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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 [1]. 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 [2]. 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 [2]. 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 [3], and later Östlund and Rommer [4] (in the context of one-dimensional quantum systems) showed that in the thermodynamic limit, CTMRG and

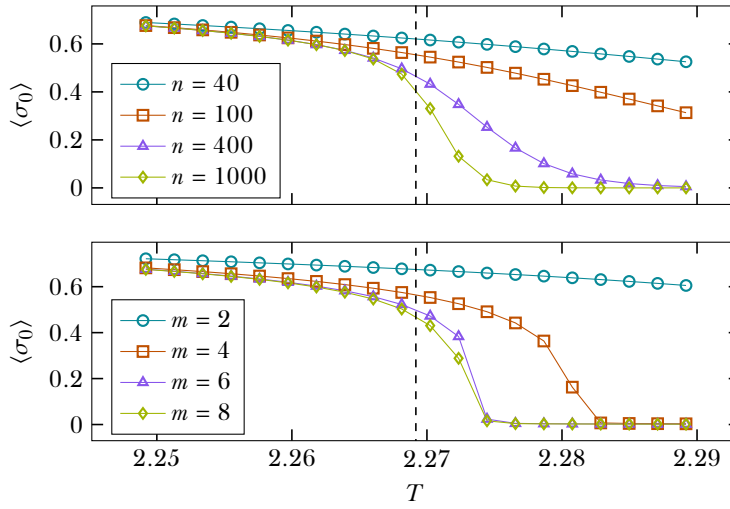

Figure 1.1: Upper panel: expectation value of the central spin $\langle\sigma_0\rangle$ after n CTMRG steps. m is chosen such that the truncation error is smaller than 10^{-6}. Lower panel: $\langle\sigma_0\rangle$ for systems with bond dimension m.

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 [5]. 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 [6]

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

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.

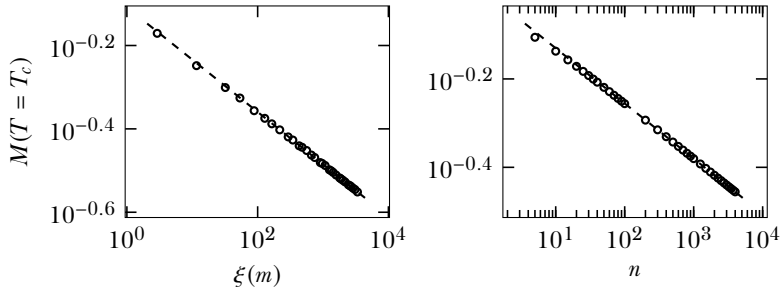

Figure 1.2: Left panel: fit to the relation in Equation 1.6, yielding $\frac{\beta}{\nu} \approx 0.125(5)$. The data points are obtained from simulations with $m = 2, 4, \ldots, 64$. The smallest 10 values of m have not been used for fitting, to diminish correction terms to the basic scaling law. Right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

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

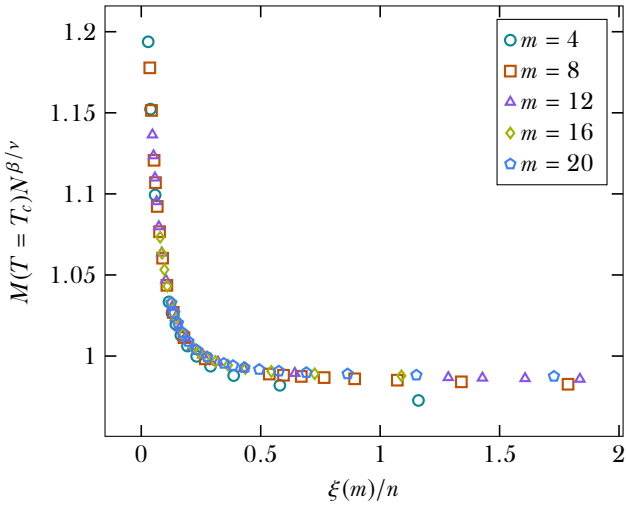

Figure 1.3: Scaling function $\mathcal{G}(\xi(m)/N)$ given in Equation 1.8.

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.

