UNIVERSITEIT GENT

Master Engineering Physics

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Master desertatoin

Thesis Tensor networks

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Academic supervisor: prof.

Contents

Todo list

1 Introduction

write this

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

2 Models

2.1 Ising model

2.1.1 Classical Ising

The classical ising model is given by the following hamiltonian:

$$H = -J \left(\sum_{<ij>} \sigma_i \sigma_j + g \sum_i \sigma_i \right) \tag{1}$$

where $< ij >$ 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:

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

2.1.2.1 1D Phase Diagram

2.1.2.2 2D Phase Diagram

2.2 Heisenberg

The heisenberg model is given by:

$$\hat{H} = - \left(\sum_{<ij>} J_x \sigma_i^z \sigma_j^z + J_y \sigma_i^y \sigma_j^y + J_z \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^z \right) \tag{3}$$

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.

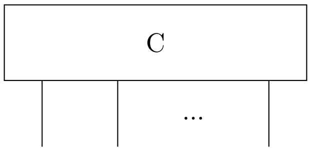


Figure 1: Caption

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

$$|\Psi\rangle = \sum_{i_1 i_2 \cdots i_n} C^{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \tag{4}$$

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:

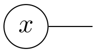
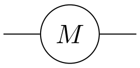
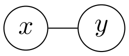
$$C^{i_1 i_2 \cdots i_n} = C^{1}{}^{i_1}_{\alpha_1} C^{2}{}^{i_2}_{\alpha_1 \alpha_2} \cdots C^{n}{}^{i_n}_{\alpha_{n-1}} \tag{5}$$

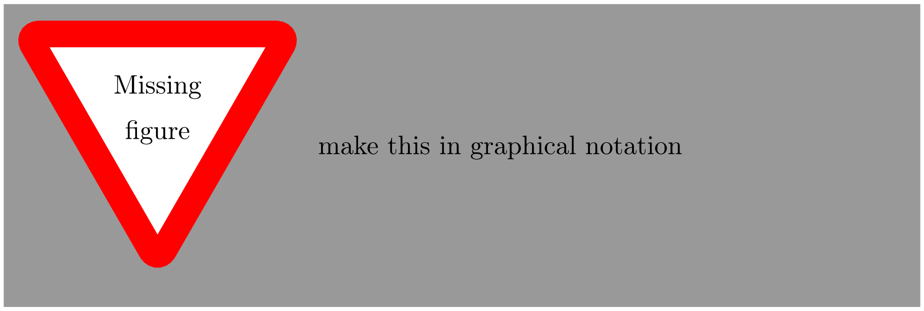
Where summation over shared indices is implied. It is always possible to find such an representation by means of matrix decomposition. The summation over α_i are called virtual bond and their dimension is denoted by χ.

Explicit translational invariance is given by tensor $C^i_{\alpha\beta}$ 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:

$$|\Psi\rangle = \mathrm{Tr}\left(C^{i_1} C^{i_2} \cdots C^{i_n}\right) |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \tag{6}$$

Table 1: Caption

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



make this in graphical notation

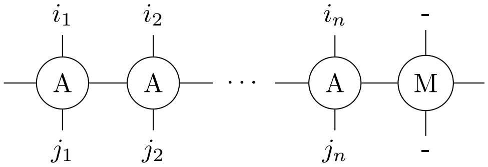
4.2 graphical notation

Tensor networks can be written in a graphical notation. The legs f 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:

$$\begin{aligned}\hat{O} = \sum Tr(A^{i_1 j_1} A^{i_2 j_2} \cdots A^{i_n j_n} M) \\ \times |i_1\rangle \langle j_1| \otimes |i_2\rangle \langle j_2| \otimes \cdots \otimes |i_n\rangle \langle j_n|\end{aligned} \tag{7}$$



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 introdcution

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

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

The first line is the partition function for clasical discrete systems. The index n runs of all possible microstates. It is know that the propability to find the system in a given microstates is given by:

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

An useful quantity is the density matrix ρ.

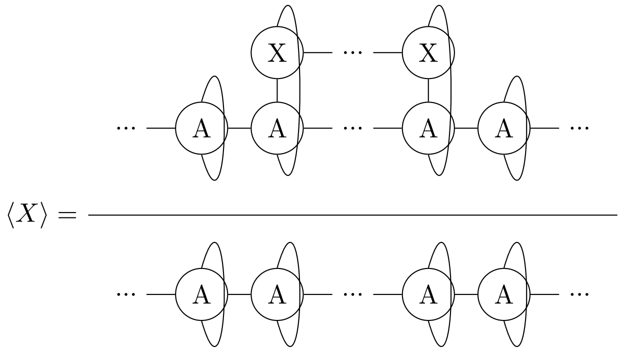
$$
\begin{aligned}
\rho &= \sum_j p_i \left|\Psi_j\right\rangle \left\langle\Psi_j\right| \\
&= \sum_j \frac{e^{-\beta \hat{H}}}{Z} \left|\Psi_j\right\rangle \left\langle\Psi_j\right|
\end{aligned}
\tag{10}
$$

With this notation

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

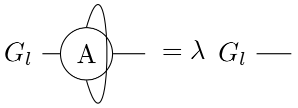
5.2 Calculation with MPO in 1D

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

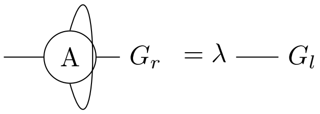


(12)

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.

