Monte Carlo Simulations of the 3-State Potts Model in 2D

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Abstract

Populaire Samenvatting

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Introduction

Phase transitions are an everyday part of life, the most well known being the transition of water into water vapor or ice into water. They also occur in more abstract contexts such as networks of neurons.[22]

Although there are some systems that can be exactly solved and thus be studied at the phase transition, many more can not, and thus different methods have to be employed to understand the phase transitions. In this thesis we will use Monte Carlo simulations to study the critical behaviour of the Potts model. We proceed as follows:

In Chapter 1 we consider exactly what properties a phase transitions has. We see that the behaviour of of many thermodynamic properties of a system at criticality can be described by critical exponents. These exponents are closely related to each other. We also consider the two-dimensional Ising model in zero-field, which has been solved exactly and for which the critical exponents are known. Then we have a look at the Potts model, its definition and some conjectures concerning properties of the phase transition.

In Chapter 2 we look at the theory behind simulating lattice systems using Monte Carlo simulations. We define the Metropolis algorithm, what shortcomings it has and how those shortcomings can be amended by using the Wolff algorithm. We also consider some optimizations for the simulations.

Chapter 3 lays out the way to analyze the data obtained from the simulation. Some care has to be taken to use statistically independent measurements. We also look at resampling methods used to calculate properties of the system that depend in a complicated way on the measured quantities. The critical temperature is found by using Binder cumulants, while critical exponents are found using finite size scaling arguments.

In Chapter 4 the results of applying the methods from Chapter 3 are presented for the two-dimensional Ising and Potts models. The measured values for the critical temperatures and exponents agree well with the exact solution (for the Ising model) and other simulation and conjectures (for the Potts model).

In Chapter 5 we summarize the results and give an outlook for further work.

Due to the strong computational component of this project, a significant chunk of code is not included here. A repository containing Python and Cython[1] code as well as the data sets that were generated may be found at `github.com/teunzwart/bachelor-project`, including a basic guide on how to use it.

Set repository to non-private.

Finally I would like to thank my supervisor, dr. Phillipe Corboz, for introducing me into the field of computational physics and patiently explaining statistical analysis of Monte Carlo data. I would also like to thank Edan Lerner for acting as my second assessor.

[1] Cython is a Python module that allows the inclusion of static types and other C features in Python code and converts the resulting code into valid C, which is then normally compiled. Especially for-loop heavy code may become 300 times faster. See `cython.org`

Chapter 1

Models and Critical Phenomena

1.1 Phase Transitions and Critical Phenomena

To determine when a phase transition has taken place, we consider the order parameter. In ferromagnetic systems such as iron, as well as in the systems we will study in this work, this is the magnetization. On one side of the phase transition a non-zero magnetization is present. As the iron is heated, it moves past its Curie temperature and the magnetization does become zero. More generally we consider an order parameter ϕ which is a quantity that is non-zero on one side of the phase transition, and vanished on the other side. Usually the order parameter is zero on the high temperature side of the phase transition. (See fig. 1.1. The Ising model is considered in more detail in section 1.2.) The temperature at which the order parameter becomes zero is the critical temperature T_c.

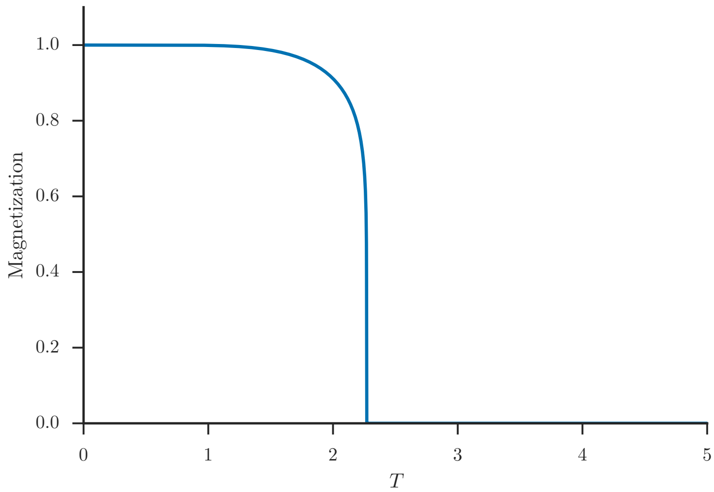

Figure 1.1: The magnetization of the two-dimensional Ising model. Notice how the magnetization is finite on one side of the phase transition, but zero on the other side.

