

# Contents

<b>1</b>	<b>Methods</b>	<b>1</b>
1.1	Abstract . . . . .	1
1.2	Technical details . . . . .	1
1.3	Convergence criteria . . . . .	2
	1.3.1 Simulations with finite bond dimension . . . . .	2
	1.3.2 Simulations with finite system size . . . . .	3
1.4	Spectrum of the corner transfer matrix . . . . .	4
	1.4.1 Analytical results for the Ising model . . . . .	4
	<b>Bibliography</b>	<b>9</b>

# 1

## Methods

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### 1.1 Abstract

We describe the technical details of the algorithms used to compute quantities of interest. We report the convergence behaviour of the algorithms and discuss validity and sources of error.

### 1.2 Technical details

For the models treated in this thesis, the corner transfer matrix  $\mathcal{A}$  and the row-to-row transfer matrix  $T$  are symmetric. But due to the accumulation of machine-precision sized errors in the matrix multiplication and singular value decomposition, this will, after many algorithm steps, no longer be the case. In order for results to remain valid, we manually enforce symmetricity after each step.

The tensor network contractions at each algorithm step will cause the elements of  $\mathcal{A}$  and  $T$  to tend to infinity, which means that they will at some point exceed the maximum value of a floating point number as it can be stored in memory. But because the elements of  $\mathcal{A}$  and  $T$  represent Boltzmann weights, they can be scaled by a constant factor, which allows us to prevent this overflow if we use a suitable scaling. For example by requiring that

$$\mathrm{Tr} \mathcal{A}^4 = 1, \tag{1.1}$$

so that the interpretation of  $\mathcal{A}^4$  as a reduced density matrix of an effective one-dimensional quantum is valid.

## 1.3 Convergence criteria

### 1.3.1 Simulations with finite bond dimension

The convergence of the CTMRG algorithm with fixed bond dimension  $m$  (the infinite system algorithm) can be defined in multiple ways (*cite*). In this thesis, the convergence after step  $i$  of the algorithm is defined as

$$c_i = \sum_{\alpha=1}^m |s_{\alpha}^{(i)} - s_{\alpha}^{(i-1)}|, \quad (1.2)$$

where  $s_{\alpha}$  are the singular values of the corner transfer matrix  $\mathcal{A}$ . If the convergence falls below some threshold  $\epsilon$ , the algorithm terminates.

The assumption is that once the singular values stop changing to some precision, the optimal projection is sufficiently close to its fixed point and the transfer matrices  $\mathcal{A}$  and  $\mathcal{T}$  represent an environment only limited by the length scale given by  $m$ , i.e.

$$\xi(m) \ll N \quad (1.3)$$

is satisfied.

#### Convergence at the critical point of the Ising model

The convergence is shown in Figure 1.1. It is clear that the phenomenological law

$$\log c_n \propto n \quad (1.4)$$

holds to high precision, with the slope depending on  $m$ . Deviations only occur at values of  $c$  of around  $10^{-12}$ .

The convergence of the various quantities as function of the number of algorithm steps is shown in Figure 1.2. For all quantities  $Q$ , the absolute relative difference with the final algorithm step

$$\Delta Q_{\text{rel}}(n) = \left| \frac{Q(n) - Q(n = 10^5)}{Q(n = 10^5)} \right| \quad (1.5)$$

is shown. Again, a law of the form

$$\log(\Delta Q_{\text{rel}}) \propto n \quad (1.6)$$

seems to hold.