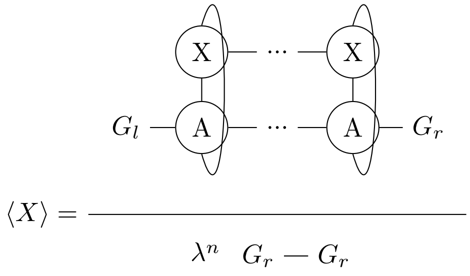


(13)



(14)

Equation eq. (12) can now be easily caclulated:



(15)

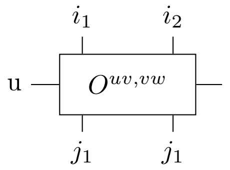
6 contruction MPO

6.1 Mpo manipulations

The manipulations of MPO's is done by manipulating the tensor into a matrix, performing some matrix calculations and casting it back into it's original form.

This section gives some examples how these manipulations are done in practice:

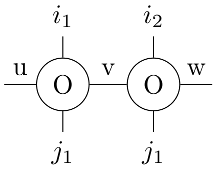
6.1.1 decomposition



$$= O^{i_1 i_2 j_1 j_2}_{\alpha_u \gamma_w}$$

$$\begin{aligned} &\cong O^{uw}_{(\alpha_u i_1 j_1)(\gamma_w i_2 j_2)} \\ &= O^{uv}_{(\alpha_u i_1 j_1)\beta_v} O^{vw}_{\beta_v (\gamma_w i_2 j_2)} \end{aligned} \qquad (16)$$

$$\cong$$



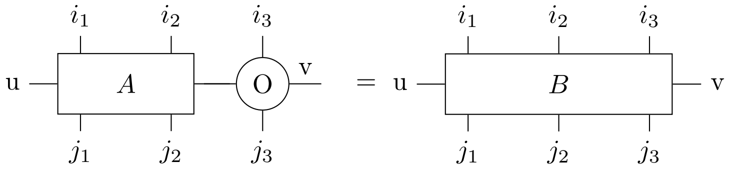
Step 2 reshapes and groups the indices to one index. The dimension of this index is the sum of the seperate dimensions. Step 3 decomposes the matrix into a product of 2 matrices. The exact nature of this decomposition is dicussed further. The last step transforms the indices back to separate legs.

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

$$\dim v = \min(\dim u, \dim v) + 2 \dim i \qquad (17)$$

6.1.2 inverse

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

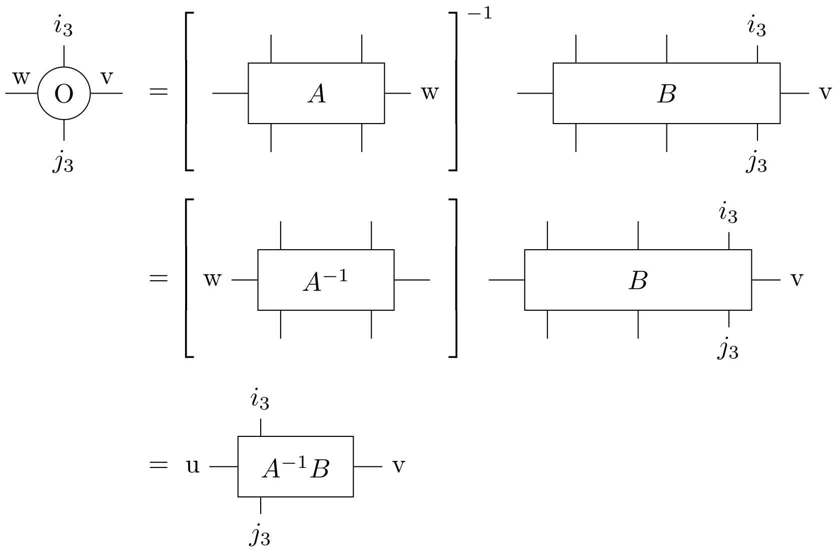


(18)

Again, the indices can be taken toghether in the following way: $\alpha = (u i_1 i_2 j_1 j_2)$ and $\beta = (i_3 j_3 v)$:

$$A_{\alpha\gamma} O_{\gamma\beta} = B_{\alpha\beta} \qquad (19)$$

This will be denoted by



(20)

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/

6.1.3 virtual levels and matrisation

explain

6.1.3.1 Matrisation 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 :

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

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

$$\begin{aligned} l &= \begin{bmatrix} 1 & 0 & \cdots \end{bmatrix} \\ r &= l^T \end{aligned} \tag{22}$$

