Cluster Expansion of Thermal States using Tensor Networks

David Devoogdt

Academic year 2020-2021

Abstract

Simulating many-body quantum systems is one of the challenges faced by modern Physics. One particular problem is computing the operator $e^{-\beta \hat{H}}$, which is used to compute the partition function of a quantum model. This function is needed to make prediction about the macroscopic behaviour of quantum systems. Of particular interest are the phase transitions. The dissertation introduces the rich field of tensor networks as a method to perform these calculations. The physics of strongly correlated matter is discussed. The main contribution of this work, the novel cluster expansions, are described, together with the computational tools to solve the equations efficiently. The results are promising. Large imaginary time steps can be taken. Calculating of the phase transition of transversal field Ising model in 2D produces results that can challenge recent developments in literature.

1 Overview

Understanding the many-body quantum problem remains a challenge. Strongly correlated matter has many interesting phases which are not yet understood, including high-T superconductors, topological ordered phases, quantum spin liquids [2]. One method to simulate these materials numerically are tensor networks. This work introduces a new method to calculate the exponential of a Hamiltonian with local interactions. This allows to evolve a quantum state in time and calculate the macroscopic properties at a finite temperature. As an example. The new method is used to calculate phase transitions of the transversal Ising model.

2 Tensor Networks

2.1 MPS

Matrix Product States (MPS) form an ansatz to describe the

$$|\Psi\rangle = \sum_{i_1 i_2 \cdots i_n} C^{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \quad (1)$$

The tensor C needs d^n numbers to describe the full wave function. In uniform MPS, the tensor $C^{i_1 i_2 \cdots i_n}$ is subdivided into the product of n tensors C and a matrix M that contains the boundary conditions

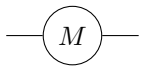
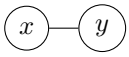
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M). \quad (2)$$

If M is the identity matrix, the chain is closed cyclically. Tensor networks are typically denoted in their graphical form (see table 1). External lines denote free indices, connected lines implies a summation over the shared line, analogous to matrix multiplication. Equation (2) is in this graphical notation becomes

. (3)

An MPS has 2 dimension, the physical dimnsion of the particles $d = dim\,(|i_2\rangle)$ and the dimension χ of the bonds between the tensors. The cluster expansion will rely on "virtual levels". This is the division of the MPS in blocks, analogous to dividing a matrix into block matrices. Every virtual level has its own associated dimension

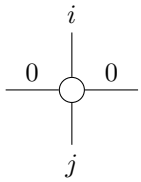
Table 1: Examples of graphical notation.

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

2.2 MPO

A matrix procuct operator (MPO), is similar to an MPS but has 2 physical legs i and j. The following compact notation is used in this paper

$$O^{00} = \quad = . \tag{4}$$



This is the MPO with virtual level 0 and physical indices i and j, which will both be omitted. Non-zero virtual indices are shown, and summation over virtual level is implied. Summation over shared virtual bond 1 on 2 neighbouring sites is denoted as

$$O^{01}O^{10} = \overset{1}{\quad}. \tag{5}$$

While contraction over all possible virtual levels on 3 sites is denoted by

. (6)

3 Cluster Expansion

The novel method to construct a PEPO $e^{-\beta\hat{H}}$ with cluster expansions. An example is given by eq. (6). This was first introduced in [3]. The goal is capture the exponential of the Hamiltonian operator $\hat{H}$

$$\hat{H} = -J\left(\sum_{<ij>} H_2^i H_2^j + \sum_i H_1^i\right) \tag{7}$$

This Hamiltonian consists of 1 and 2 site operators. Of course more general Hamiltonians can also be used. The notation for the contraction of the tensor network will also be used to denote the Hamiltonian evaluated on the given geometry

$$\begin{aligned} H\left(\quad\right) = & H_1 \otimes 1 \quad \otimes 1 \\ & +1 \quad \otimes H_1 \otimes 1 \\ & +1 \quad \otimes 1 \quad \otimes H_1 \\ & +H_2 \otimes H_2 \otimes 1 \\ & +1 \quad \otimes H_2 \otimes H_2 \\ & . \end{aligned} \tag{8}$$

3.1 Idea

The main idea is to make an extensive expansion by adding blocks which solve the model exactly on a local patch. Crucially, the expansion is not in the inverse temperature β but in the size of the patches. The local patches are separated by a virtual level 0 bond. To make this somewhat more precise, the first steps of the expansion are shown here. The smallest patch, i.e. 1 site, encodes the exponential of that Hamiltonian

$$= \exp\left(-\beta H(\quad)\right). \tag{9}$$

If there were no 2 site interactions, this already captures the full diagonalisation. Of course, such a model wouldn't be useful. The next step is to introduce 2 site interactions, where the one site interactions are subtracted from the diagonalised Hamiltonian.

