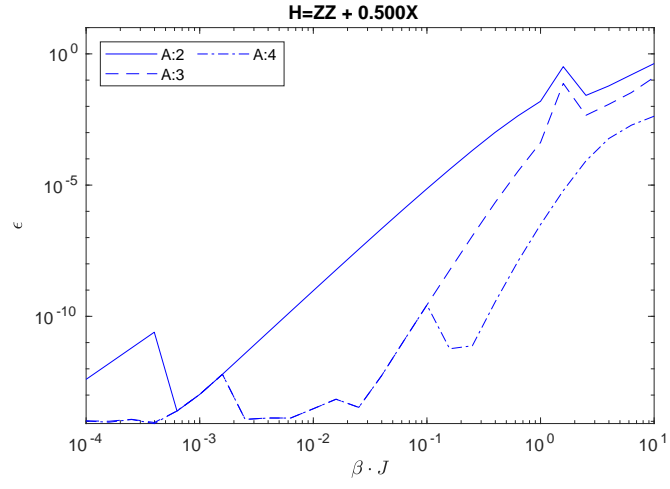
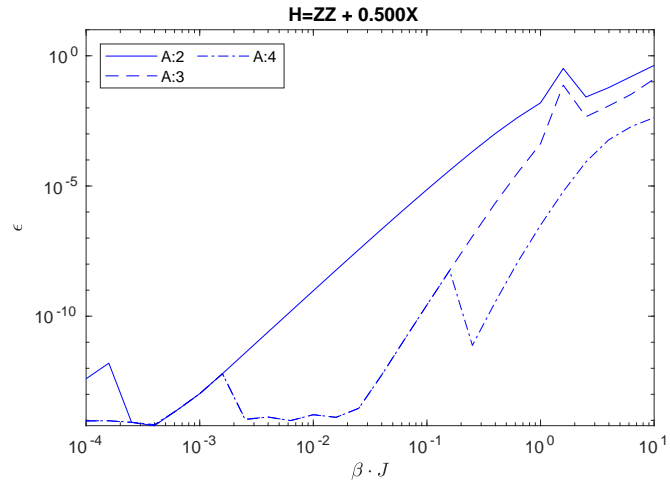


Figure 2: A figure with two subfigures



(c) 10^{-12}



(d) 10^{-13}

Figure 2: A figure with two subfigures

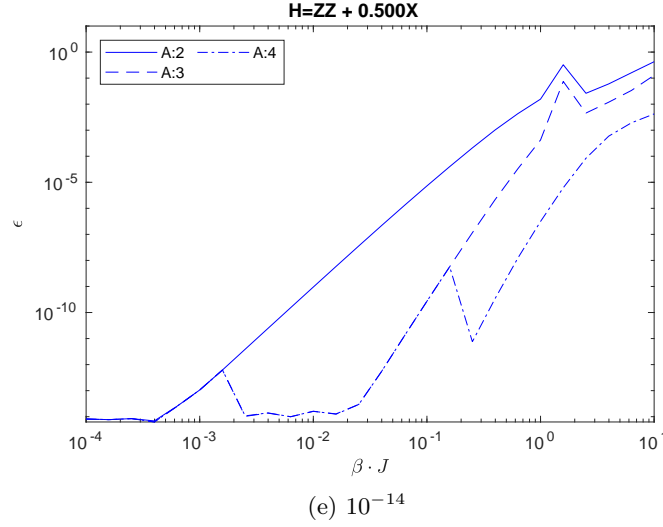


Figure 2: A figure with two subfigures

The following split is made: $O^{mn} \cong U^n$ and $O^{n0} \cong \Sigma V^\dagger$. In this way the inverse exists and doesn't need any calculation: $O^{mn} = U^\dagger$.

implement
this!