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

6.2 Time evolution methods

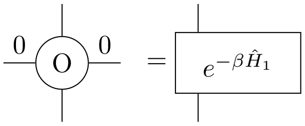
6.3 Cluster expansion

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 folowing form is assumed

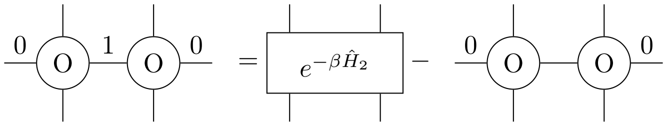
$$\hat{H}_n = \sum_{i=1}^{n-1} \hat{h}_{i,i+1} + \sum_{i=1}^{n} \hat{h}'_i \tag{23}$$

Virtual level zero is defined as follows:



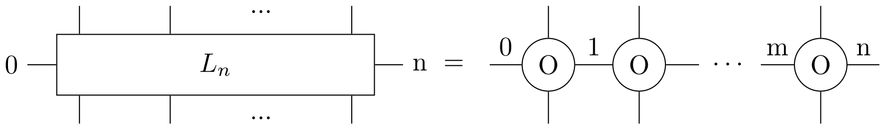
(24)

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



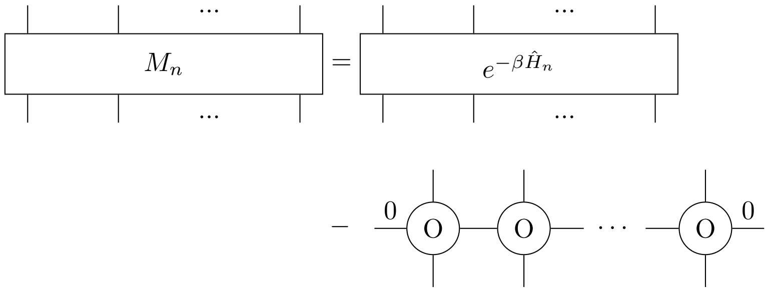
(25)

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.



(26)

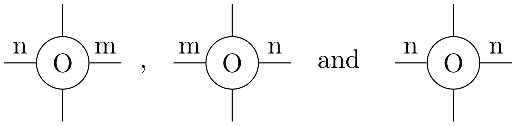
M_n is the difference between the exponentiated hamiltonian for n sites and the contraction of the MPO over all the currently assigned combinations of virtual levels.



(27)

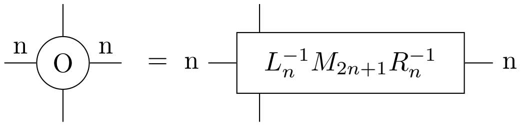
6.3.1 Type A

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



with $n \in \mathbb{N}_0$ and $m = n - 1$.

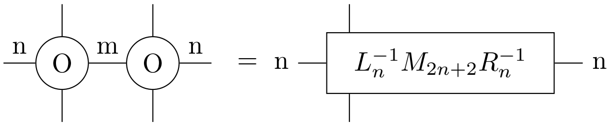
6.3.1.1 O^{nn} The O^{nn} block is defined by eq. (28)



(28)

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

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



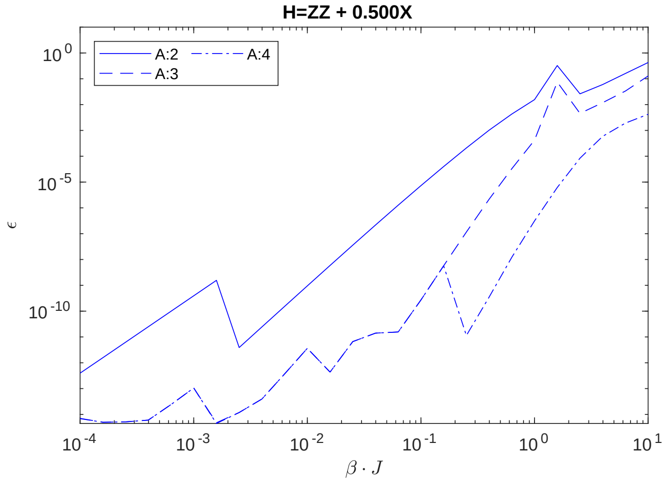
(29)

The individual elements O^{mn} and O^{nm} are obtained by doing an svd decoposition.

