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# 1

## Critical behaviour and finite-size scaling

---

### 1.1 Abstract

In this chapter, we introduce the central concepts in critical phenomena and finite-size scaling.

We follow the excellent review by Barber [1] and chapter five of Cardy's book [2].

### 1.2 Phase transitions

When matter exhibits a sudden change in behaviour, often characterized by a discontinuity or divergence of one or more thermodynamic quantities, we say it undergoes a *phase transition*.

A quantity that signifies this change is called an *order parameter*, which can take vastly different forms across systems and transitions. For example, for the transition of a ferromagnet, the order parameter is the net magnetization of the system, while for a percolation transition, it is the size of the largest connected graph.

For a historical account of the classification of phase transitions, see [3]. At the present time, we distinguish between two different types [4].

When some thermodynamic quantity changes discontinuously, i.e. shows a jump, we call the transition *first order*. In contrast, during a *continuous* phase transition a variable undergoes change continuously. The point at which a continuous phase transition occurs, is called the critical point.

The two-dimensional Ising model (*ref here*) in a magnetic field shows both types of transition. At zero magnetic field and  $T = T_c = 1/(\log(1 + \sqrt{2}))$ , the magnetization changes from zero for  $T > T_c$  to a finite value for  $T < T_c$  in a continuous manner.

Below the critical temperature  $T_c$ , when the magnetic field  $h$  tends to zero from  $h > 0$ , the magnetization tends to a positive value. Conversely, when the magnetic field tends to zero from  $h < 0$ , the magnetization tends to a negative value. Thus, across the region  $h = 0, T < T_c$  the system undergoes a first-order phase transition.

### 1.2.1 Finite systems

We will now argue that a phase transition cannot occur in a finite system, but only happens when the number of particles tends to infinity.

Because thermodynamic quantities are averages over all possible microstates of a system, those quantities are completely defined in terms of the system's partition function, or equivalently its free energy.

Since in a finite system, the partition function is a finite sum of exponentials, it is analytic (infinitely differentiable). Hence, thermodynamic quantities cannot show true discontinuities and the phase transitions described in the above section do not occur.

pictures?

## 1.3 Critical behaviour

We will now focus our attention on continuous phase transitions, more specifically the one that occurs in the two-dimensional Ising model. Before we discuss the behaviour of the free energy around the critical point, we briefly summarize how the thermodynamic limit is approached far away from it. Here, we largely follow [1].

We assume that the free energy per site in the thermodynamic limit

$$f_\infty(T) = \lim_{N \rightarrow \infty} \frac{F(T, N)}{N} \quad (1.1)$$

exists, and is not dependent on boundary conditions. By definition, it is not analytic in a region around the critical point.

Outside that region, however, we can write

$$F(T, N) = Nf_\infty(T) + o(N), \quad (1.2)$$

where correction terms  $g(N)$  of  $o(N)$  (little-o of  $N$ ) obey

$$\lim_{N \rightarrow \infty} \frac{g(N)}{N} = 0. \quad (1.3)$$

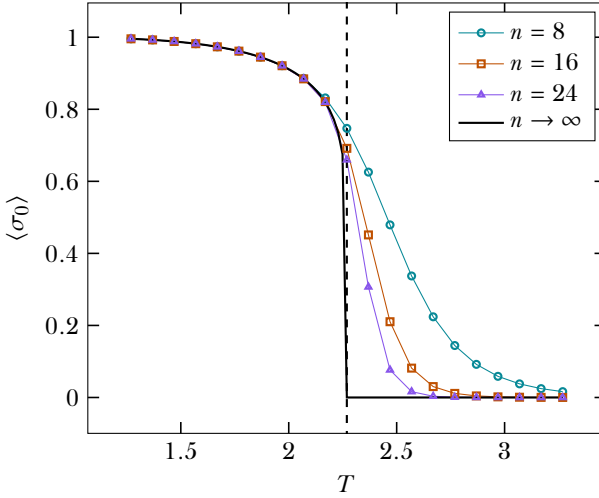


Figure 1.1: The magnetization of the central spin for small lattices with boundary spins fixed to +1. The black line is the exact solution in the thermodynamic limit.

These corrections, of course, do depend on boundary conditions.

Equation 1.2 is valid only outside the critical region precisely because  $F(T, N)$  is analytic *everywhere*, and  $f_\infty(T)$  is only analytic away from the critical point.

The behaviour of  $F(T, N)$  (and hence, all thermodynamic quantities) at criticality is approached is described by *finite-size scaling*.