7.2.2.1 dimension From the construction the bond dimension grows from the left to the right. For the last step, there are only d^2 non zero singular values. Each steps adds d^2 to the dimension. For the last step, only d^2 non zero singular values need to be kept. With the following notation:

$$\begin{array}{c}
 i \\
 | \\
 \text{m} \text{---} \bigcirc \text{---} \text{n} \\
 | \\
 j
 \end{array} = A_{(\alpha ij)\beta}^m$$

$$\begin{array}{c}
 i \\
 | \\
 \text{n} \text{---} \bigcirc \text{---} 0 \\
 | \\
 j
 \end{array} = B_{(\alpha ij)\beta}^n$$
(34)

The bond dimension of lower virtual levels can be reduced if we can solve the following equations simultaneously:

Then the MPO doesn't change if there are matrices A'^n , A'^{n+1} and B'^n such that

$$\begin{aligned}
 S &= A^m A^n = A'^m A'^n \\
 T &= A^m B^n = A'^m B'^n
 \end{aligned}$$
(35)

Such matrices with optimal bond dimension can be found with generalised SVD. Generalised SVD decomposes 2 matrices as follows:

$$\begin{aligned} S^\dagger &= (U\Sigma_1)Q^\dagger \\ T^\dagger &= (V\Sigma_2)Q^\dagger \end{aligned} \quad (36)$$

The new bond dimension is the $\dim n' = d^2 \cdot \min(\dim n - 1, \dim(n + 1))$. The dimension is higher than type A.

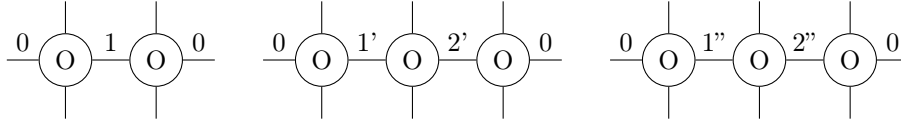
meer
uitleg gsvd
<https://nl.mathworks.com/>

7.2.2.2 discussion This type has no parameters to fine tune. The only blocks appearing in this series expansion are explicitly calculated to lower the remaining error. The inverse is well defined. It is expected that the error increases strictly with increasing temperature and keeps decreasing for higher orders.

7.2.3 Type C

This type implements the same strict type as Type B, but in a different way. No calculation is involved, except the calculation of the the exponentiated hamiltonian to certain order. The following kind of MPO strings are allowed:

primed vir-
tual levels



and so forth. All but one MPO elements are chosen to be the identity matrix. The middle one is the exponentiated hamiltonian with reshaped legs.

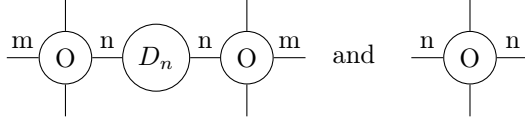
Primed levels are in fact just non overlapping virtual levels. They can be mapped to normal virtual levels.

7.2.3.1 discussion As can be expected from the construction, the bond dimension grows very fast. This type is just as precise as Type B, and will not be reported in the section 8.1. This type could be improved by compressing the MPO at intermediate stages before adding a new primed level. This would likely not improve the speed and dimension of Type B.

quantify

7.2.4 Type D

This type uses a different setup which tries to capture the best of both Type A and B. Type could handle long range correlation better because of the introduction of O^{nn} , but the inverse was not necessarily well defined. Type B had well conditioned inverses, but performed in most of the cases worse. The block appearing in type D are as follows:



Similar to type A,

$$\begin{array}{c} \text{m} \\ | \\ \bigcirc \\ | \\ \text{m} \end{array} \begin{array}{c} \text{n} \\ | \\ \bigcirc \\ | \\ \text{n} \end{array} \begin{array}{c} \text{n} \\ | \\ \bigcirc \\ | \\ \text{n} \end{array} = \begin{array}{c} \text{n} \\ | \\ \boxed{L_n^{-1} M_{2n+2} R_n^{-1}} \\ | \\ \text{n} \end{array} \quad (37)$$

$$= U \Sigma V^\dagger$$

Matrix D_n is the singular value diagonal matrix divided by a normalisation factor ϕ . Both U and V are multiplied by $\sqrt{\phi}$.