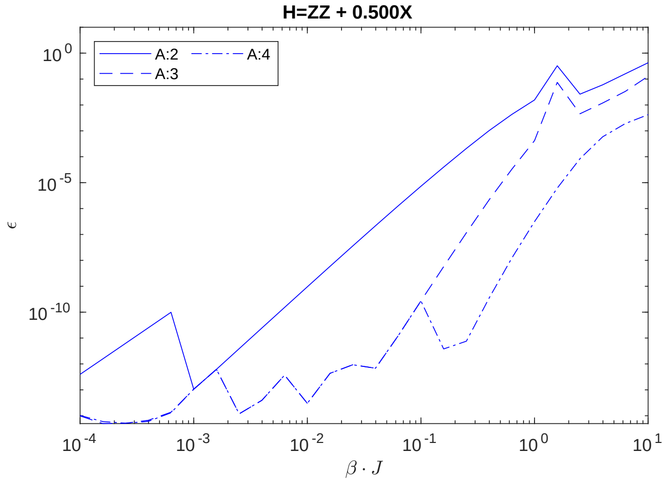
During the svd the bond dimension can be lowered by only keeping the rows and colums belonging to $\sigma > \sigma_0$. This also helps the invertibility. Increasing σ_0 reduces the precision of the MPO. This can be seen in fig. 2. A good tradeoff seems to be $\sigma_0 = 10^{-12}$. There is almost no precision loss vor small β, while for intermediate it performs optimal for intermediate β.

symmetric split S, invertibility lowest eiges, eigensplit, order cutoff

toon figuurtjes met verschillende sigma 0 voor $t_i sing$

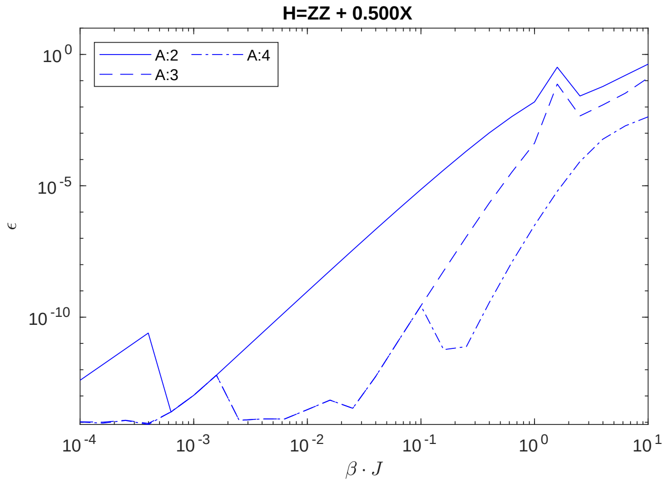


(a) 10^{-10}

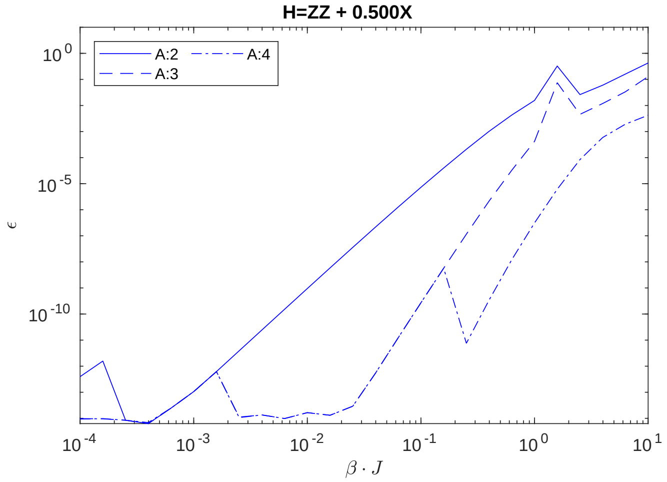


(b) 10^{-11}

Figure 2: A figure with two subfigures

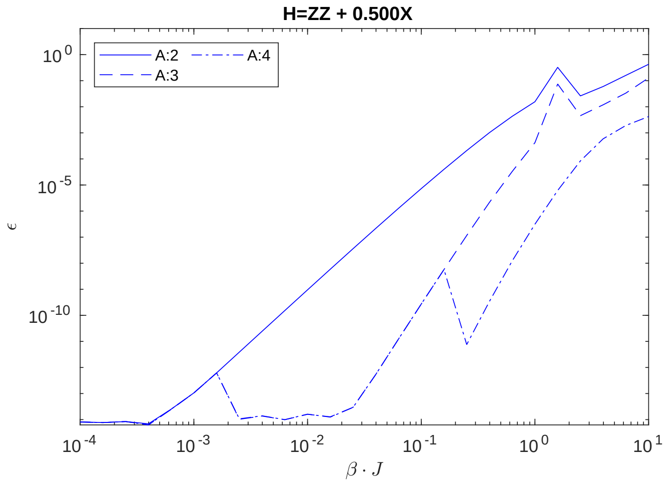


(c) 10^{-12}



(d) 10^{-13}

Figure 2: A figure with two subfigures



(e) 10^{-14}

Figure 2: A figure with two subfigures

As can be seen in **??**, mainly the construction for small values of β get affected by the choice of σ_0.