When we consider phase transitions, we distinguish two different kinds. The phase transition associated with freezing water is what is called first-order. As the critical temperature is crossed the water molecules move from a disordered phase into an ordered crystal phase. As this happens, energy is emmited in the form of latent heat. This is defined as

$$l = \int_{T_c-}^{T_c+} c(T)\,\mathrm{d}T, \tag{1.1}$$

with l the latent heat and $c(T)$ the heat capacity of the system. In first order transition the order parameter is discontinous at T_c.[6] In the rest of this work we only consider second-order transitions, for which the latent heat is zero and the order parameter, but not the rate of change of the order parameter is continuous at T_c.

While the latent heat of a transition may be zero, this need not be the case for the heat capacity of the system or other thermodynamic properties such as the magnetic susceptibility. Often the heat capacity diverces as $c \propto |T - T_c|^{-\alpha}$. We call α a critical exponent. Because for continuous phase transitions the latent heat has to vanish by definition, α has to be smaller than 1, because otherwise the integral of eq. (1.1) diverges. No divergence occurs if $\alpha < 0$. In the limiting case that $\alpha = 0$, we can consider the divergence of the specific heat to be logarithmic since

$$\log\left(\frac{1}{x}\right) = \lim_{\alpha \to 0+} \frac{1}{\alpha}\left(x^{-\alpha} - 1\right), \tag{1.2}$$

where $x = |T - T_c| / T_c$. Theoretically and experimentally we find that the exponent governing divergence is the same both above and below T_c.[6]

1.1.1 Correlation Functions

For the systems we would like to consider it is often interesting to quantify how different parts of system relate to each other. In fact we will see that this correlation proves critical when choosing an appropriate algorithm to numerically study systems around the critical temperature (section 2.2.1). To quantify the correlations in a system we define the two-point correlation function[6], which, to illustrate some properties of the correlation function, we first define for a system of spins:

$$G^{(2)}(\mathbf{i}, \mathbf{j}) = \langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle. \tag{1.3}$$

Here $\mathbf{i}$ and $\mathbf{j}$ are the position vectors of the spins at locations i and j respectively. The angle brackets denote thermal averaging. Because the system is often translationally invariant as well as isotropic, meaning it has no preferred direction, such as in a crystal lattice or in disordered systems, $G^{(2)}$ often depends only on $|\mathbf{i} - \mathbf{j}|$

In the general case the two-point correlation function is defined as

$$G^{(2)}(r) = \langle \boldsymbol{\phi}(0) \cdot \boldsymbol{\phi}(\mathbf{r}) \rangle, \tag{1.4}$$

where ϕ is the order parameter of the system. Below T_c the system is ordered and $G^{(2)}$ is large for all r. In the example using spins given above, this means almost all spins are aligned. A more useful quantity in this case is the connected correlation function

$$G_c^{(2)} = \langle \boldsymbol{\phi}(0) \cdot \boldsymbol{\phi}(\mathbf{r}) \rangle - \left|\langle \phi \rangle\right|^2. \tag{1.5}$$

By subtracting the thermally averaged value of the order parameter from the two-point correlation function, we can ignore the general alignment of the order parameter and only have fluctuations in the order parameter contribute.

When T/T_c is either large or small $G_c^{(2)}$ is small. Precisely at the critical temperature $G_c^{(2)}$ has the form

$$G_c^{(2)} \propto \frac{1}{r^{d-2+\eta}}, \tag{1.6}$$

with d the dimensionality of the system and η another critical exponent. Far away from T_c $G_c^{(2)}$ can not be approximated by a power law, but for $|T - T_c|/T_c \ll 1$ $G_c^{(2)}$ has the form

$$G_c^{(2)} \propto \frac{e^{-r/\xi}}{r^{d-2+\eta}}. \tag{1.7}$$

ξ denotes the correlation length. Fluctuations of the order parameter up to this length scale are common, but larger fluctuations are exponentially suppressed. The correlation length diverges as T_c is approached from above or below, according to

$$\xi \propto |T - T_c|^{-\nu}, \tag{1.8}$$

where ν is another critical exponent.