### 1.3.1 Finite-size scaling

Figure 1.1 shows the behaviour of the order parameter obtained by exact diagonalization of the partition function of small lattices. It is clear that far from the critical point, the order parameter is essentially not dependent on system size, while in critical region there are significant deviations from the thermodynamic behaviour.

One can now define two characteristic temperatures [5, 1]. The first being the cross-over temperature  $T_X$  at which finite-size effects become important,

which is predicted to scale as

$$|T_X - T_c| \propto N^{-\theta}. \quad (1.4)$$

$\theta$  is called the cross-over or rounding exponent.

The second characteristic temperature is the pseudocritical temperature, denoted by  $T^\star$ . It can be defined in several ways, one being the point where the order parameter becomes almost zero, or the point where the heat capacity

$$C = T^2 \frac{\partial^2 F}{\partial T^2} \quad (1.5)$$

reaches its maximum.  $T^\star$  can be regarded as the point where the finite system in some sense comes closest to undergoing a transition.

Generally  $T^\star$  will not equal  $T_X$ . Furthermore,  $T^\star$  depends on boundary conditions: periodic or fixed boundary conditions will nudge the system into an ordered state, therefore  $T^\star > T_c$ . Free boundary conditions will cause the system to favor disorder and the pseudocritical temperature to be lowered.

In any case, it is predicted that

$$|T^\star - T_c| \propto N^{-\lambda}. \quad (1.6)$$

It is generally accepted that [1]

$$\lambda = \theta. \quad (1.7)$$

Furthermore, if one assumes that finite-size effects become important once the correlation length of the system becomes of order of the system size, i.e. [5]

$$\xi(T_X(N)) \propto N, \quad (1.8)$$

then the correlation length exponent  $\nu$ , given by

$$\xi(T) \propto |T - T_c|^{-\nu} \quad (1.9)$$

is, by using Equation 1.4, related to  $\theta$  as

$$\theta = \frac{1}{\nu}. \quad (1.10)$$

### 1.3.1.1 The finite-size scaling ansatz

The behaviour of a system of finite size  $N$  is expected to be a function of the ratio

$$y = \frac{N}{\xi(T)}, \quad (1.11)$$

where  $\xi(T)$  is the correlation length of the thermodynamic system [6].

Footnote about systems that are not completely finite, but finite in one direction.

With the assumption in Equation 1.8, this means that in the limit  $y \gg 1$ , we expect to see thermodynamic behaviour, while for  $y \ll 1$ , the finite system size should enter in the analysis.

To see exactly how this happens, consider as an example the order parameter  $M$ , which in the thermodynamic limit, close to the critical point obeys

$$M(T) \propto \begin{cases} (-t)^\beta & \text{if } T \leq T_c, \\ 0 & \text{if } T \geq T_c, \end{cases} \quad (1.12)$$

where we have defined the reduced temperature

$$t = \frac{T - T_c}{T_c}. \quad (1.13)$$

Assuming the correlation length diverges algebraically

$$\xi(T) \propto |t|^{-\nu}, \quad (1.14)$$

for  $T < T_c$  we have

$$M(T) \propto \xi(T)^{-\beta/\nu}. \quad (1.15)$$

The *finite-size scaling ansatz* now says that for finite systems

$$M(T, N) = N^{-\beta/\nu} \mathcal{F}(y), \quad (1.16)$$

with the requirement that for  $N \rightarrow \infty$ , it should reproduce the thermodynamic behaviour in Equation 1.15, leading to

$$\lim_{y \rightarrow \infty} \mathcal{F}(y) \propto y^{\beta/\nu}. \quad (1.17)$$

At the critical point, however, the bulk correlation length diverges and the only relevant length scale is  $N$ , so that we must have

$$M(T = T_c, N) \propto N^{-\beta/\nu}, \quad (1.18)$$

from which it follows that

$$\lim_{y \rightarrow 0} \mathcal{F}(y) = \text{const.} \quad (1.19)$$

### 1.3.1.2 Extracting exponents from numerical simulation

To extract critical exponents from (finite) numerical simulations, Equation 1.16 may be written as

$$M(T, N) = N^{-\beta/\nu} \mathcal{G}(tN^{1/\nu}) \quad (1.20)$$

where it is used that (per Equation 1.14)

$$y = \frac{N}{\xi(T)} \propto t^\nu N, \quad (1.21)$$

and the new scaling function is customarily written as having argument  $tN^{1/\nu} = (t^\nu N)^{1/\nu}$ .