6.3.2 Truncation

6.3.2.1 O^{nn} Intoduction of a O^{nn} 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.

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

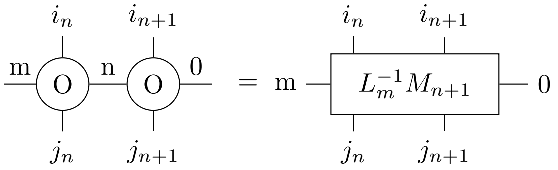
6.3.2.2 O^{mn} and O^{nm}

nog niet gevodnen

zeggen wat allemaal niet werkt

6.3.3 Type B

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

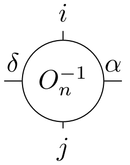


$$\cong X_{(\alpha_m i_n j_n)(i_{n+1}j_{n+1})}$$
$$= U^n \Sigma V^\dagger \tag{30}$$

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: $O^{mn} = U^\dagger$. Take has to be taken with the indices to apply the inverse.

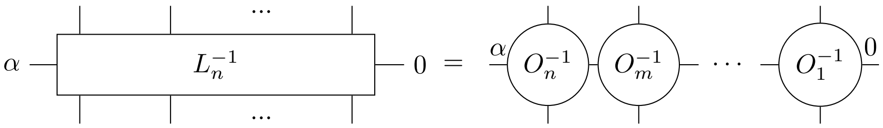
$$\begin{aligned} U^n_{(\alpha ij)\beta}A_{\beta\gamma} &= B_{\alpha ij\gamma} \\ A_{\delta\gamma} &= U^{n\dagger}_{\delta(\alpha ij)}B_{\alpha ij\gamma} \end{aligned} \tag{31}$$

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



$$\cong U^{n\dagger}_{\delta ij\alpha} \tag{32}$$

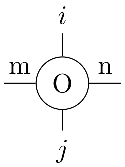
With the notation from eq. (20) we have:



(33)

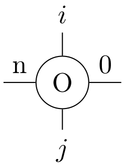
The inverse can be applied sequentially.

6.3.3.1 dimension From the construction the bond dimension grows from the left to the right. Again $\dim n = d^{2n}$. However this can be reduced if we can solve the following equations simultaneously:



$$= A^{m}_{(\alpha ij)\beta}$$

(34)



$$= B^{n}_{(\alpha ij)\beta}$$

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

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

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

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

As expected, the bond dimension is the $\dim n' = \min(d^2 \dim m, \dim(n+1)d^2)$.

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

6.3.3.2 discussion

6.3.4 Type C

primed virtual levels

6.3.5 Type D

dit erin zeten of niet?? type05

7 Benchmarking

7.1 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:

$$R = d^{2n} \times 16 bytes \tag{37}$$

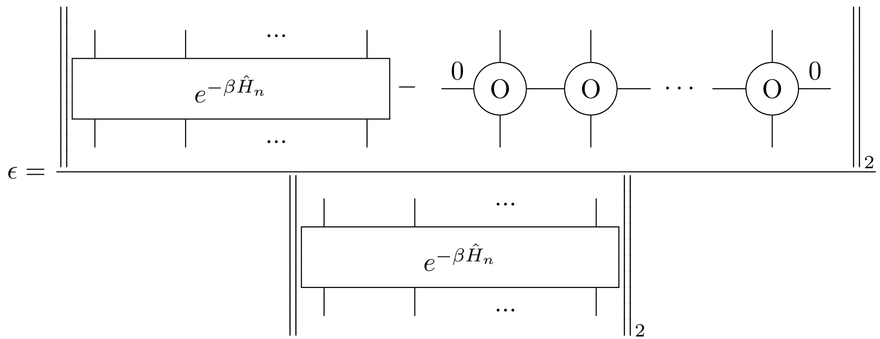
Which means a 14 site chain already takes up GB of RAM.

time complexity algoritms

7.1.1 norms

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

trace norm, schatten p norm, ...



(38)

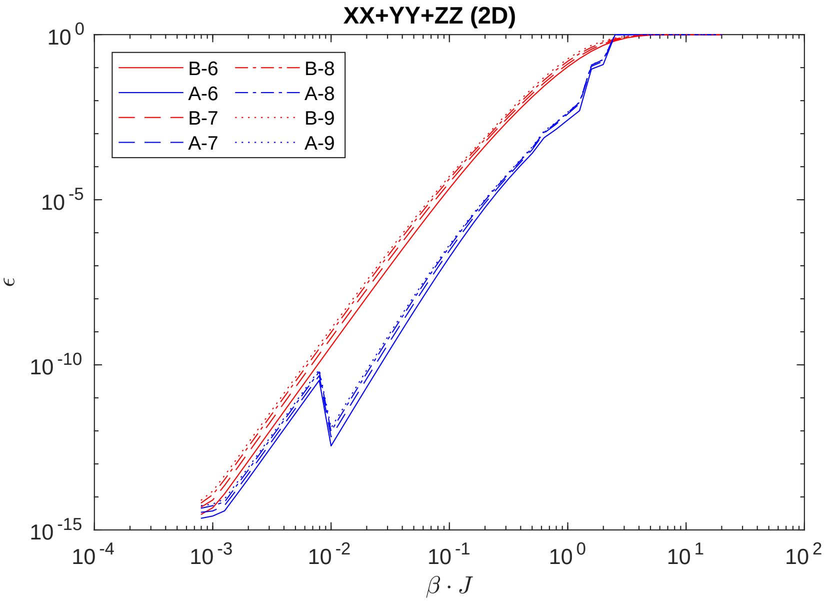
7.2 system size and cyclicity

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.

