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Methods

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 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 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 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

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

so that the interpretation of 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

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

where s_α are the singular values of the corner transfer matrix A. If the convergence falls below some threshold ϵ, 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 A and T represent an environment only limited by the length scale given by m, i.e.

$$\xi(m) \ll N \tag{1.3}$$

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

$$\log c_n \propto \alpha(m) n \tag{1.4}$$

holds to high precision, with deviations only occuring 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

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

is shown. Again, a law of the form

$$\log(\Delta Q_{\mathrm{rel}}) \propto n \tag{1.6}$$

seems to hold.

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

$$\Delta Q(\epsilon) = M(\epsilon) - M(10\epsilon), \tag{1.7}$$

i.e. the change of quantity Q when we decrease the threshold ϵ 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

$$\Delta Q(\epsilon) = \alpha_1(m)\epsilon, \tag{1.8}$$

whereas the free energy follows a quadratic relationship

$$\Delta f(\epsilon) = \alpha_2(m)\epsilon^2. \tag{1.9}$$

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

$$Q(\epsilon \to 0) = Q(\epsilon_{\min}) + \sum_{\epsilon = \frac{\epsilon_{\min}}{10}, \frac{\epsilon_{\min}}{100}, \ldots} \Delta Q(\epsilon), \tag{1.10}$$

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

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

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

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

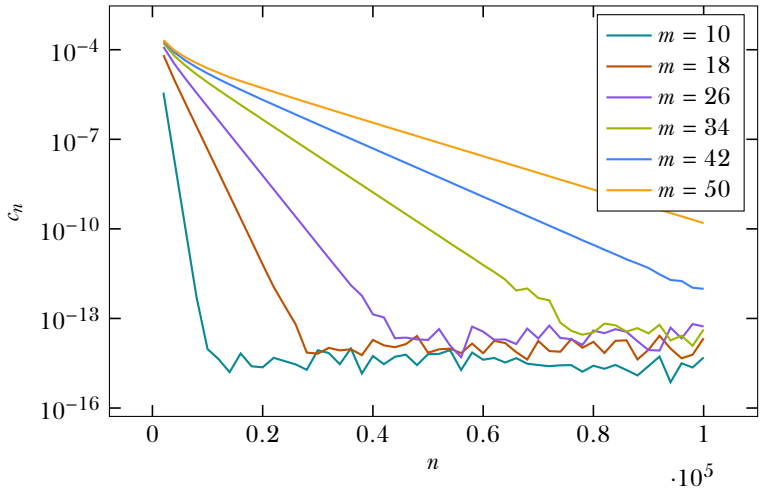

Figure 1.1: Convergence as defined in Equation 1.2 versus n, the number of ctmrg steps.

is seen to hold.

What is α? Refer to section where you discuss the spectrum of the reduced density matrix.

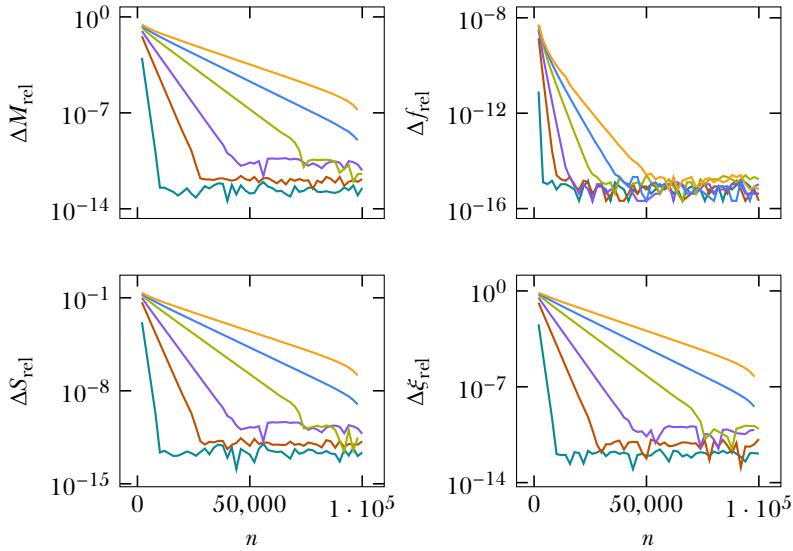

Figure 1.2: Absolute relative difference of quantities (see Equation 1.5). Same legend as Figure 1.1.

