1
Results

1.1 Abstract

Cite more

We present finite-size scaling results using the corner transfer matrix renormalization group method on two-dimensional classical square lattices [12]. We compare the results of conventional finite-size scaling in the system size N with scaling in the number of states kept during the renormalization step of the algorithm, denoted by m. Such a comparison was first done in [11]. We highlight the areas in which method excels over the other.

Calculate critical temperature and exponents using information that is directly extractable from the corner transfer matrix.

1.2 Introduction

The first direct comparison of finite-size scaling in the system size N with scaling in the bond dimension of the corner transfer matrix renormalization group method m was done in [11]. In explaining the basic concepts, we largely follow this paper.

The error in the approximation of the partition function (and thus all thermodynamic quantities) in the thermodynamic limit with the corner transfer matrix method depends on two characteristic length scales. The first is the size of the system N. After n steps of the infinite-system algorithm, we have

$$N = 2n + 1. \tag{1.1}$$

The second length scale is related to the finite bond dimension m. Baxter [2], and later Östlund and Rommer [14] (in the context of one-dimensional quantum systems) showed that in the thermodynamic limit, CTMRG and

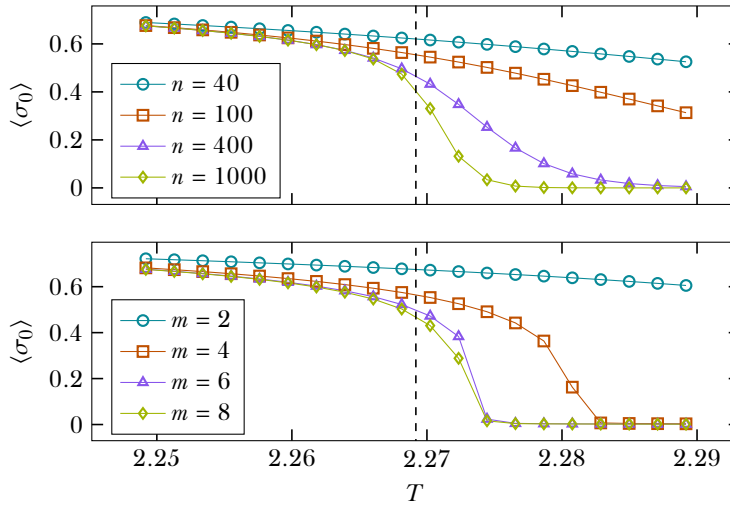

Figure 1.1: Upper panel: expectation value of the central spin $\langle\sigma_0\rangle$ after n CTMRG steps. m is chosen such that the truncation error is smaller than 10^{-6}. Lower panel: $\langle\sigma_0\rangle$ for systems with bond dimension m.

DMRG are variational optimizations in the space of matrix product states.

Can extend this idea a bit.

It is known that an MPS-ansatz with finite bond dimension inherently limits the correlation length of the system to a finite value [20]. Hence, thermodynamic quantities obtained from the CTMRG algorithm with finite m, in the limit $N \to \infty$, cannot diverge and must show finite-size effects similar to those of some effective finite system of size $N_{\text{eff}}(m)$ depending on the bond dimension m.

Figure 1.1 shows the behaviour of the order parameter of the two-dimensional Ising model for systems of finite-size, where m has been chosen such that the truncation error is smaller than 10^{-6}, and for systems of finite m, where the result is converged in the system size N. The results look very similar and support the above claim.

Order parameter is not the same as magnetization central spin. Where to explain this?

1.2.1 Definition of N_{eff} in terms of the correlation length at T_c

In the thermodynamic limit (corresponding to infinite m and N), we have the following expression for the correlation length of a classical system [3]

$$\xi(T) = \frac{1}{\log\left(\frac{T_0}{T_1}\right)}. \tag{1.2}$$

Here, T_0 and T_1 are the largest and second-largest eigenvalues of the row-to-row transfer matrix T, respectively. With N tending towards infinity and finite m, near the critical point $\xi(T)$ should obey a scaling law of the form

$$\xi(T, m) = N_{\text{eff}}(m)\mathcal{F}(N_{\text{eff}}(m)/\xi(T)) \tag{1.3}$$

with

$$\mathcal{F}(x) = \begin{cases} \text{const} & \text{if } x \to 0, \\ x^{-1} & \text{if } x \to \infty. \end{cases} \tag{1.4}$$