7.2.4.1 discussion It's not completely clear what the values of ϕ should be. If ϕ is too large, large chains are not suppressed. If ϕ is too small, the O^{nn} blocks will become large and hence the chain will diverge again. A reasonable value is the sum of the singular values.

other things
could be
tried here,
WIP

7.2.4.2 matrisation The cost of this type lies in the fact that it has no compact way of casting it to a matrix. The following works, but has quite a large dimension:

O_{00}	O_{01}	$-2O_{01}$	O_{01}	$O_{01} D_1^{1/2}$
O_{10}	O_{12}	$-2O_{12}$	O_{12}	
	O_{21}			
O_{10}				
	O_{21}			
O_{10}			O_{11}	
	O_{21}		O_{22}	
$D_1^{1/2} O_{10}$				$D_1^{-1/2} O_{12} D_2^{1/2}$
			$D_2^{1/2} O_{21} D_1^{-1/2}$	

fix this

7.3 Implementation details

7.3.1 Source code structure

7.3.2 internal representation

7.3.3 normalisation factor

7.3.4 buffering results

8 Benchmarking

8.1 dioganalsation

The performance of the MPO construction can be compared with the exact diagonalisation of the hamiltonian for a given number of sites. To obtain a faithful results, the number of sites should be as high as possible. In practice, diagonalisation of large matrices becomes slow and memory consuming. The size grows exponentially in the number of sites: $d^n \times d^n$. A double takes 8 bytes of memory. A Rough estimated of the amount of RAM R needed to store this complex array is:

$$R = d^{2n} \times 16 \text{bytes} \quad (38)$$

Which means a 14 site chain already takes up GB of RAM.

8.1.1 norms

The schatten 2 norm is used in the following analysis, denoted by $\|\cdot\|_2$. In the figures the relative error ϵ is reported.

$$\epsilon = \frac{\left\| \left(e^{-\beta \hat{H}_n} - \left(\begin{array}{c} 0 \\ \bigcirc \end{array} \begin{array}{c} 0 \\ \bigcirc \end{array} \dots \begin{array}{c} 0 \\ \bigcirc \end{array} 0 \end{array} \right) \right\|_2}{\left\| e^{-\beta \hat{H}_n} \right\|_2} \quad (39)$$

time complexity algorithms

trace norm, schatten p norm, ...

make version for cyclic

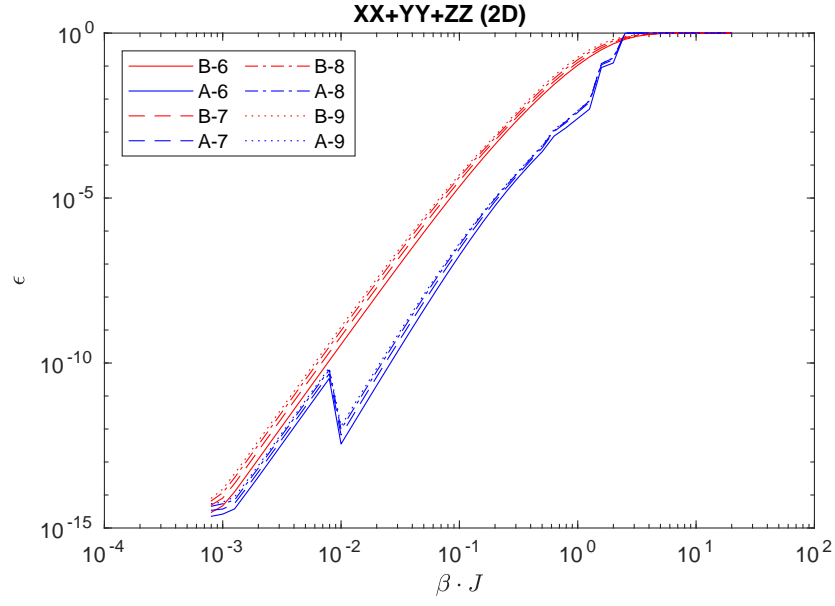
8.1.1.1 system size and cyclicity This norm can only be calculated for a finite number of sites. The influence of the number of sites for a linear and cyclic fig. 3 . As expected, the cyclic norm represents large systems better for

the same number of sites. The linear norm keeps increasing with every added site.