To make an estimate of a quantity in the limit  $N \rightarrow \infty$ , or equivalently  $\epsilon \rightarrow 0$ , we can study the change in a quantity as function of the convergence threshold  $\epsilon$ . We define

$$\Delta Q(\epsilon) = M(\epsilon) - M(10\epsilon), \quad (1.7)$$

i.e. the change of quantity  $Q$  when we decrease the threshold  $\epsilon$  by an order of magnitude. The results in Figure 1.3 show that, remarkably, the order parameter, entropy and correlation length to high precision follow the linear relationship

$$\Delta Q(\epsilon) = \alpha_1(m)\epsilon, \quad (1.8)$$

whereas the free energy follows a quadratic relationship

$$\Delta f(\epsilon) = \alpha_2(m)\epsilon^2. \quad (1.9)$$

This means that we can confidently extrapolate the value of a quantity in the fully converged limit as

$$Q(\epsilon \rightarrow 0) = Q(\epsilon_{\min}) + \sum_{\epsilon = \frac{\epsilon_{\min}}{10}, \frac{\epsilon_{\min}}{100}, \dots} \Delta Q(\epsilon), \quad (1.10)$$

where  $\epsilon_{\min}$  is the lowest threshold used in simulation, and  $\Delta Q(\epsilon)$  is determined by fitting to suitable higher values of the threshold.

technically this is not correct for the already converged values of  $m$

Cross check with correlation length, report on boundary conditions

### 1.3.2 Simulations with finite system size

In the finite-system algorithm, we want to reliably extrapolate quantities in the bond dimension  $m$ . The convergence behaviour is shown in Figure 1.4. For each quantity  $Q$ , we plot the absolute relative difference with the value at the highest  $m$

$$\Delta Q_{\text{rel}}(m) = \left| \frac{Q(m) - Q(m = 200)}{Q(m = 200)} \right| \quad (1.11)$$

versus the bond dimension  $m$ .

The plateaus of  $m$ -values that barely increase the precision are due to the degeneracies in the spectrum of the reduced density matrix. Apart from this structure, the law

$$\Delta Q_{\text{rel}}(m) \propto m^{\alpha(N)} \quad (1.12)$$

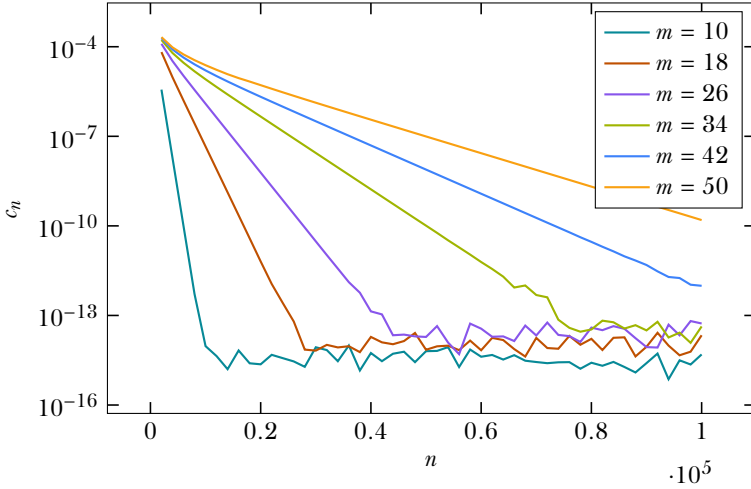


Figure 1.1: Convergence as defined in Equation 1.2 versus  $n$ , the number of CTMRG steps. Up until very small values of  $c_n$ , the convergence is monotonically decreasing and obeys a logarithmic law with slope depending on  $m$ .

is seen to hold for high enough  $m$  for the order parameter, free energy and entropy.

What is  $\alpha$ ? Refer to section where you discuss the spectrum of the reduced density matrix. log log law doesn't seem to work out for correlation length. why??

## 1.4 Spectrum of the corner transfer matrix

### 1.4.1 Analytical results for the Ising model

In what follows, we largely follow [2, 4].