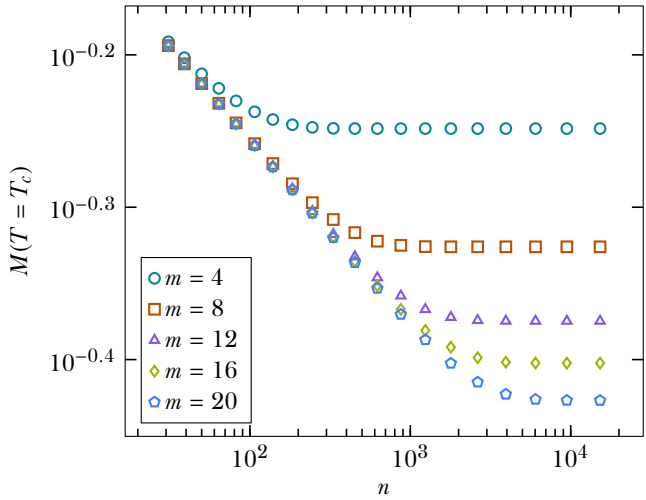

Figure 1.4: Behaviour of the order parameter at fixed m as function of the number of renormalization steps n. For small n, all curves coincide, since the system size is the only limiting length scale. For large enough n, the order parameter is only limited by the length scale $\xi(m)$. In between, there 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.

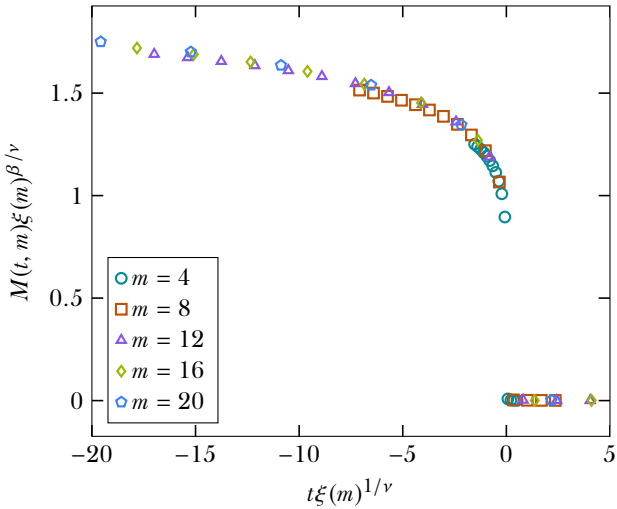

Figure 1.5: Scaling function $\mathcal{P}(t\xi(m)^{1/\nu})$ in Equation 1.10.

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 [7, 8, 9].

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 $\alpha = 1, \ldots, m$.

Empirically, MPS ground states of critical systems do not reach their maximum entropy $\log m$, but one may still assume

$$S_A \propto S_A^{\max}(m) \tag{1.14}$$

close to criticality, which directly implies the relationship

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

Numerical evidence of this fact was first given by the authors of [10], who found

$$\xi(m) \propto m^{1.3} \tag{1.16}$$

for a gapless system of free fermions, using DMRG calculations. Later, using the iTEBD algorithm [11], the authors of [12] presented numerical evidence for such a relation for the Ising model with transverse field and the Heisenberg model, with

$$\kappa_{\text{Ising}} \approx 2, \tag{1.17}$$

$$\kappa_{\text{Heisenberg}} \approx 1.37. \tag{1.18}$$

A quantitative theory of this behaviour was given in [13]. Assuming the energy density as function of the effective correlation length ξ takes the form

$$E(\xi) = E_\infty + \frac{A}{\xi^2} + \frac{B}{\xi} P_r(m), \tag{1.19}$$

where

$$P_r(m) = \sum_{\alpha=m}^{\infty} \omega_\alpha \tag{1.20}$$

is the residual probability. Using results in [14] for the spectrum of ρ_A in limit $m \to \infty$, ξ is found to obey Equation 1.15 with

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

yielding

$$\kappa_{\text{Ising}} = 2.034\ldots, \tag{1.22}$$

$$\kappa_{\text{Heisenberg}} = 1.344\ldots, \tag{1.23}$$

which are in good agreement with the findings in [12].

1.3.1 Classical analogue of entanglement entropy

The key point of the corner transfer matrix renormalization group method [15, 1] is that it unifies White's density matrix renormalization group method [16] with Baxter's corner transfer matrix approach [17, 3], through the identification (in the isotropic case)

$$\rho_{\text{half-chain}} = A^4. \tag{1.24}$$

This allows one to define a 2D classical analogue to the half-chain entanglement entropy of a 1D quantum system

$$S_{\text{classical}} = -\operatorname{Tr} A^4 \log A^4 = -\sum_{\alpha=1}^{m} \nu_\alpha^4 \log \nu_\alpha^4, \tag{1.25}$$

where ν_α are the eigenvalues of the corner transfer matrix A. In the CTMRG algorithm, A is kept in diagonal form, making $S_{\text{classical}}$ trivial to compute.