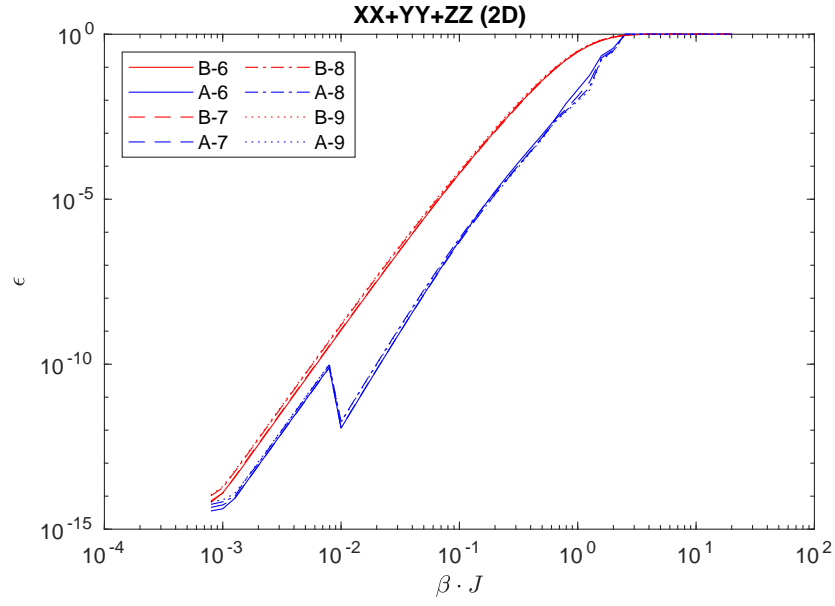
Calculating the cyclic norm comes at the extra cost of contracting a cyclic tensor network.

In this chapter, the cyclic norm will be given for $M=8$ sites.

calculate
complexity



(a) test



(b) test

Figure 3: test

8.1.2 Ising

The first model used to benchmark the different types of MPO's is the transversal ising model. For type A the ϵ increases with β . As expected, the relative error decreases with increasing order.

The behaviour of type B is more chaotic. The error increases no longer monotonously. For small values of β , the order is truncated.

For type 5 fig. 5, there is a consistent improvement over type B.

larger orders
need reim-
plementation
(non matrix
based)