For Ising model on a square lattice, we have [1]

$$\hat{\rho} = \hat{A}^4 = \exp(-\hat{H}_{\text{CTM}}), \quad (1.13)$$

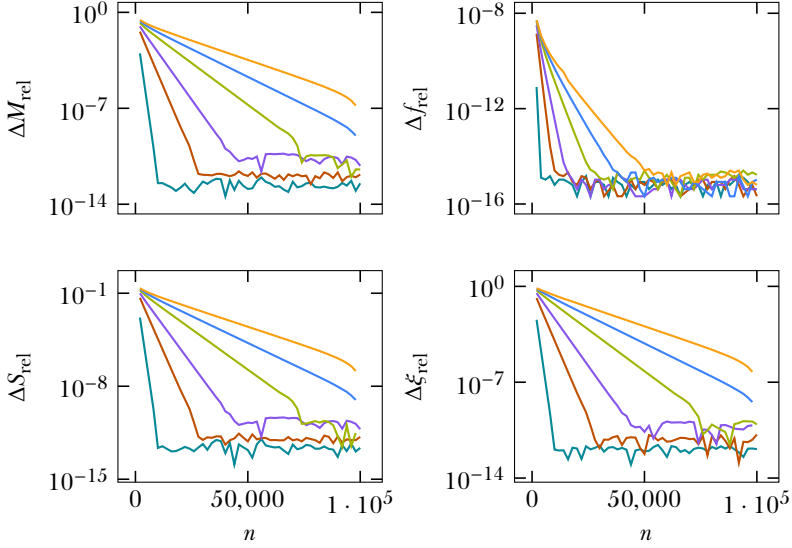


Figure 1.2: Absolute relative difference of quantities (see Equation 1.5). Same legend as Figure 1.1.

where

$$\hat{H}_{\text{CTM}} = \sum_{l=0}^{\infty} \epsilon_l(T) c_l^\dagger c_l, \quad (1.14)$$

with  $c_l$  and  $c_l^\dagger$  fermionic annihilation and creation operators and

$$\epsilon_l = \begin{cases} (2l+1)\epsilon(T) & \text{if } T > T_c, \\ 2l\epsilon(T) & \text{if } T < T_c. \end{cases} \quad (1.15)$$

In other words, the reduced density matrix (or equivalently, the corner transfer matrix  $\mathcal{A}$ ) can be written as a density matrix of an effective free fermionic Hamiltonian with equally spaced excitations.

What does this mean for the spectrum of  $\mathcal{A}$ ? If we assume a free boundary, we have to distinguish between the ordered and disordered phase.

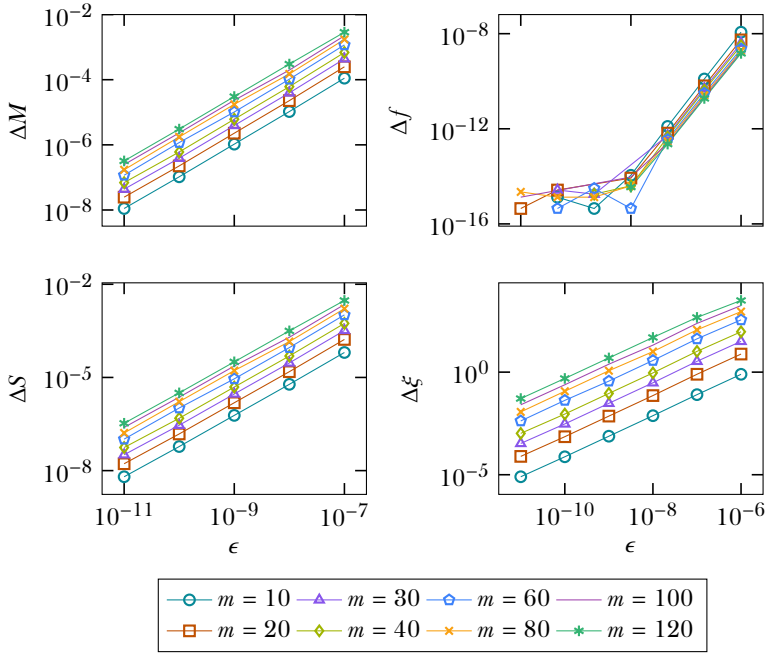


Figure 1.3: Stepwise differences upon decreasing the threshold  $\epsilon$  by an order of magnitude, as in Equation 1.7. For the order parameter, entropy and correlation length, a linear relationship holds to high precision, while for the free energy the relationship is quadratic.