$$\begin{aligned} \overset{1}{\quad} = \exp -\beta H(\quad) \\ -\overset{0}{\quad} \end{aligned} \tag{10}$$

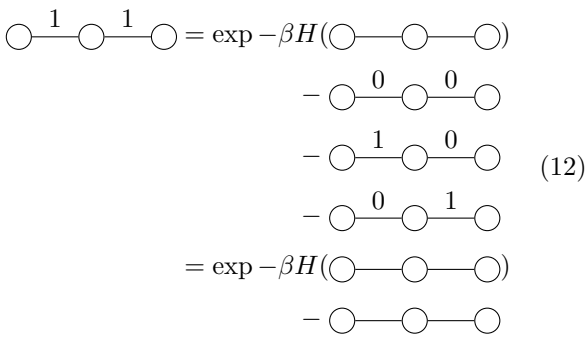
Contraction of larger network lead to many terms, such as

. (11)

The beauty of this lays in the fact that disconnected regions(regions separated by level 0) combine in exactly the right way to capture the terms appearing in

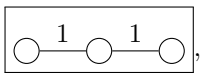
the series expansion of the exact tensor exponential. [3] Only the terms of the exponential which acts on 3 or more neighbouring sites at once, are not accounted for.

Notice that in eq. (10), 2 new blocks are introduced. The dimension of virtual level 1 needs to be d^2, with d the dimension of physical level. Although different possible constructions, already differ in the next step, one more step is added to make te construction and notation clear.



(12)

This is called an cluster expansion of order 3, because there are 3 connected sites solved exactly. The right-hand side of eq. (12) can be ommited, as it is just evaluating the exponentiated Hamiltonian on the same geometry as the left hand side and substructing all possible contractions of the blocks which were added previously. This very compact notation will be able to capture the essence of the different constructions. Because it is important for the remainder of the chapter, it is stressed that for an equation similar to



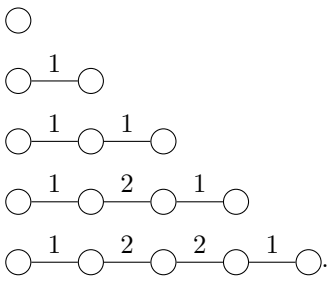
, (13)

the right-hand side of eq. (12) is implied. In the following section, different types will be discussed. For every chain lenght, a new block is defined. This could be done in numerous ways. The different types will be discussed in the next sections.

3.2 1D

3.2.1 Type A

The first few blocks in the cluster expansion are

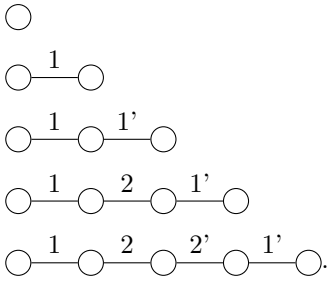


(14a)
(14b)
(14c)
(14d)
(14e).

Virtual level l needs a bond dimension of d^{2l} to solve the equations. The introduction of O^{nn} blocks lead to long chains. This could result in diverging behaviour for cyclic systems.

3.2.2 Type E

To remedy this behaviour, type E only has these blocks

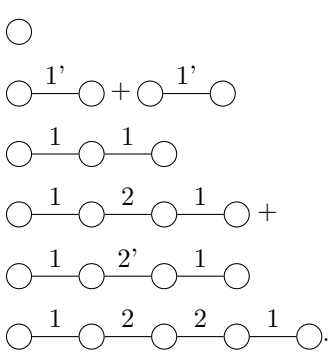


(15a)
(15b)
(15c)
(15d)
(15e).

The bond dimension χ is twice as large, because for every virtual level there is also a primed level. With these blocks, it is impossible to make a patch longer than what is solved explicitly. This generalises well to higher dimension.

3.2.3 Type F

Both type A and F have potentially ill conditioned inverses. The blocks of type F are



(16a) (16b) (16c) (16d) (16e)

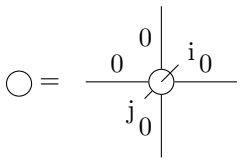
The blocks O^{nn+1} are unitary up to a constant factor. The primed blocks solve the chains of even order. This requires twice the bond dimension of type A, but is guaranteed to have well conditioned inverses.

3.3 2D

In hindsight of the results, the construction in 2D is a generalisation of type A. The linear blocks, which are given by a tree graph, will be a direct generalisation. The non-linear blocks are used to account for loops.