Hence, the effective length scale corresponding to the finite bond dimension m is proportional to the correlation length of the system at the critical point $t = 0$.

$$N_{\text{eff}}(m) \propto \xi(T = T_c, m). \tag{1.5}$$

Under this assumption, the order parameter should obey the following scaling relation at the critical temperature

$$M(T = T_c, m) \propto \xi(T = T_c, m)^{-\beta/\nu}. \tag{1.6}$$

The left panel of Figure 1.2 shows that this scaling relation holds. The fit yields $\frac{\beta}{\nu} \approx 0.125(5)$, close to the true value of $\frac{1}{8}$.

The right panel shows the conventional finite-size scaling relation

$$M(T = T_c, N) \propto N^{-\beta/\nu}, \tag{1.7}$$

yielding $\beta/\nu \approx 0.1249(1)$, which can be systematically improved by fitting to larger system sizes, obtained with a fixed truncation error.

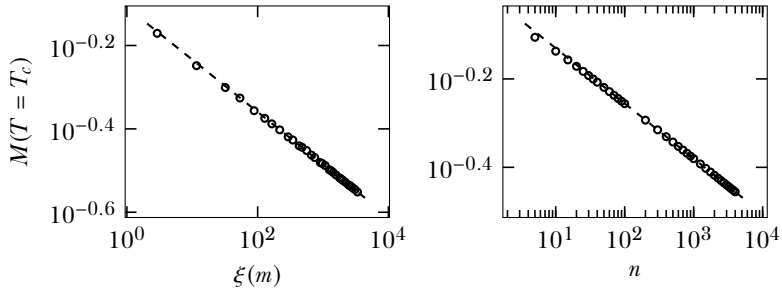

Figure 1.2: Left panel: fit to the relation in Equation 1.6, yielding $\frac{\beta}{\nu} \approx 0.125(5)$. The data points are obtained from simulations with $m = 2, 4, \ldots, 64$. The smallest 10 values of m have not been used for fitting, to diminish correction terms to the basic scaling law. Right panel: fit to conventional finite-size scaling law given in Equation 1.7.

In the case of scaling in correlation length $\xi(m)$, the exponent does not improve when taking bigger values of m, while keeping the termination criterion (relative change of singular values) fixed. This points to a flaw in the termination criterion of the algorithm.

Furthermore, the correlation length $\xi(m)$ shows characteristic half-moon patterns on a log-log scale, stemming from the degeneracies in the corner transfer matrix spectrum. This makes the data harder to interpret, since the effect of increasing m depends on how much of the spectrum is currently retained.

Talk about how to alleviate this partially by using entropy S as length scale.

To further test the hypothesis that N and $\xi(m)$ are the only relevant length scales, the authors of [11] propose a scaling relation for the order parameter M at the critical temperature of the form

$$M(N, m) = N^{-\beta/\nu} \mathcal{G}(\xi(m)/N) \tag{1.8}$$

with

$$\mathcal{G}(x) = \begin{cases} \text{const} & \text{if } x \to \infty, \\ x^{-\beta/\nu} & \text{if } x \to 0, \end{cases} \tag{1.9}$$

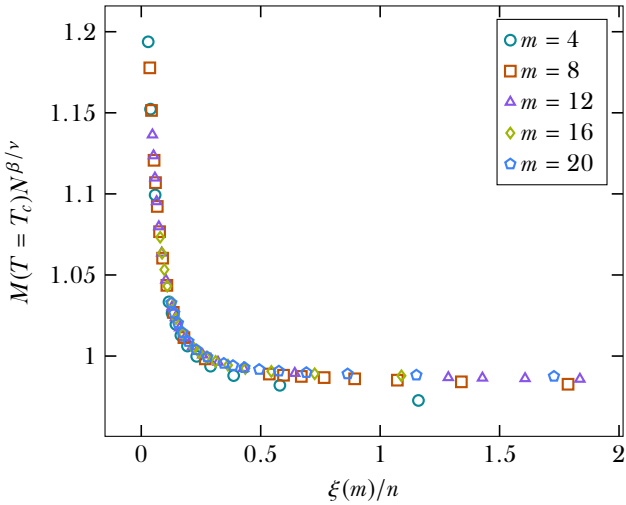

Figure 1.3: Scaling function $\mathcal{G}(\xi(m)/N)$ given in Equation 1.8.

meaning that Equation 1.8 reduces to Equation 1.7 in the limit $\xi(m) \gg N$ and to Equation 1.6 in the limit $N \gg \xi(m)$. Figure 1.3 shows that the scaling relation of Equation 1.8 is justified.