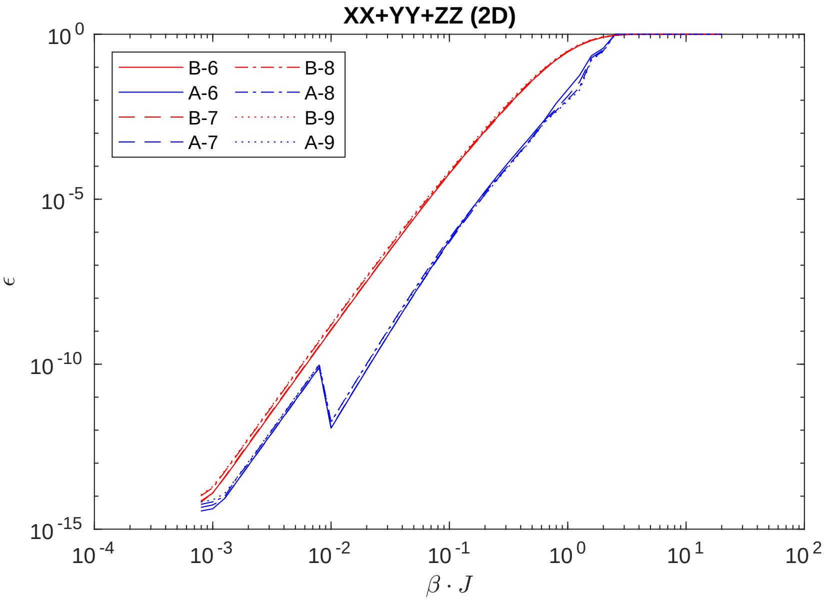
Calculating the cyclic norm comes at the extra cost of contracting a cyclic tensor network.

calculate complexity

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



(a) test



(b) test

Figure 3: test

7.2.1 Ising

7.2.1.1 optimal model parameters 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.

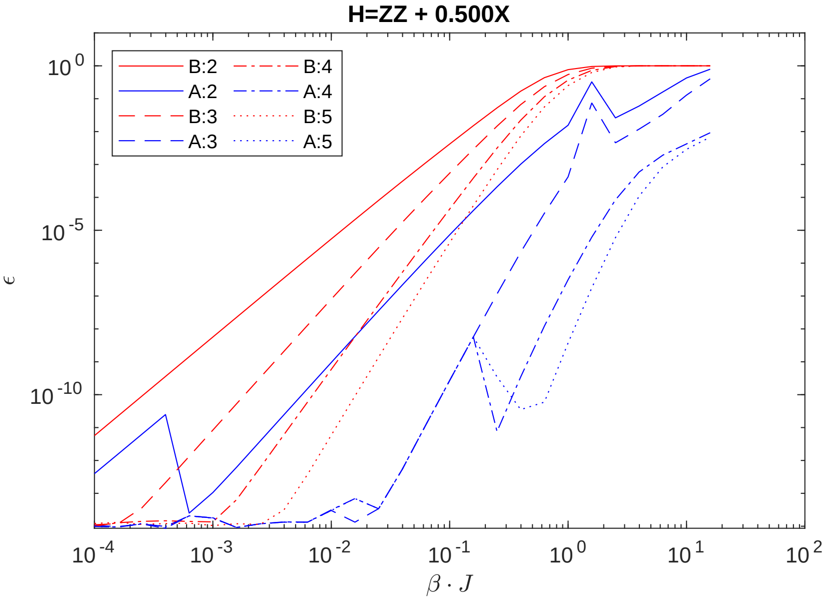


Figure 4: Comparison type A and B for Transversal Ising

7.2.2 Heisenberg

For the Heisenberg model, type A is also an improvement over type B. For large values of β, type A is not able to reproduce the exact