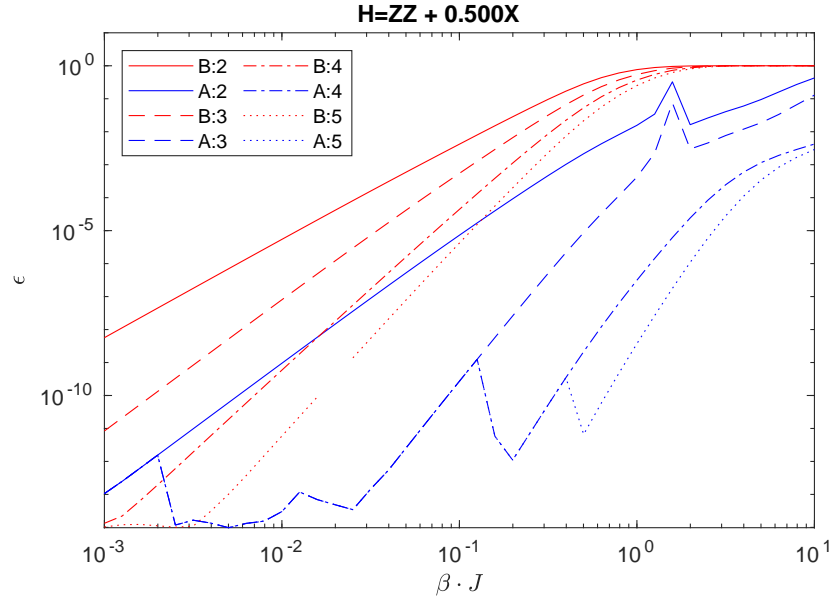


Figure 4: Comparison type A and B for Transversal Ising

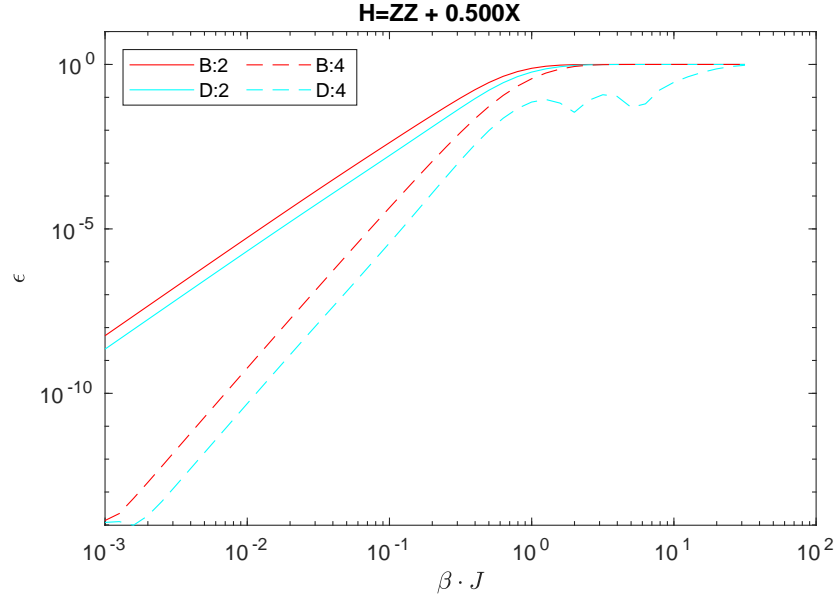


Figure 5: Comparison type C and B for Transversal Ising

8.1.3 Heisenberg

For the Heisenberg model, type A is also an improvement over type B. For large values of β , increasing the order does not help. Type 5 fig. 7 is more promising, but higher orders require too much memory to simulate.