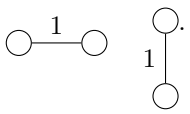
3.3.1 Linear blocks

The generalisation of an MPO to 2D is called a PEPO (project entangle pair operator). These PEPO's are graphically depicted by the same symbol



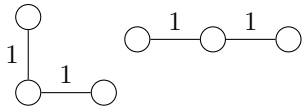
(17)

The construction starts of as



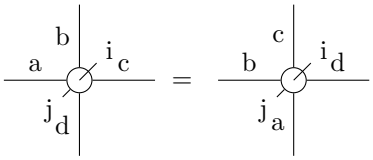
(18)

For the order 3 blocks, 6 different options are possible. They are



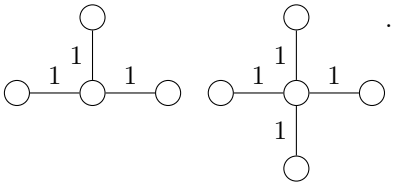
(19)

and rotations over 90 degrees. Solving all blocks such that



(20)

reduced the number of blocks that need to be solved significantly. Also T and + blocks should be added

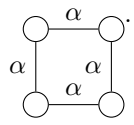


(21)

From here on, it can again be generalised to longer chains and +'s. Care has to be taken to construct the blocks in the right order.

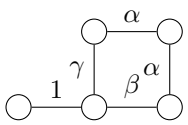
3.3.2 Nonlinear blocks

Not all finite size patches are covered with the blocks introduced in the previous section. The lowest order block not covered is



(22)

This is a nonlinear equation, and will be treated separatey in section 3.4. All virtual levels for solving loops are denoted by Greek letters. For $d = 2$, the bond dimension of α can be as low as 6. To connect the loops to the linear blocks, corner pieces similar to



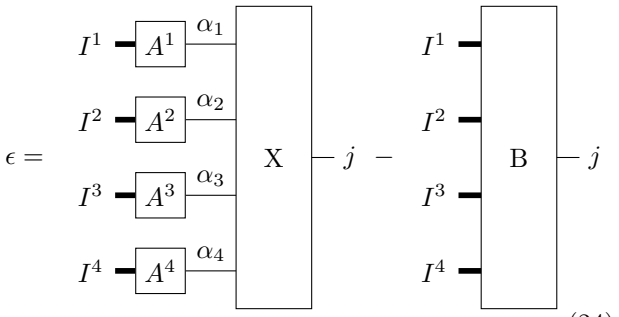
(23)

are used. Directly connecting to $O^{\alpha\alpha 01}$ also solves the local patch, but cause diverging results when 2 or more corner pieces with extensions connect. One corner can connect to 2 chains, with length of the same order as the linear blocks. Going further is possible, comes at an ever increasing bond dimension cost.

3.4 Solvers

3.4.1 Linear Solver

Now that it is clear how the construction works, we focus on how to solve them numerically. Let's focus on the block $X = O^{1111}$ from eq. (21). The involved tensor are reshaped and reordered to bring it in the following form



(24)

Here B is the exponentiated Hamiltonian the + geometry minus the contraction of all previous added blocks. ϵ is the residual error, and should be zero up to machine precision when the solver is finished. Solving this equation by inverting the matrices A^i separately results in numerical unstable results, due to the ill conditioned chains. In practice this instability starts happening at virtual level 2. Taking the pseudoinverse of the tensor product $A = A^1 \otimes A^2 \otimes A^3 \otimes A^4$ resolves the problem, but is computationally too expensive. The problem is resolved by taking the SVD decomposition of each matrix $A^i = U^i \Sigma^i V^{i\dagger}$. The unitary matrices are inverted by taking the Hermitian transpose, and the sparse matrix $\Sigma = \Sigma^1 \otimes \Sigma^2 \otimes \Sigma^3 \otimes \Sigma^4$ is pseudoinverted.

3.4.2 Nonlinear Solver

A nonlinear solver takes steps in the direction that lowers the residual error ϵ. This procedure can be sped up if the gradient is known. Inspection of eq. (24) shows that the derivative $\frac{\partial \epsilon_{I^1 I^2 I^3 I^4 j}}{X_{\alpha_1\alpha_2\alpha_3\alpha_1}} = A_{I^1 I^2 I^3 I^4 \alpha_1\alpha_2\alpha_3\alpha_4 j}$. Or more simply contraction of the network but with X removed. This can be extended to more complex situation with the chain rule.

3.4.3 Truncation

The highest virtual level can be truncation in bond dimension. Introducing a block to solve a chain longer than the last exactly solved blocks leads to diverging results

4 Results

The cluster expansions are tested in 2 ways. In 1D and 2D, the error ϵ is calculated by comparing the contracted PEPO against the exact exponential.