Figure 1.4 shows the cross-over behaviour from the N-limiting regime, where $M(N, m) \propto N^{-\beta/\nu}$ to the $\xi(m)$-limiting regime, where $M(N, m)$ does not depend on N.

1.2.2 Scaling relations away from the critical point

In general, the position of the critical point is not known. In that situation, the scaling relation in Equation 1.8 cannot be used to calculate thermodynamic information. Instead, in the limit $N \to \infty$, we should have

$$M(t, m) \propto \xi(m)^{-\beta/\nu} \mathcal{P}(t\xi(m)^{1/\nu}), \tag{1.10}$$

which is confirmed in Figure 1.5.

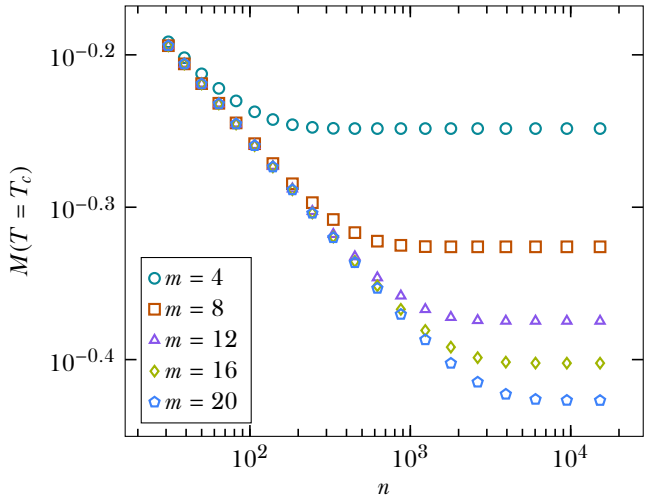

Figure 1.4: Behaviour of the order parameter at fixed m as function of the number of renormalization steps n. For small n, all curves coincide, since the system size is the only limiting length scale. For large enough n, the order parameter is only limited by the length scale $\xi(m)$. In between, there is a cross-over described by $\mathcal{G}(\xi(m)/N)$, given in Equation 1.8.

However, in practice this is still problematic, since $\xi(m)$ is defined at the critical point. Thus, we must find a way to define the length scale corresponding to a finite bond dimension m without making use of the position of the critical point.

1.3 Finite-entanglement scaling and its relation to two-dimensional classical lattices

Another way to understand the fact that the CTMRG method with finite m can never accurately represent systems at criticality, is by looking at the entanglement properties of the ground state of the corresponding one-dimensional quantum systems.

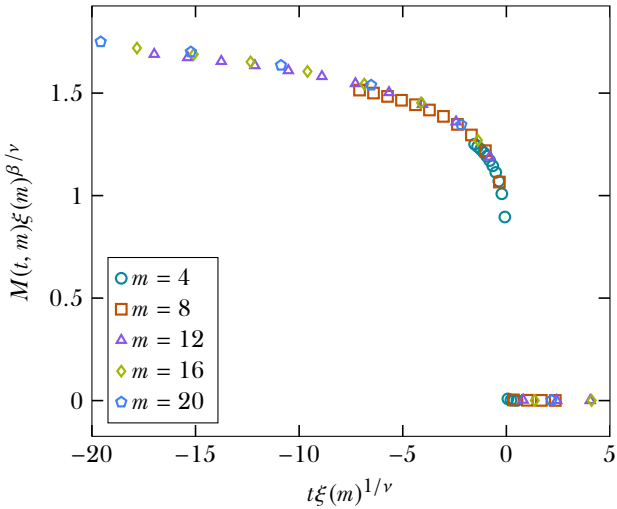

Figure 1.5: Scaling function $\mathcal{P}(t\xi(m)^{1/\nu})$ in Equation 1.10.