The critical exponents  $\beta$  and  $\nu$  and the critical temperature can now be extracted by asserting that the numerical data for different system sizes should collapse on a single curve

$$\mathcal{G}(tN^{1/\nu}) = M(T, N)N^{\beta/\nu}. \quad (1.22)$$

The authors of [7] propose a measure of the fitness  $P(\beta, \nu, T_c)$  of such a data collapse

$$P(\beta, \nu, T_c) = \frac{1}{\mathcal{N}_{\text{overlap}}} \sum_p \sum_{j \neq p} \sum_{i_{\text{overlap}}} |M(t_{ij}, N_j)N_j^{\beta/\nu} - \mathcal{E}_p(t_{ij}N_j^{1/\nu})|, \quad (1.23)$$

where for each system size  $N_p$ , the data points collected for the other system sizes  $N_j$  that overlap (that is, fall between any two data points collected for  $N_p$ ) are compared with the interpolation  $\mathcal{E}_p(t_{ij}N_j^{1/\nu})$  between those two data points.  $\mathcal{N}_{\text{overlap}}$  is the number of overlapping pairs.

It is clear that

$$P(\beta, \nu, T_c) \geq 0 \quad (1.24)$$

and the optimal values for  $\beta$ ,  $\nu$  and  $T_c$  minimize  $P(\beta, \nu, T_c)$ .

This measure for the data collapse is found, for data collected for this thesis, to work significantly better than other proposed measures such as fitting a polynomial or order 3-8 through all data points.



## 2

### Finite- $m$ scaling in the CTMRG algorithm

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abstract bla bla

Up until now, we have developed our scaling analysis in terms of a finite system size  $N$ . But the approximation of the infinite-system partition function with the CTMRG algorithm depends on two parameters; the system size  $N$  and the bond dimension  $m$ .

A finite bond dimension  $m$  carries a characteristic length scale. Baxter [8], and later Östlund and Rommer [9] (in the context of one-dimensional quantum systems) showed that in the thermodynamic limit, CTMRG and 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 [10, 11]. Hence, thermodynamic quantities obtained from the CTMRG algorithm with finite  $m$ , in the limit  $N \rightarrow \infty$ , 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 3.1 shows the behaviour of the order parameter of the two-dimensional Ising model for systems of finite-size, where the result is converged in  $m$ , and for systems of finite  $m$ , where the result is converged in the system size  $N$ . The results look very similar and support the claim that there are two relevant length scales in the critical region, namely the system size  $N$  and the length scale associated to the finite bond dimension  $m$ .

#### 2.1 Definition of the effective length scale in terms of the correlation length at $T_c$

The first direct comparison of finite-size scaling in the system size  $N$  with scaling in the bond dimension of the CTMRG method  $m$  was done in [12].

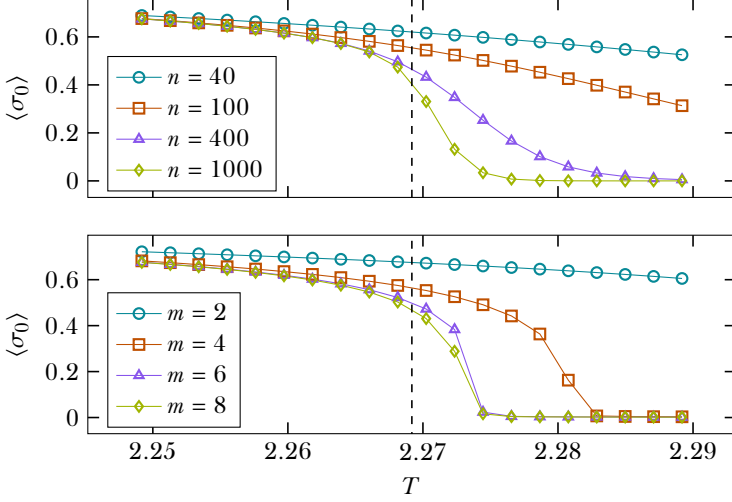


Figure 2.1: Upper panel: expectation value of the central spin  $\langle \sigma_0 \rangle$  after  $n$  CTMRG steps.  $m$  is chosen such that the truncation error is smaller than  $10^{-6}$ . Lower panel:  $\langle \sigma_0 \rangle$  for systems with bond dimension  $m$ .