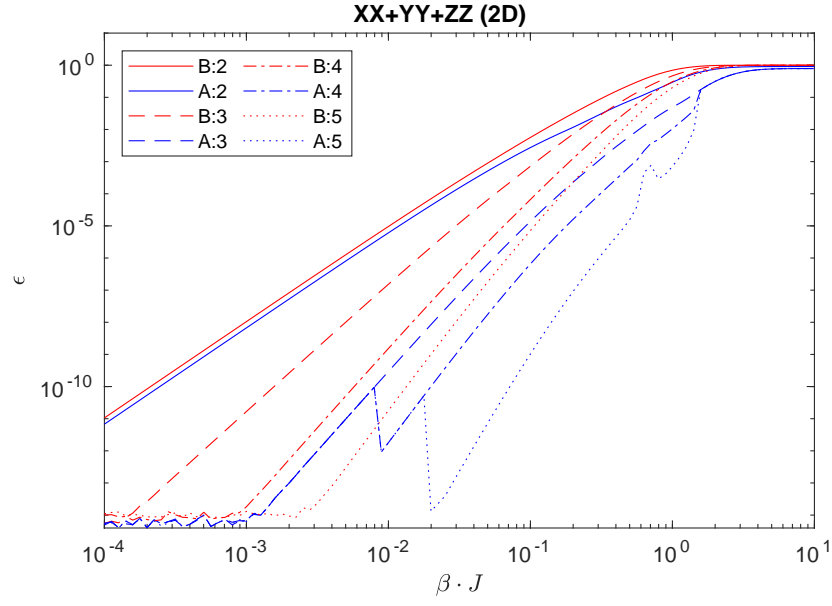


Figure 6: Comparison type A and B for Heisenberg

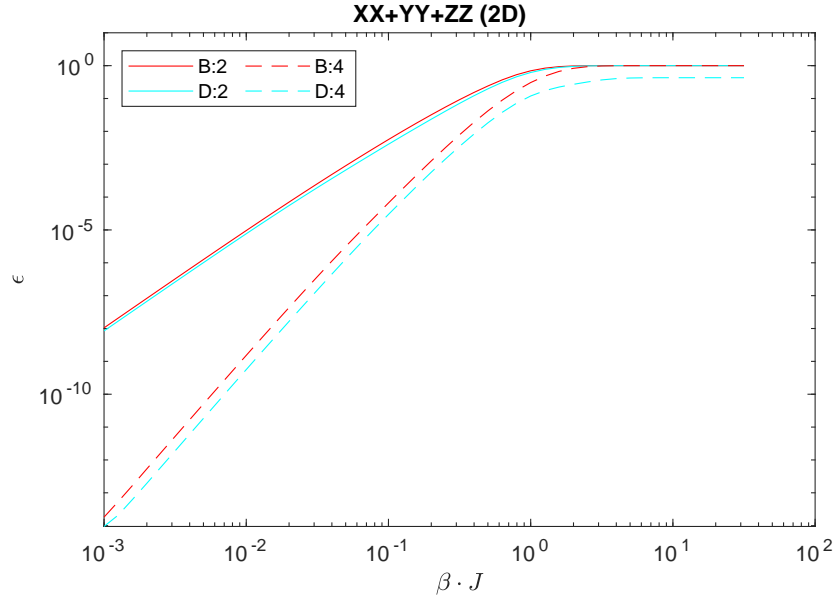


Figure 7: Comparison type C and B for Heisenberg

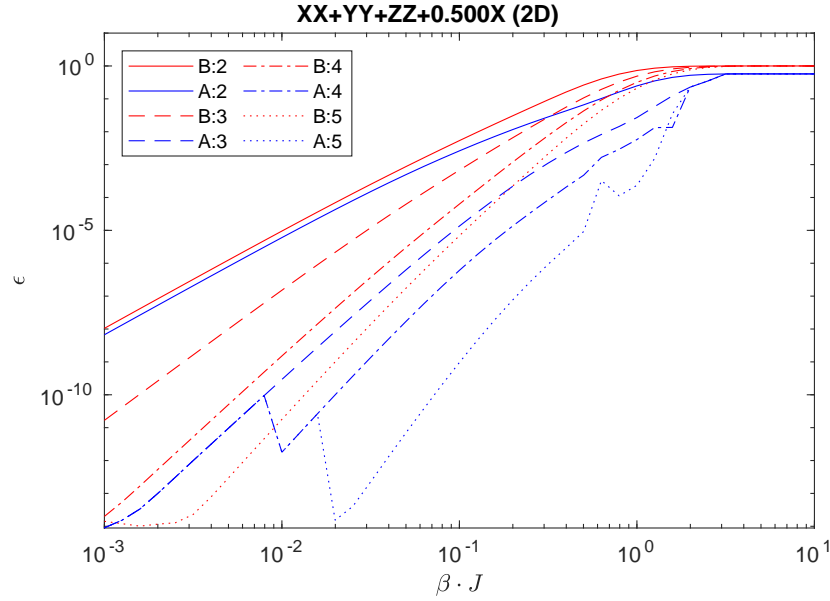


Figure 8: transversal XXX

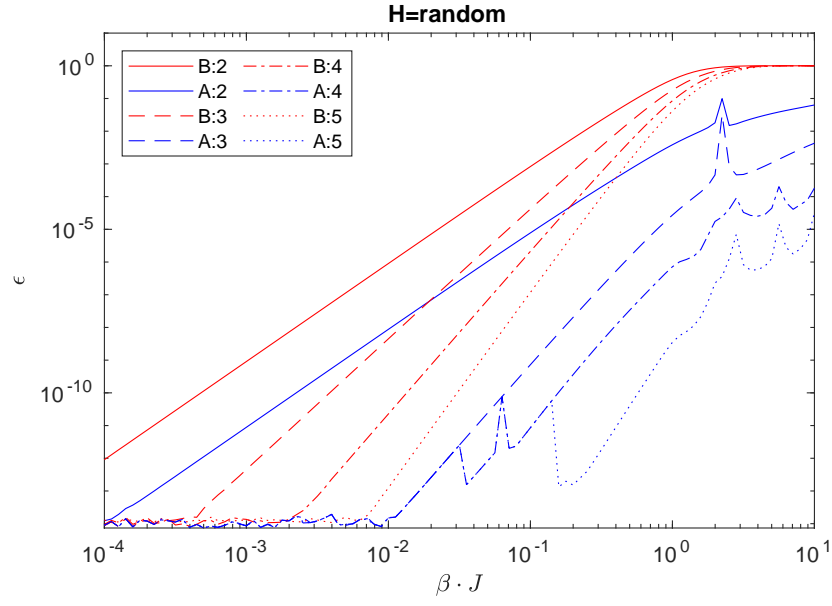
run with
M=11

8.1.4 Random

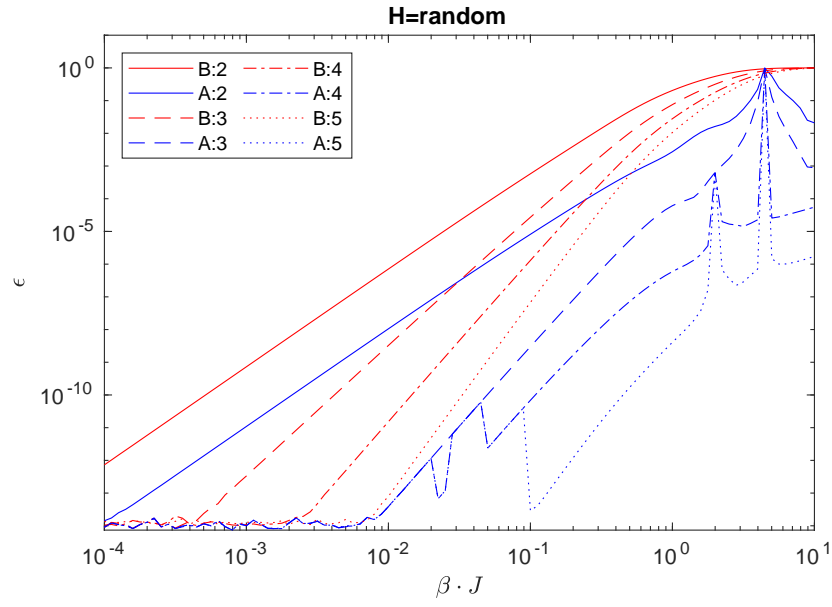
To give a representative overview for random hamiltonians, several simulations were run. The single site and nearest neighbour hamiltonians are generated by making hermitian matrices with random real and complex numbers between -1 and 1. In order to compare the different graphs, the energy scale is set such that the norm of the 2 site hamiltonian is 1.

Clearly, the performance of type B is almost independent on the chosen random variables. For type A there is more variation. Still, A performs almost always better than B. For some random models, such as fig. 9b, the order is truncated at low order for high temperatures (see peak at $\beta J \approx 4$). It's unclear why this behaviour emerges. Manually overriding the sefagaurd mechanism