In [18], numerical evidence is given for the validity of Equation 1.25 for a wide range of models, and the concept is generalized to higher dimensions. For an overview of applying corner transfer matrices in higher dimensions and to quantum systems, see [19].

1.3.2 Locating the critical point with the entanglement spectrum

Since phase transitions of quantum systems can be located by studying their entanglement spectrum (*cite here*), classical systems may be investigated in the same way through the correspondence in Equation 1.24. This is an alternative to the usual approach of studying an order parameter or derivatives of thermodynamical observables (*cite here?*).

Examples of studies using the spectrum of the corner transfer matrix to analyze two-dimensional classical systems are [20, 21, 22].

- [18]: refs [42] and [12] contain many papers which study the phenomenon of pinpointing a phase transition without using physical observables (i.e. entanglement, spectrum, fidelity instead.)
- [23]: for XY and Ising model, proves that next-to-nearest neighbor entanglement peaks at critical point (though not nearest-neighbor entanglement.)

1.3.3 Numerical results

We now check the validity of Equation 1.15 in the context of the CTMRG method for two-dimensional classical systems. Similar checks were done for one-dimensional quantum systems in [12].

Directly checking Equation 1.15 yields $\kappa = 1.93$, see top left panel of Figure 1.6. Under the assumption of Equation 1.15, we have the following scaling laws at the critical point

$$M(m) \propto m^{-\beta\kappa/\nu} \tag{1.26}$$

$$f(m) - f_{\text{exact}} \propto m^{(2-\alpha)\kappa/\nu} \tag{1.27}$$

for the order parameter and the singular part of the free energy, respectively. A fit to $M(m)$ yields $\kappa = 1.93$ and a fit to $f(m) - f_{\text{exact}}$ yields $\kappa = 1.90$. See the top right and bottom left panels of Figure 1.6. Here, we have used $\beta = 1/8$, $\nu = 1$ and $\alpha = 0$ for the Ising model.

Tell that the κ law is indeed valid, since it is a good fit.

We may use Equation 1.11 and Equation 1.25 to check the relation

$$S_{\text{classical}} \propto \frac{c\kappa}{6} \log m, \tag{1.28}$$

which also yields $\kappa = 1.93$, where $c = 1/2$ for the Ising model. See bottom right panel of Figure 1.6.

We may directly verify the value of the central charge c associated with the conformal field theory at the critical point by fitting to

$$S_{\text{classical}} \propto \frac{c}{6} \log \xi(m), \tag{1.29}$$

which yields $c = 0.501$, shown in the left panel of Figure 1.7.

The right panel of Figure 1.7 shows the fit to the scaling relation in N (or, equivalently the number of CTMRG steps n)

$$S_{\text{classical}} \propto \frac{c}{6} \log N, \tag{1.30}$$

which yields $c = 0.498$.

To verify if the point of maximum entropy

$$T^\star(m) = \max_T S(T, m) \tag{1.31}$$

is a good definition of the pseudocritical point, we fit the relation

$$T^\star - T_c \propto \xi(m)^{-1/\nu}. \tag{1.32}$$

which yields $\widetilde{T}_c = 2.2692$ and $\nu = 0.997$ when the length scale $\xi(T^\star, m)$ is used, shown in the left panel of Figure 1.8. Here, $\widetilde{T}_c$ denotes the critical temperature found by minimising the norm of squares of a fit of the form given in Equation 1.32. In finding the position of the pseudoccritical temperature $T^\star$, a tolerance of 10^{-6} was used.

If, however, the length scale $\xi(m, T_c)$ at the actual critical point is used, a much worse fit is obtained, yielding $\widetilde{T}_c = 2.2691$ and $\nu = 0.90$, shown in the right panel of Figure 1.8.

This signifies the value of $\xi(T^\star, m)$ is heavily dependent on $T^\star$, and using the length scale at the actual pseudocritical temperature found somehow offsets the error on its position.

this is unclear.

Assuming Equation 1.15, Equation 1.32 becomes

$$T^\star - T_c \propto m^{-\kappa/\nu}, \tag{1.33}$$

which yields *values*, shown in the bottom left panel of Figure 1.8.

As a cross check, we can fit instead to scaling relation of the pseudocritical temperature for finite N

$$T^\star - T_c \propto N^{-1/\nu} \tag{1.34}$$

yielding *values*. See the bottomr right panel of Figure 1.8.