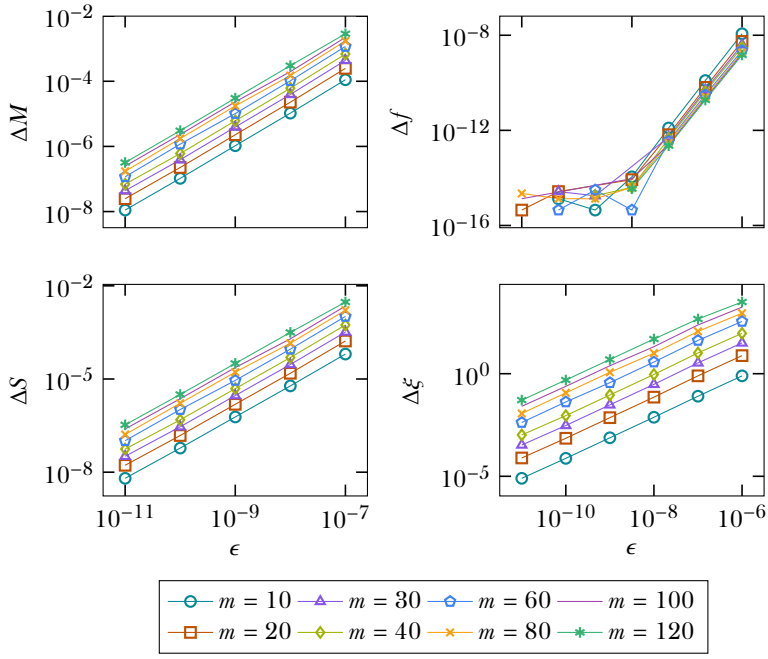

Figure 1.3: Stepwise differences upon decreasing the threshold ϵ by an order of magnitude, as in Equation 1.7.

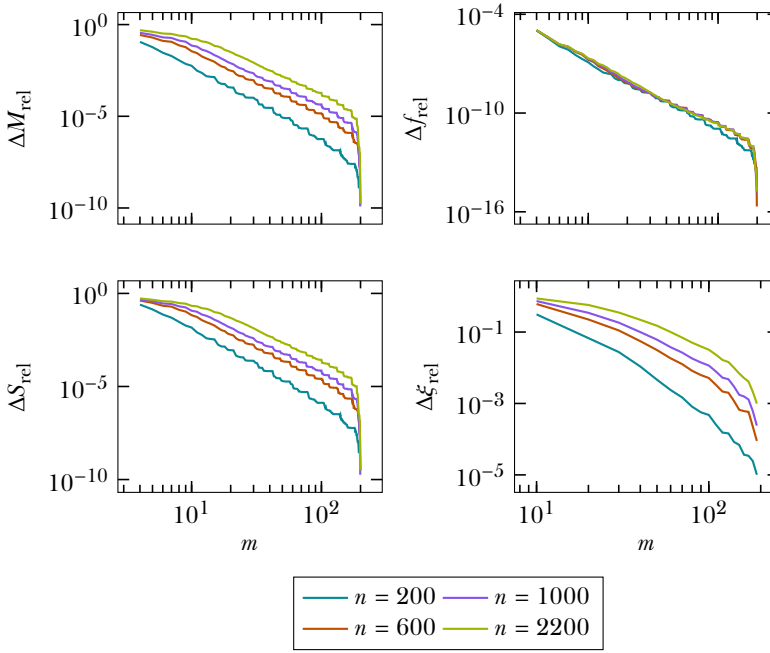

Figure 1.4: hallooooo