In the thermodynamic limit (corresponding to infinite  $m$  and  $N$ ), we have the following expression for the correlation length of a classical system [13]

$$\xi(T) = \frac{1}{\log\left(\frac{T_0}{T_1}\right)}. \quad (2.1)$$

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

$$\xi(T, m) = N_{\text{eff}}(m) \mathcal{F}(N_{\text{eff}}(m)/\xi(T)) \quad (2.2)$$

with

$$\mathcal{F}(x) = \begin{cases} \text{const} & \text{if } x \rightarrow 0, \\ x^{-1} & \text{if } x \rightarrow \infty. \end{cases} \quad (2.3)$$

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  $t = 0$ .

$$N_{\text{eff}}(m) \propto \xi(T = T_c, m). \quad (2.4)$$

Look ahead to replicating this in results section?

## 2.2 Relation to finite-entropy scaling and the exponent $\kappa$ .

The first numerical evidence of a law for the correlation length at the critical point of the form

$$\xi(m) \propto m^\kappa \quad (2.5)$$

was given by the authors of [14], who found

$$\kappa \approx 1.3 \quad (2.6)$$

for a gapless system of free fermions, using DMRG calculations. Later, using the iTEBD algorithm [15], the authors of [16] presented numerical evidence for such a relation for the Ising model with transverse field and the Heisenberg model, with

$$\kappa_{\text{Ising}} \approx 2, \quad (2.7)$$

$$\kappa_{\text{Heisenberg}} \approx 1.37. \quad (2.8)$$

### 2.2.1 Quantitative theory for $\kappa$

A quantitative theory of the existence of an exponent  $\kappa$  was given in [17]. We reproduce the argument, which is presented in the language of one-dimensional quantum systems, below.

We start by noting that in the critical region, the entanglement of a half-infinite subsystem  $A$  diverges as

$$S_A \propto \mathcal{A}(c/6) \log(\xi), \quad (2.9)$$

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 [18, 19, 20].

Recalling the definition of the entanglement entropy

$$S_A = -\text{Tr}(\rho_A \log \rho_A) = -\sum_{\alpha} \omega_{\alpha} \log \omega_{\alpha}, \quad (2.10)$$

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  $\rho_A$ , is limited by

$$S_A^{\max}(m) = \log m \quad (2.11)$$

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

This is, incidentally, another way to see that DMRG or CTMRG, or any other algorithm which produces ground states with a matrix-product structure have an inherently finite correlation length.

The leading energy correction to the free energy per site of a one-dimensional quantum system at a conformally invariant critical point at finite temperature  $T$  in the thermodynamic limit is [21]

$$f(T) = f_0 + aT^2 + \mathcal{O}(T^3). \quad (2.12)$$

Due to the quantum-classical correspondence, this is equivalent to a two-dimensional classical  $N \times \infty$  lattice with strip width  $N = 1/T$ . This implies also that the correlation length of a critical one-dimensional quantum system at finite temperature cannot diverge and goes as  $\xi \propto 1/T$ . In terms of this finite correlation length, Equation 2.12 is written as

$$f(\xi) = f_\infty + \frac{A}{\xi^2} + \mathcal{O}\left(\frac{1}{\xi^3}\right). \quad (2.13)$$

Empirically, optimized ground states with a matrix-product structure at criticality do not simply maximize their entropy, as they should if we take Equation 2.13 to be true for ground states with a matrix-product structure.

We will now show that Equation 2.13 needs, in fact, an additional term due to the matrix-product structure with finite bond dimension  $m$ .

The ground state with finite correlation length and energy density as in Equation 2.13 has a Schmidt decomposition that in principle can have infinitely many terms

$$|\psi_0\rangle = \sum_{n=1}^{\infty} \lambda_n |\psi_n^L\rangle |\psi_n^R\rangle, \quad (2.14)$$

where  $|\psi_n^L\rangle$  and  $|\psi_n^R\rangle$  are states of the left and right infinite half-chains. Normalization requires

$$\sum_n \lambda_n^2 = 1. \quad (2.15)$$

The ground state with a matrix-product structure with finite bond dimension  $m$  has an additional constraint: its Schmidt decomposition carries only the  $m$   $|\psi_n\rangle$  with largest  $\lambda_n$ . It is written as

$$|\psi_0^{\text{MPS}}\rangle = \frac{\sum_{n=1}^m \lambda_n |\psi_n^L\rangle |\psi_n^R\rangle}{\sqrt{\sum_{n=1}^m \lambda_n^2}}. \quad (2.16)$$