- validate pseudocritical point by matching it to pseudocritical point given by correlation length and magnetization (how?)
- scaling of pseudocritical point $T^\star - T_c \propto m^{-\kappa/\nu}$.

1.4 To do

Articles to cite:

- [24]: assumes existence of κ and compares finite-size scaling with finite-m scaling for 1D quantum systems with periodic boundary conditions.
- [9]: proves relation for classical eight vertex model

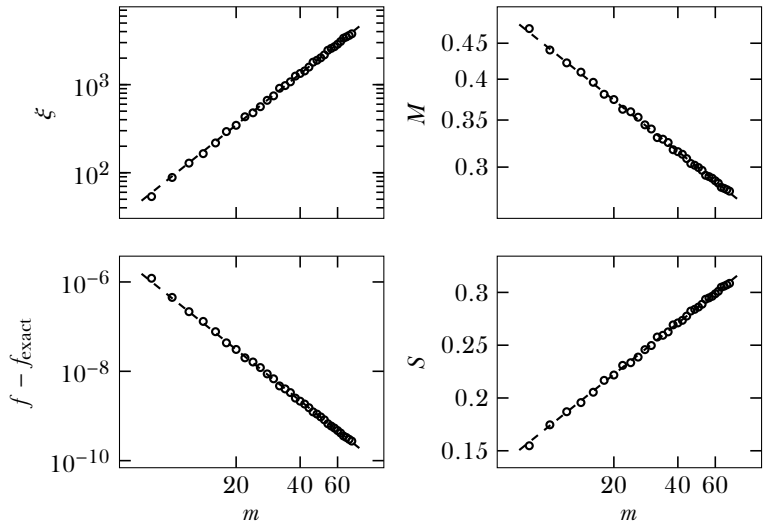

Figure 1.6: Numerical evidence for Equation 1.15, Equation 1.26, Equation 1.28, yielding, from left to right and top to bottom, $\kappa = \{1.93, 1.93, 1.90, 1.93\}$.

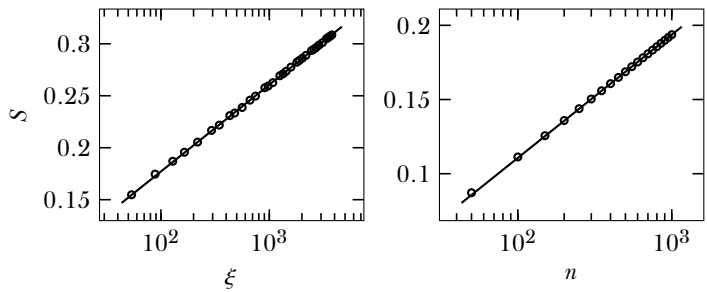

Figure 1.7: Left panel: numerical fit to Equation 1.29, yielding $c = 0.501$. Right panel: numerical fit to Equation 1.30, yielding $c = 0.498$.

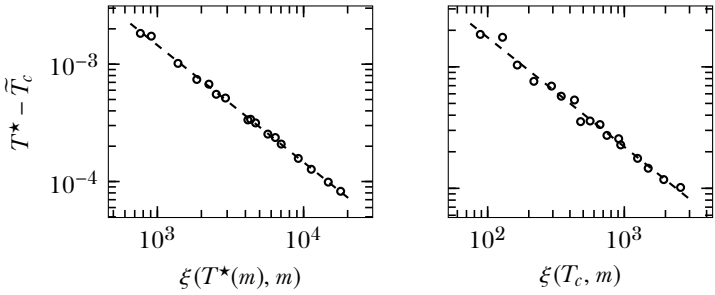

Figure 1.8: Left panel: numerical fit to Equation 1.32 with $\xi(T^\star(m), m)$ used as relevant length scale. Right panel: same fit but using $\xi(T_c, m)$, the correlation length at the exact critical point.

Things to check

- does $S(T^\star, m) \propto \log \xi(T^\star, m)$ hold?
- does $S(T^\star, N) \propto \log N$ hold better than $S(T_c, N) \propto \log N$?
- does fitting $T_c - T^\star(N)$ to N give better results than fitting against $S(T^\star, N)$?
- how does $T^\star(m)$ from entropy compare against $T^\star$ found from max correlation length, or vanishing magnetization?
- optimize κ for scaling of pseudo critical point?
- find $T^{\star,N}$ for larger N for ising model.

Plots to make:

- $T^\star - T_c$ vs N
- $S(T_c, N) \propto \log N$
- generally, why should there be a difference between using entropy at critical point vs using entropy at pseudocritical point? How does each one scale?

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