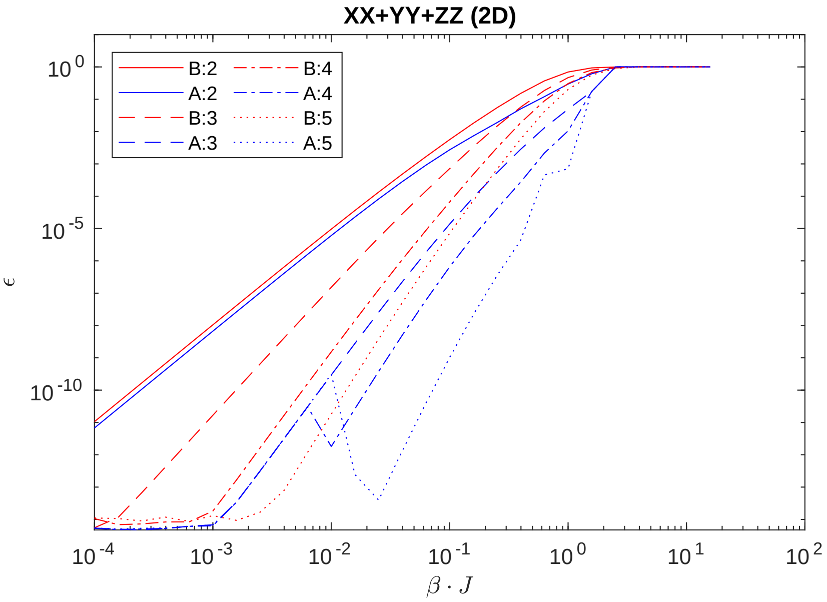


Figure 5: Comparison type A and B for Heisenberg

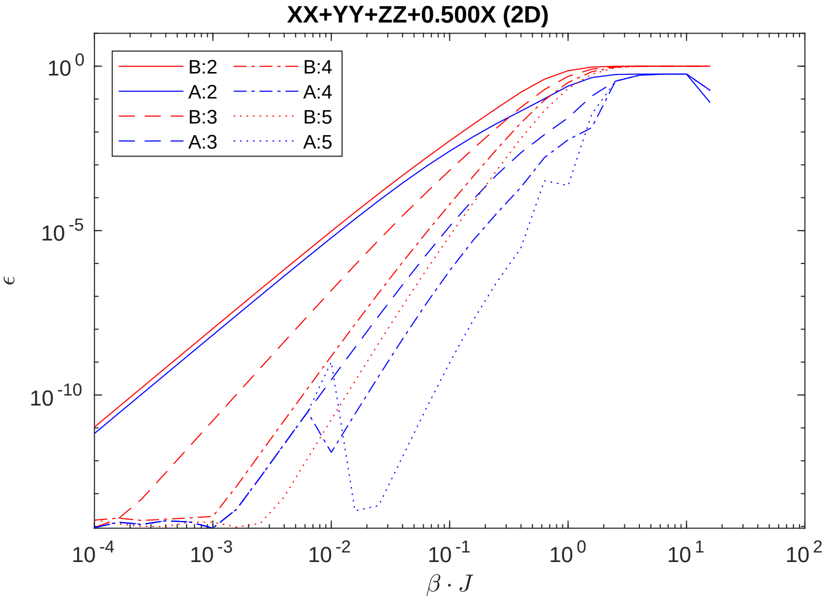


Figure 6: transversal XXX

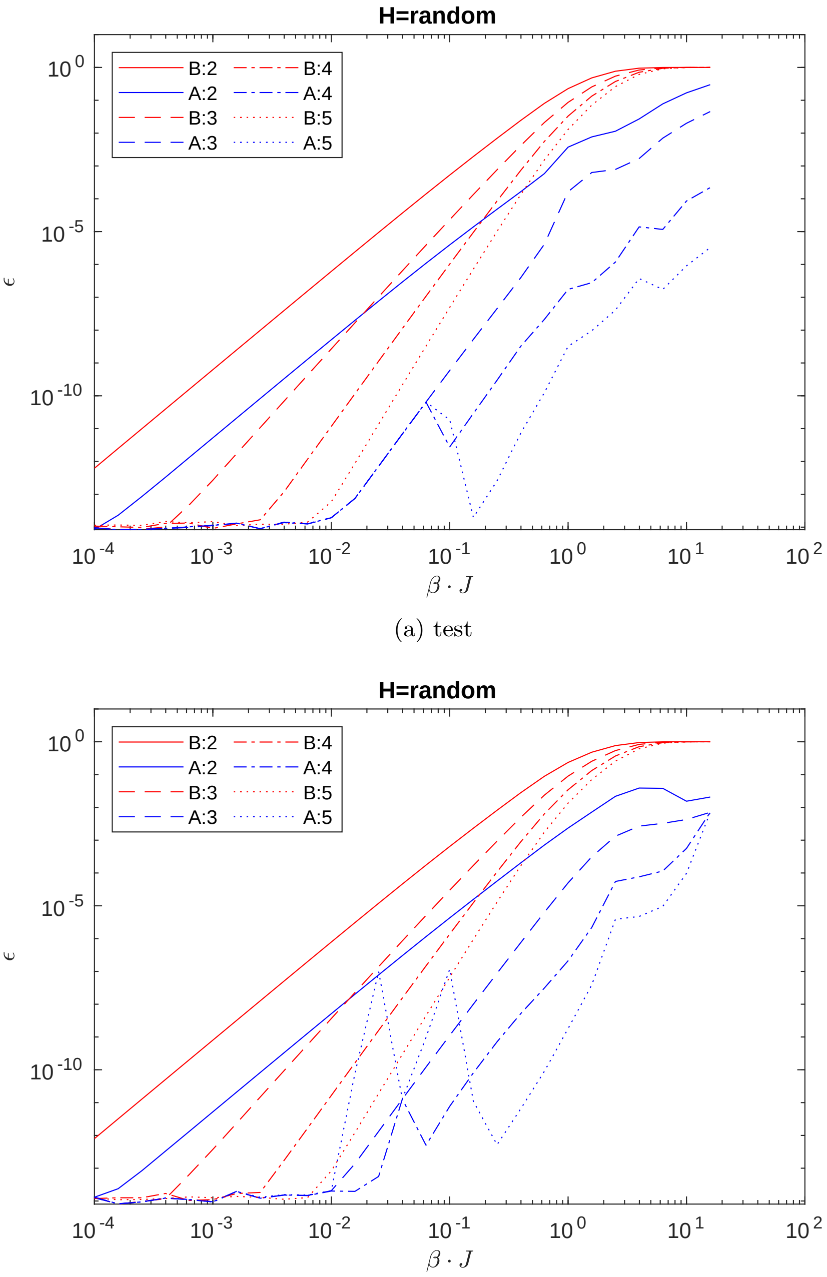
run with M=11

7.3 Random

To give a representative overview for random hamiltonians, several simulations were run. The single site and nearest neighbourgh 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 engergy 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. As