To find the extra energy cost of only keeping the first  $m$  terms in the Schmidt decomposition, note that in the limit of  $m$  large,  $|\psi_0^{\text{MPS}}\rangle$  almost entirely overlaps with  $|\psi_0\rangle$ , hence can be written as

$$|\psi_0^{\text{MPS}}\rangle = \sqrt{1 - \epsilon^2} |\psi_0\rangle + \epsilon |\psi_{\text{ex}}\rangle, \quad (2.17)$$

where  $|\psi_{\text{ex}}\rangle$  is some excited state and  $\epsilon \ll 1$ . This leads to an energy of

$$E_0^{\text{MPS}} = \langle \psi_0^{\text{MPS}} | \hat{H} | \psi_0^{\text{MPS}} \rangle = E_0 + \epsilon^2 (E_{\text{ex}} - E_0), \quad (2.18)$$

with

$$\epsilon^2 = \left( 1 - \langle \psi_0 | \psi_0^{\text{MPS}} \rangle^2 \right) = 1 - \sum_{n=1}^m \lambda_n^2 \equiv P_{\text{res}}(m). \quad (2.19)$$

Here, we have defined the residual probability  $P_{\text{res}}$ , also known as the truncation error, as the part of the spectrum that is thrown away.

If we now assume that  $E_0 - E_{\text{ex}}$  is proportional to the energy gap  $\Delta$ , which scales as [22, 23, 24]

$$\Delta \propto \frac{1}{\xi}, \quad (2.20)$$

we arrive at

$$E_0^{\text{MPS}} = E_\infty + \frac{A}{\xi^2} + \frac{BP_{\text{res}}(m)}{\xi}. \quad (2.21)$$

It is clear that when the correlation length is very large, by Equation 2.9 the entropy and  $P_{\text{res}}(m)$  must be too. So, the third term in Equation 2.21 dominates.

If the correlation length is small, the second term dominates. The correlation length that belongs to the MPS ground state with fixed  $m$  is the optimum that minimizes this expression.

The details of the calculation, which can be found in the supplementary material of [17], depend on the asymptotic form of  $P_{\text{res}}$ , found in [25]. In the limit  $m \rightarrow \infty$ , the correlation is indeed of the form in Equation 2.5 with

$$\kappa = \frac{6}{c \left( \sqrt{12/c} + 1 \right)}, \quad (2.22)$$

which is in good agreement with the values found in [16].

Refer back to chapter on spectrum of CTM

# 3

## Results

---

### 3.1 Abstract

Cite more

We present finite-size scaling results using the corner transfer matrix renormalization group method on two-dimensional classical square lattices [26]. 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 [12]. 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.

### 3.2 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 [12]. 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

$$N = 2n + 1. \tag{3.1}$$

The second length scale is related to the finite bond dimension  $m$ . Baxter [8], and later Östlund and Rommer [9] (in the context of one-dimensional quantum systems) showed that in the thermodynamic limit, CTMRG and

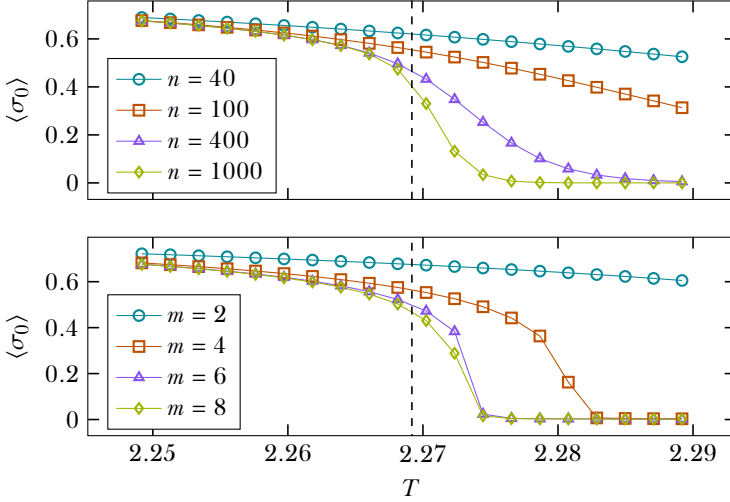


Figure 3.1: Upper panel: expectation value of the central spin  $\langle \sigma_0 \rangle$  after  $n$  CTMRG steps.  $m$  is chosen such that the truncation error is smaller than  $10^{-6}$ . Lower panel:  $\langle \sigma_0 \rangle$  for systems with bond dimension  $m$ .

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 [10]. Hence, thermodynamic quantities obtained from the CTMRG algorithm with finite  $m$ , in the limit  $N \rightarrow \infty$ , 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 3.1 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?