1.1.2 Scaling Laws

We can define three other critical exponents. For the magnetic susceptibility we have

$$\chi \propto |T - T_c|^{-\gamma}, \tag{1.9}$$

while for the magnetization of a system we have

$$m \propto |T - T_c|^{\beta} \qquad \mathrm{T} \to \mathrm{T_c} \text{ from below.} \tag{1.10}$$

Finally we can define a critical exponent for the magnetization in a non-zero magnetic field (the previous five critical exponents assumed $B = 0$). Precicesly at T_c

$$m \propto B^{1/\delta} \qquad \mathrm{B} \to 0. \tag{1.11}$$

These six critical exponents are not independent of each other but are related through scaling laws. Given these scaling laws only two critical exponents need to be known to determine all others as well. They are:

$$\alpha + 2\beta + \gamma = 2 \tag{1.12}$$
$$\alpha + \beta(\delta + 1) = 2 \tag{1.13}$$
$$(2 - \eta)\nu = \gamma \tag{1.14}$$
$$\nu d = 2 - \alpha, \tag{1.15}$$

with d the dimensionalty of the system.[3, 6, 14]

1.1.3 Universality

One property of critical phenomena that simplifies their study is the concept of universality. This is the independence of many thermodynamic properties on the exact details of the hamiltonian of the system. They will only depend on the dimensionality of the system and symmetries of the Hamiltonian Consider the hamiltonian

$$H(s) = H_0(s) + \lambda H_1(s), \tag{1.16}$$

where s denotes the state of the system, H_0 is a part with a given symmetry, and H_1 does not have that symmetry. The critical exponents then only depend on λ in that they have one value when $\lambda = 0$ and another when $\lambda \neq 0$. This also means that, if both H_0 and H_1 have the same symmetries, then, if H_0 is some simple hamiltonian while H_1 is more complicated, it is possible to obtain the critical exponents of a system using the simple part while stripping the more complicated part. This may significantly ease the determination of critical exponents when performing simulations. Different systems with the same critical exponents are said to be in the same universality class. It is believed (and experimentally established with error) that such diverse systems as carbon dioxide, xenon and the three-dimensional Ising model are in the same universality class.[3]

1.2 The Two-Dimensional Ising Model

To validate methods to determine critical exponents for systems that are not exactly solvable, a control system that is exactly solved is useful. To that end we study the two-dimensional Ising model in zero-field, first solved exactly in 1944 by Lars Onsager.[18] It describes a square lattice with nearest neighbour interactions, where each lattice point has with it associated a number (which we will refer to as spin) which may either be +1 or -1 and was originally meant as a model for magnets. The Hamiltonian in zero-field is[15]

$$H = -J_1 \sum_{j=1}^{\mathcal{M}} \sum_{k=1}^{\mathcal{N}} \sigma_{j,k}\sigma_{j,k+1} - J_2 \sum_{j=1}^{\mathcal{M}} \sum_{k=1}^{\mathcal{N}} \sigma_{j,k}\sigma_{j+1,k}, \tag{1.17}$$

with $\mathcal{M}$ and $\mathcal{N}$ the extent of the lattice in the x- and y-directions respectively and J_1 and J_2 the interaction strength between neighbours in respectively the x- and y-directions. In the case where the interaction strength in both directions is the same the Hamiltonian becomes[17]