blabla

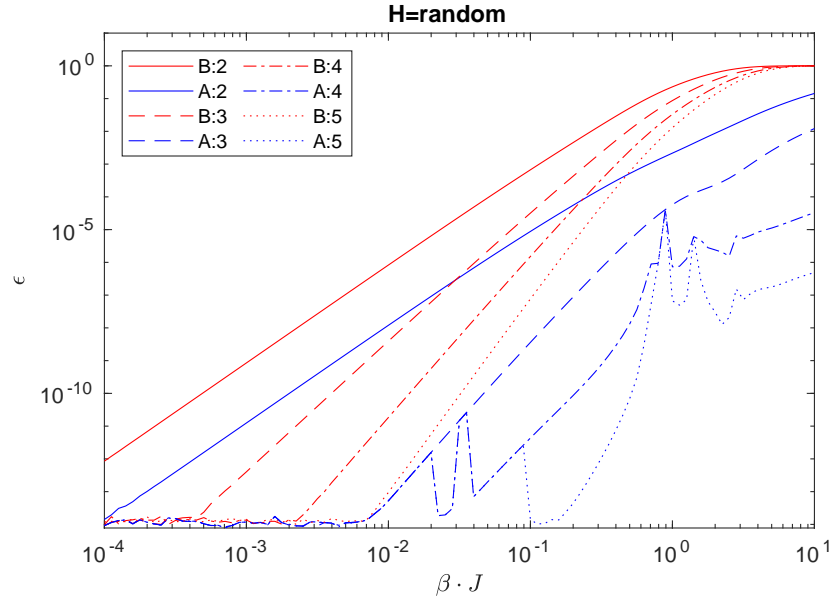


(a) test

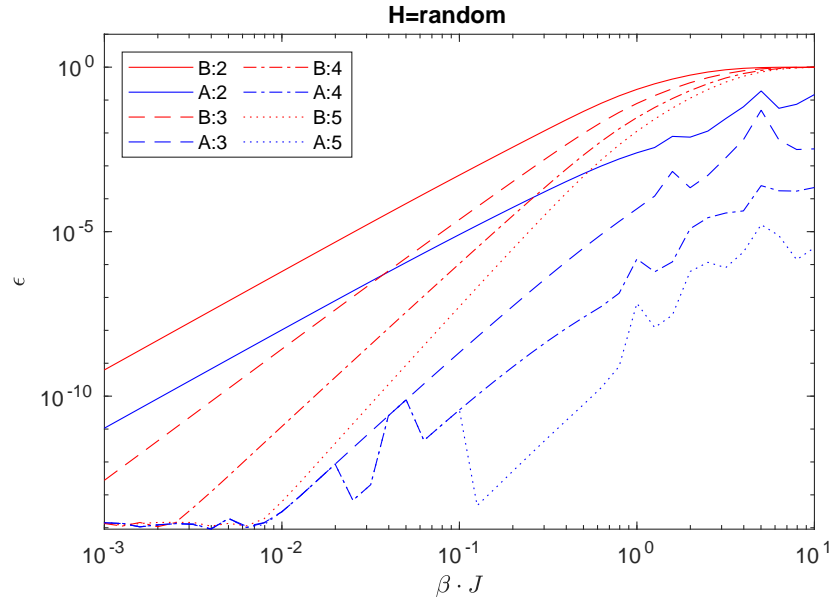


(b) test

Figure 9: test



(c) test



(d) test

Figure 9: test (cont.)

Also here type D improve the results of type B. For high β truncation seems

necessary.

nog niet
klaar

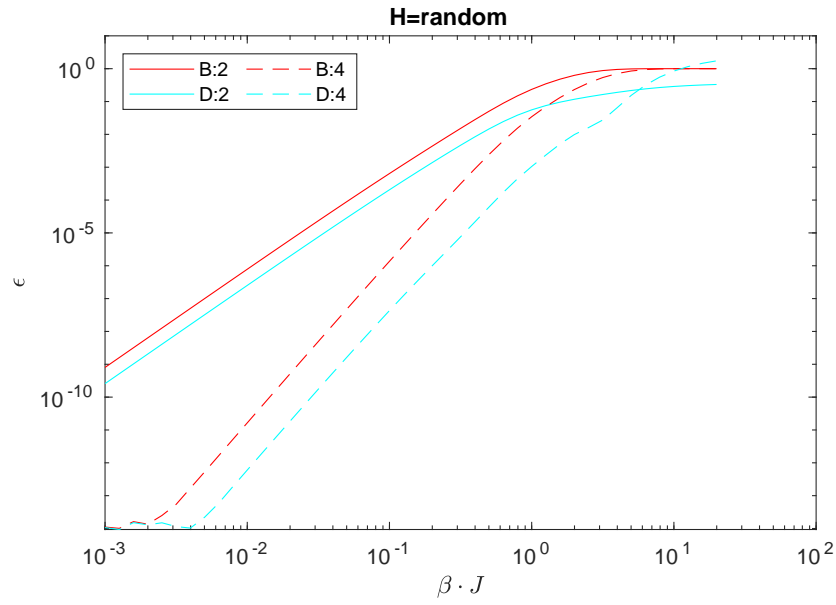


Figure 10: Comparison type C and B for random Hamiltonian

8.2 analytical results

References

- [1] B. Vanhecke, M. Damme, L. Vanderstraeten, F. Verstraete, Symmetric cluster expansions with tensor networks (12 2019).