### 3.2.1 Definition of 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 [13]

$$\xi(T) = \frac{1}{\log\left(\frac{T_0}{T_1}\right)}. \quad (3.2)$$

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

$$\xi(T, m) = N_{\text{eff}}(m) \mathcal{F}(N_{\text{eff}}(m)/\xi(T)) \quad (3.3)$$

with

$$\mathcal{F}(x) = \begin{cases} \text{const} & \text{if } x \rightarrow 0, \\ x^{-1} & \text{if } x \rightarrow \infty. \end{cases} \quad (3.4)$$

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  $t = 0$ .

$$N_{\text{eff}}(m) \propto \xi(T = T_c, m). \quad (3.5)$$

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

$$M(T = T_c, m) \propto \xi(T = T_c, m)^{-\beta/\nu}. \quad (3.6)$$

The left panel of Figure 3.2 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

$$M(T = T_c, N) \propto N^{-\beta/\nu}, \quad (3.7)$$

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

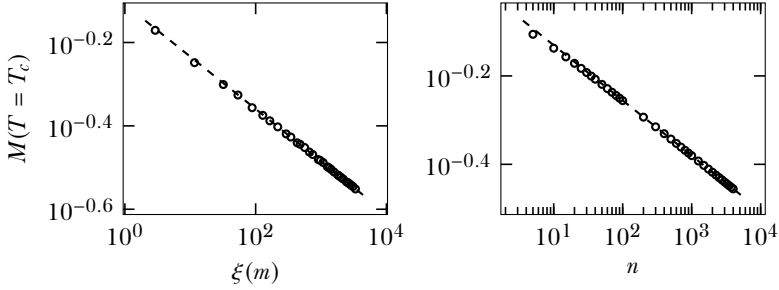


Figure 3.2: Left panel: fit to the relation in Equation 3.6, yielding  $\frac{\beta}{\nu} \approx 0.125(5)$ . The data points are obtained from simulations with  $m = 2, 4, \dots, 64$ . The smallest 10 values of  $m$  have not been used for fitting, to diminish correction terms to the basic scaling law. Right panel: fit to conventional finite-size scaling law given in Equation 3.7.

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 [12] propose a scaling relation for the order parameter  $M$  at the critical temperature of the form

$$M(N, m) = N^{-\beta/\nu} \mathcal{G}(\xi(m)/N) \quad (3.8)$$

with

$$\mathcal{G}(x) = \begin{cases} \text{const} & \text{if } x \rightarrow \infty, \\ x^{-\beta/\nu} & \text{if } x \rightarrow 0, \end{cases} \quad (3.9)$$

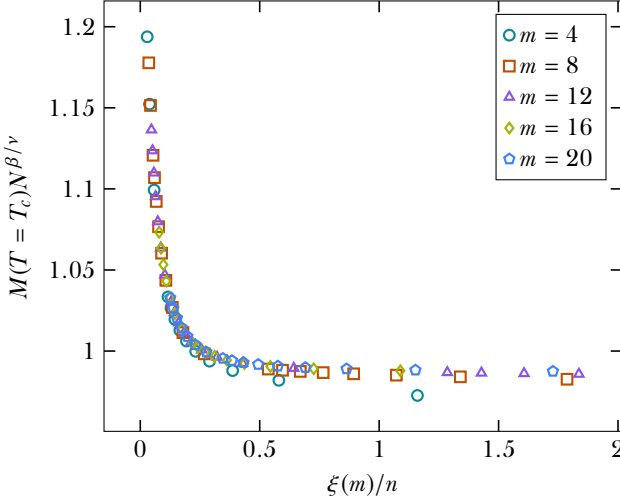


Figure 3.3: Scaling function  $\mathcal{G}(\xi(m)/N)$  given in Equation 3.8.

meaning that Equation 3.8 reduces to Equation 3.7 in the limit  $\xi(m) \gg N$  and to Equation 3.6 in the limit  $N \gg \xi(m)$ . Figure 3.3 shows that the scaling relation of Equation 3.8 is justified.

Figure 3.4 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  $N$ .

### 3.2.2 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 3.8 cannot be used to calculate thermodynamic information. Instead, in the limit  $N \rightarrow \infty$ , we should have

$$M(t, m) \propto \xi(m)^{-\beta/\nu} \mathcal{P}(t\xi(m)^{1/\nu}), \quad (3.10)$$

which is confirmed in Figure 3.5.