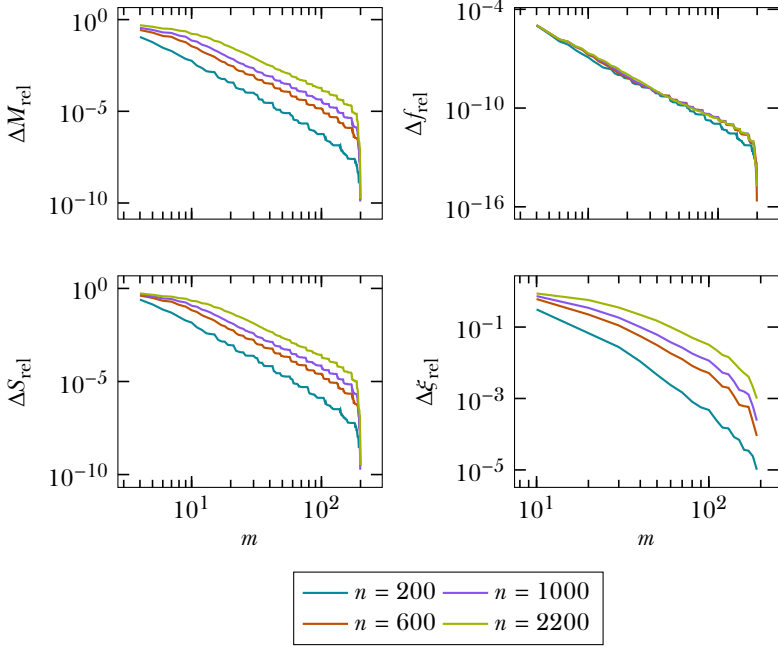


Figure 1.4: The absolute relative difference of quantities, as defined in Equation 1.11. For high enough  $m$ , it obeys a power law with varying exponent  $\alpha(N)$ . The sharp drop for the highest values of  $m$  is an artefact of the definition of  $\Delta Q_{\text{rel}}$  and the plateau-like fashion in which the value of a quantity converges, owing to the spectrum of the reduced density matrix approximated by the CTMRG algorithm. Like in the finite- $m$  case, the free energy converges much faster than the other quantities, and does so with little  $n$ -dependence. Note that  $\Delta \xi_{\text{rel}}$  does not obey a power law.



In the disordered phase, we have  $\epsilon_l = (2l + 1)\epsilon(T)$ . The ground state,  $E = 0$ , corresponds to the vacuum state of the effective system described by  $H_{\text{CTM}}$ . The single-fermion excitations give  $\epsilon, 3\epsilon, 5\epsilon, \dots$ , while two-fermion excitations give  $4\epsilon$  ( $c_0^\dagger c_1^\dagger |0\rangle$ ),  $6\epsilon$  ( $c_0^\dagger c_2^\dagger |0\rangle$ ) and  $8\epsilon$  ( $c_0^\dagger c_3^\dagger |0\rangle$  or  $c_1^\dagger c_2^\dagger |0\rangle$ ). So the first degeneracy appears at  $8\epsilon$ .  $9\epsilon$  is triply degenerate: it can be constructed with a single-fermion excitation and in two ways with a three-fermion excitation.

In the ordered phase, we have a two-fold degeneracy for every state due to symmetry. The ground state energy  $E = 0$ . After that, we can only make the levels  $2\epsilon, 4\epsilon, 6\epsilon, \dots$ . The degeneracy of the  $n$ th energy level is given by  $2p(n)$ , twice the number of partitions of  $n$  into distinct integers [okunishi1999universal]. The factor two comes from the symmetry.

To illustrate:  $c_1^\dagger c_2^\dagger |0\rangle$  and  $c_3^\dagger |0\rangle$  both have  $E = 6\epsilon$ , the third energy level (counting the vacuum as the zeroth energy level), which is to say  $p(3) = 2$  since  $\{3, 2 + 1\}$  are the ways to write 3.

## Bibliography

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