stated in the construction. no clear criterium is found for the truncation of odd orders (addition of double blocks). This can be seen for order 5 in some graphs.

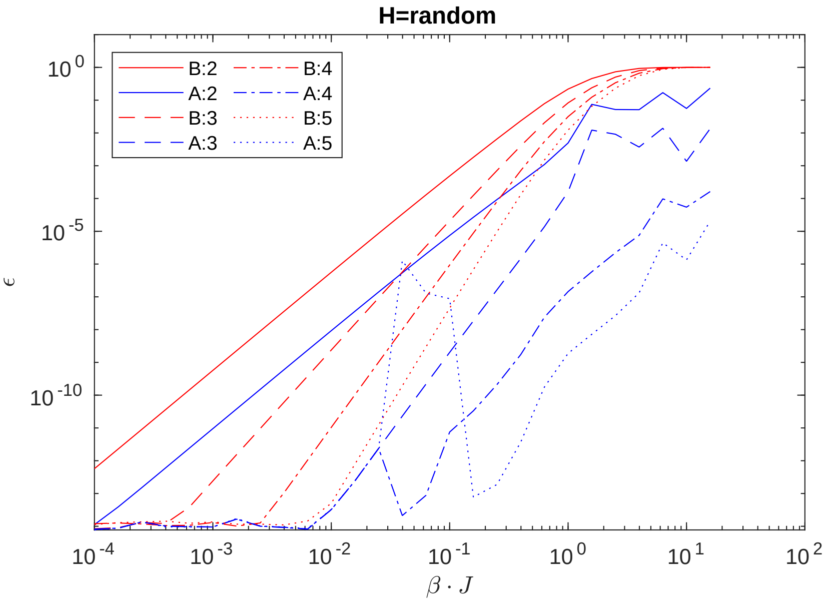
For most of the trials, orders higher than 6 get truncated.



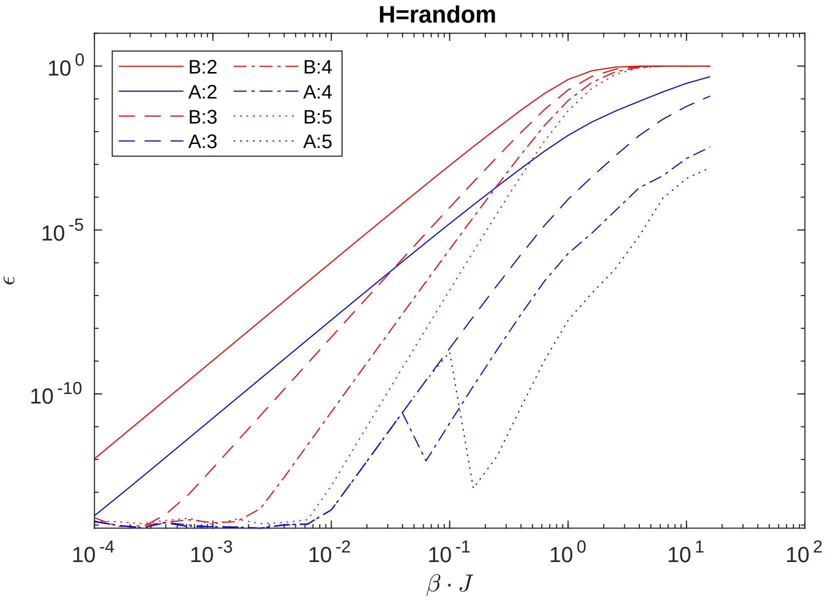
(a) test

(b) test

Figure 7: test



(c) test



(d) test

Figure 7: test (cont.)

7.4 analytical results

References

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