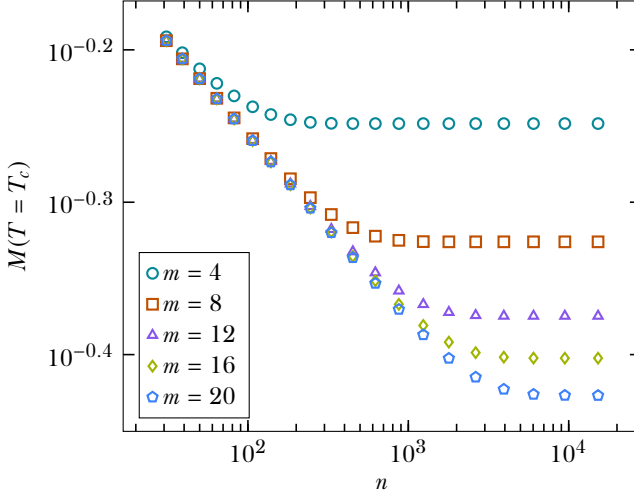


Figure 3.4: Behaviour of the order parameter at fixed  $m$  as function of the number of renormalization steps  $n$ . For small  $n$ , all curves coincide, since the system size is the only limiting length scale. For large enough  $n$ , the order parameter is only limited by the length scale  $\xi(m)$ . In between, there is a cross-over described by  $\mathcal{G}(\xi(m)/N)$ , given in Equation 3.8.

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.

### 3.2.3 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 ??. This is an alternative to the usual approach of studying an order parameter or derivatives of thermodynamical observables (*cite here?*).

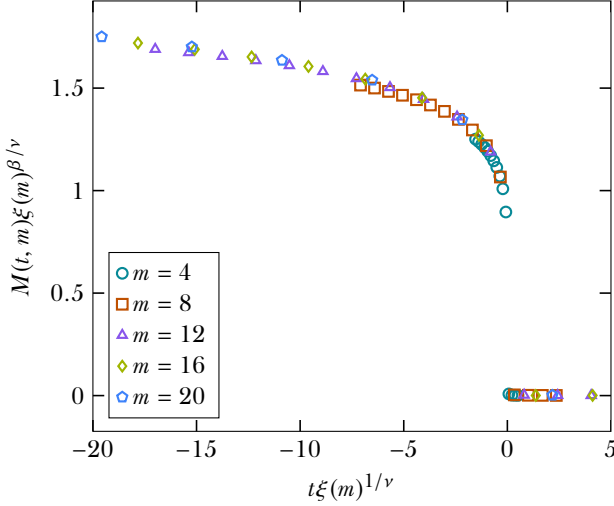


Figure 3.5: Scaling function  $\mathcal{P}(t\xi(m)^{1/\nu})$  in Equation 3.10.

Examples of studies using the spectrum of the corner transfer matrix to analyze two-dimensional classical systems are [27, 28, 29].

- [30]: 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.)
- [31]: for XY and Ising model, proves that next-to-nearest neighbor entanglement peaks at critical point (though not nearest-neighbor entanglement.)

### 3.2.4 Numerical results

We now check the validity of ?? in the context of the CTMRG method for two-dimensional classical systems. Similar checks were done for one-dimensional quantum systems in [16].

Directly checking ?? yields  $\kappa = 1.93$ , see top left panel of Figure 3.6. Under the assumption of ??, we have the following scaling laws at the critical point

$$M(m) \propto m^{-\beta \kappa / \nu} \quad (3.11)$$

$$f(m) - f_{\text{exact}} \propto m^{(2-\alpha)\kappa/\nu} \quad (3.12)$$

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 3.6. Here, we have used  $\beta = 1/8$ ,  $\nu = 1$  and  $\alpha = 0$  for the Ising model.

Tell that the  $\kappa$  law is indeed valid, since it is a good fit.

We may use Equation 2.9 and ?? to check the relation

$$S_{\text{classical}} \propto \frac{c\kappa}{6} \log m, \quad (3.13)$$

which also yields  $\kappa = 1.93$ , where  $c = 1/2$  for the Ising model. See bottom right panel of Figure 3.6.

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

$$S_{\text{classical}} \propto \frac{c}{6} \log \xi(m), \quad (3.14)$$

which yields  $c = 0.501$ , shown in the left panel of Figure 3.7.

The right panel of Figure 3.7 shows the fit to the scaling relation in  $N$  (or, equivalently the number of CTMRG steps  $n$ )

$$S_{\text{classical}} \propto \frac{c}{6} \log N, \quad (3.15)$$

which yields  $c = 0.498$ .