It is known that near the critical point, when the correlation length ξ is large but finite, the entanglement of a subsystem A scales as

$$S_A \propto \mathcal{A}(c/6)\log(\xi) \tag{1.11}$$

where $\mathcal{A}$ is the number of boundary points of A and c is the central charge of the conformal field theory at the critical point [4, 19, 6].

Recalling the definition of the entanglement entropy

$$S_A = -\operatorname{Tr}(\rho_A \log \rho_A) = -\sum_\alpha \omega_\alpha \log \omega_\alpha, \tag{1.12}$$

it is trivially seen that the entropy of a state given by the DMRG (or any other MPS), which only retains m basis states of ρ_A, is limited by

$$S_A^{\max}(m) = \log m \tag{1.13}$$

by putting $\omega_\alpha = 1/m$ for $\alpha = 1, \ldots, m$.

Thus, by assuming $S_A^{\max}(m) \propto S_A$ close to criticality, one may infer that the maximum correlation length that an MPS can capture scales as

$$\xi(m) \propto m^{\kappa}. \tag{1.14}$$

Numerical evidence of this fact was first given by the authors of [1], who found

$$\xi(m) \propto m^{1.3} \tag{1.15}$$

for a gapless system of free fermions, using DMRG calculations. Later, using the iTEBD algorithm [18], the authors of [17] presented numerical evidence for such a relation for the Ising model with transverse field and the Heisenberg model, with

$$\kappa_{\text{Ising}} \approx 2, \tag{1.16}$$

$$\kappa_{\text{Heisenberg}} \approx 1.37. \tag{1.17}$$

A quantitative theory of this behaviour was given in [16]. Assuming the energy density as function of the effective correlation length ξ takes the form

$$E(\xi) = E_\infty + \frac{A}{\xi^2} + \frac{B}{\xi} P_r(m), \tag{1.18}$$

where

$$P_r(m) = \sum_{\alpha=m}^{\infty} \omega_\alpha \tag{1.19}$$

is the residual probability. Using results in [5] for the spectrum of ρ_A in limit $m \to \infty$, ξ is found to obey

$$\xi = m^{\kappa}, \tag{1.20}$$

with

$$\kappa = \frac{6}{c(\sqrt{12/c} + 1)} + \mathcal{O}(1/\log m). \tag{1.21}$$

1.4 To do

Articles to cite:

- [17]: postulates exponent κ, provides numerical support and extracts basic results for 1D quantum systems with periodic boundary conditions. Also compares to nishino 2D results. Replicate his experiments? Because CTM seems to give different value for κ.
- [1]: establishes $\xi \propto m^{1.3}$ for correlation length of converged DMRG ground states of a gapless systems of free fermions.
- [15]: assumes existence of κ and compares finite-size scaling with finite-m scaling for 1D quantum systems with periodic boundary conditions.
- [16]: proves expression for κ in asymptotically large m limit that depends only on central charge c, but with corrections of order $1/\log(\chi)$.
- [19]: Also finds $S_A \propto \log(L)$ for 1D quantum systems.
- [4]: proves relation $S_A \propto \mathcal{A}(c/6)\log(\xi)$, with $\mathcal{A}$ the number of boundary points (verified for integrable 2d classical lattice systems).
- [6]: proves relation for classical eight vertex model

Check for validity of $\xi(m) \propto m^{\kappa}$

- entropy scaling at T_c (using exact value of c).
- correlation length scaling at T_c.
- data collapse of order parameter (using exact value of T_c, β, ν.)

1.5 Finding the critical point by maximizing entropy

Articles to cite:

- [7]: theory and numerical support for directly extracting information from ctm spectrum, equivalence to 1D quantum systems.
- [9]: characterisation of phase transition by ctm spectrum for $q = 6$ clock model.
- [8]: characterisation of phase transition by ctm spectrum for truncated tetrahedal model.
- [10]: characterisation of phase transition by ctm spectrum for Widom-Rowlinson models.

- [13]: for XY and Ising model, proves that next-to-nearest neighbor entanglement peaks at critical point (though not nearest-neighbor entanglement.)

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