4.1 Exact exponentials

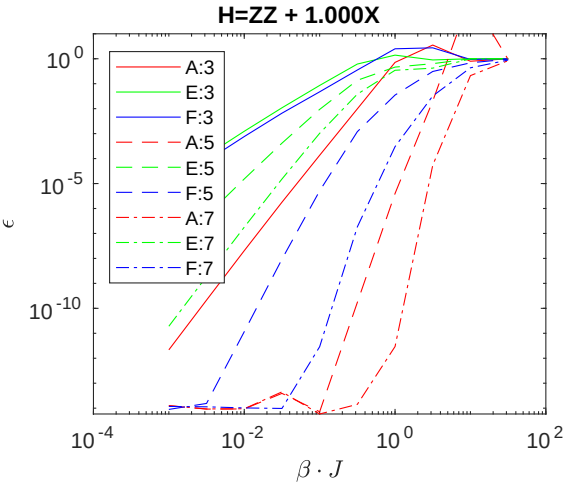


Figure 1: Comparison type A, E and F for Transversal Ising. Error evaluated on cyclic chain.

In 1D, the error is calculated on a cyclic system of 11 sites. The results are shown in fig. 1. All the cluster expansion get better with increasing order. Type A outperforms the other 2 types by quite some margin. This conclusion is also true for the Heisenberg model and random 2 site Hamiltonians. The results in 2D show a similar trend. The error in 2D is of the same order of magnitude. The plaquette term eq. (22) is needed, the extensions are optional. The results show that real time evolution ($t = -i\beta$) also performs well.

4.2 2D Transversal Ising

The transversal Ising model is of the form eq. (7), with $H_1 = g\sigma^x$ and $H_2 = \sigma^z$. For low temperature, the spins tend to align forming a magnet. For high T, the magnetisation disappears. The transversal field cause the spins to align in the direction of the transversal field. A cluster expansion of order 5 with loops is used to simulate the phase transition of the transversal Ising model at g=0 (classical) and g=2.5. The simulated magnetisation $\langle m \rangle$ and the data collapse of m, entropy S and correlation length ξ for g=2.5 is shown in fig. 2. δ is a measure for the size of the system. Figure 2 shows a very clear data collapse. For g=0, the fitted critical temperature $T_c = 2.691(9)$. Onsager's analytical solution is $T_c = 2.69185$. For $g = 2.5$, the fitted value $T_c = 1.2736(6)$ agrees well with values from literature, e.g. $T_c = 1.2737(2)$ obtained with a competing tensor network technique and $T_c = 1.2737(6)$ obtained with quantum Monte Carlo. [1] Higher precision can be achieved with cluster expansions of higher order.

5 Outlook

The results agree well with exact exponentiation and with critical values from literature, proving that these cluster expansion can compete with other methods. With current methods, it is possible to simulate the quantum critical point of the Ising model. The linear blocks and plaquette term seem to be sufficient to make an accurate cluster expansion, making the generalisation to 3D within reach.

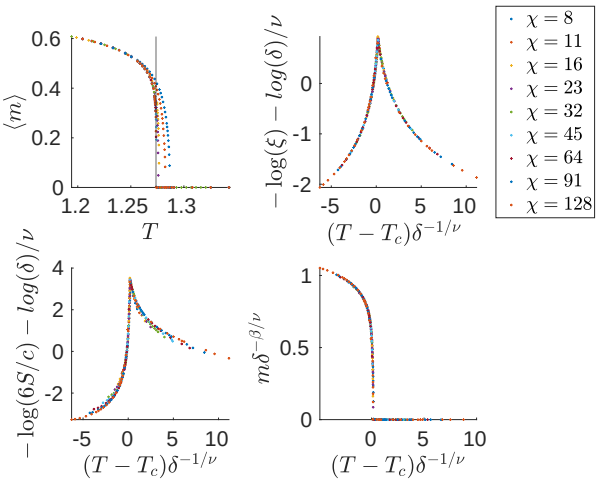


Figure 2: Data collapse for $g = 2.5$ phase transition of transversal Ising Model. Data points are taken from $T \in [T_c - 0.08, T_c + 0.08]$.

References

[1] Piotr Czarnik and Philippe Corboz. Finite correlation length scaling with infinite projected entangled pair states at finite temperature. *Physical Review B*, 99:245107, 2019.

[2] Román Orús. A practical introduction to tensor networks: Matrix product states and projected entangled pair states, oct 2014.

[3] Bram Vanhecke, Laurens Vanderstraeten, and Frank Verstraete. Symmetric cluster expansions with tensor networks. *Physical Review A*, 103(2), 2021.