To verify if the point of maximum entropy

$$T^*(m) = \max_T S(T, m) \quad (3.16)$$

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

$$T^* - T_c \propto \xi(m)^{-1/\nu}. \quad (3.17)$$

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 3.8. Here,  $\widetilde{T}_c$  denotes the critical temperature found by minimising the norm of squares of a fit of the form given in Equation 3.17. In finding the position of the pseudocritical 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 3.8.

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 3.17 becomes

$$T^\star - T_c \propto m^{-\kappa/\nu}, \quad (3.18)$$

which yields *values*, shown in the bottom left panel of Figure 3.8.

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

$$T^\star - T_c \propto N^{-1/\nu}, \quad (3.19)$$

yielding *values*. See the bottom right panel of Figure 3.8.

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

### 3.3 To do

Articles to cite:

- [32]: assumes existence of  $\kappa$  and compares finite-size scaling with finite- $m$  scaling for 1D quantum systems with periodic boundary conditions.
- [20]: proves relation for classical eight vertex model

Things to check

- does  $S(T^\star, m) \propto \log \xi(T^\star, m)$  hold?

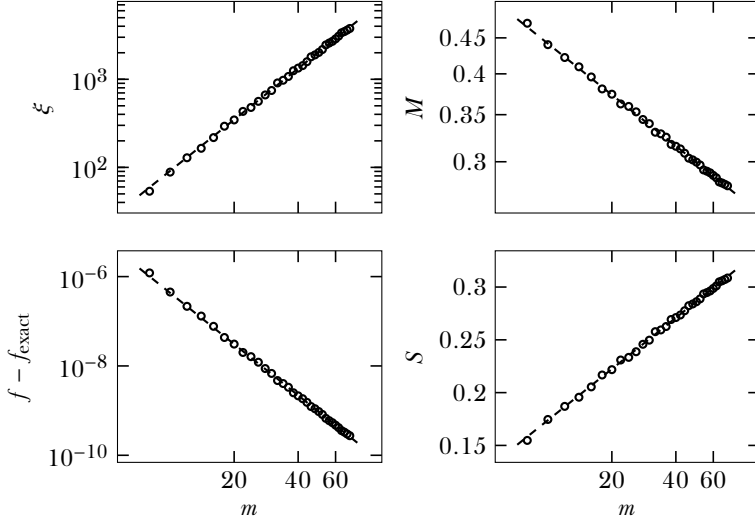


Figure 3.6: Numerical evidence for ??, Equation 3.11, Equation 3.13, yielding, from left to right and top to bottom,  $\kappa = \{1.93, 1.93, 1.90, 1.93\}$ .

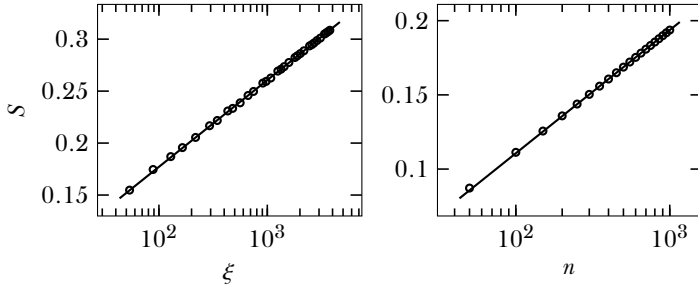


Figure 3.7: Left panel: numerical fit to Equation 3.14, yielding  $c = 0.501$ . Right panel: numerical fit to Equation 3.15, yielding  $c = 0.498$ .



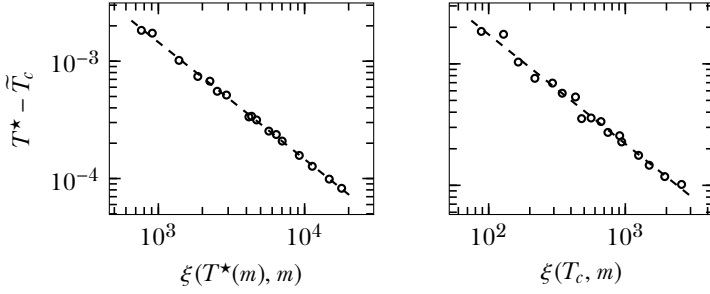


Figure 3.8: Left panel: numerical fit to Equation 3.17 with  $\xi(T^*(m), m)$  used as relevant length scale. Right panel: same fit but using  $\xi(T_c, m)$ , the correlation length at the exact critical point.

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

Plots to make:

- $T^* - T_c$  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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