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j, \tag{1.18}$$

where the bracket denotes summation over nearest neighbours.[1] In the ferromagnetic ground state ($J > 0$) all spins on the lattice are aligned in one of two possible directions (the direction is chosen when the mirror symmetry in the lattice plane is spontaneously broken as the lattice cools). The Hamiltonian is subject to toroidal boundary conditions in both directions, meaning $\sigma_{1,k} = \sigma_{\mathcal{M}+1,k}$ and $\sigma_{j,1} = \sigma_{j,\mathcal{N}+1}$. We are interested in the thermodynamic properties of the Ising Model. To that end we define the partition function

$$\begin{aligned} Z &= \sum_{\sigma=\pm 1} e^{-\beta H} && (1.19) \\ &= \sum_{\sigma=\pm 1} \prod_{j=1}^{\mathcal{M}} \prod_{k=1}^{\mathcal{N}} e^{\beta J_1 \sigma_{j,k}\sigma_{j,k+1}} \prod_{j=1}^{\mathcal{M}} \prod_{k=1}^{\mathcal{N}} e^{\beta J_2 \sigma_{j,k}\sigma_{j+1,k}}, && (1.20) \end{aligned}$$

with $\beta = 1/k_B T$ and the sum running over every possible orientation of the spins on the lattice. Solving this requires a non-trivial amount of effort and it is best to refer to either Onsager[18], who systemically added one-dimensional Ising models together to create a two dimensional lattice, or Kasteleyn as described in [15], whose approach considerably simplifies the derivation by reducing it to a combinatorial problem.

[1] Note that naively applying this Hamiltonian to calculate the lattice energy overcounts the energy by a factor of 2 since each bond is counted twice.

The derivation introduces a sign ambiguity in Z which takes some additional care to resolve, but we can avoid having to deal with this by considering the free energy F in the thermodynamic limit[2] instead of the partition function

$$\begin{aligned} F &= -\frac{1}{\beta} \lim_{\substack{\mathcal{N}\to\infty \\ \mathcal{M}\to\infty}} \frac{1}{\mathcal{M}\mathcal{N}} \log(Z_{\mathcal{M},\mathcal{N}}) \\ &= -\frac{1}{\beta}\Bigg[\log(2) + \frac{1}{2}\frac{1}{(2\pi)^2}\int_0^{2\pi} \mathrm{d}\theta_1 \int_0^{2\pi} \mathrm{d}\theta_2 \log\Bigg(\cosh(2\beta J_1)\cosh(2\beta J_2) \\ &\qquad - \sinh(2\beta J_1)\cos(\theta_1) - \sinh(2\beta J_2)\cos(\theta_2)\Bigg)\Bigg]. \end{aligned} \tag{1.21}$$

F is an analytic function of the temperature T, except at one value, which we will call the critical temperature T_c. At this temperature we can define the equality[15]

$$|z_1| = \frac{1-|z_2|}{1+|z_2|}, \text{ with } z_1 = \tanh(2\beta J_1), z_2 = \tanh(2\beta J_2). \tag{1.22}$$

Rewriting and squaring this gives

$$1 - |z_1 z_2| = |z_1| + |z_2| \rightarrow \tag{1.23}$$

$$\left(1 - z_1^2\right)\left(1 - z_2^2\right) = 4|z_1 z_2| \tag{1.24}$$

Finally, using

$$\frac{1}{2z_k}\left(1 - z_k^2\right) = \frac{1}{\sinh(2\beta J_k)}, \text{ with } k \in \{1, 2\} \tag{1.25}$$

we get the equality

$$1 = \sinh(2\beta J_1)\sinh(2\beta J_2). \tag{1.26}$$

In the case where interaction strength in both the x- and y-directions is the same ($|J_1| = |J_2| = J$) we get an expression for the critical temperature in terms of the bond energy

$$1 = \sinh(2\beta J) \rightarrow \tag{1.27}$$

$$k_B T_c = \frac{2}{\operatorname{asinh}(1)} J = \frac{2}{\log\left(1+\sqrt{2}\right)} J \approx 2.269J \tag{1.28}$$

Onsager [18] also calculated the values of the free energy, internal energy and entropy at the critical temperature[3]:

$$-\frac{f_c}{k_B T} = \frac{1}{2}\log 2 + \frac{2}{\pi} G \approx 0.929, \tag{1.29}$$

$$u_c = -\sqrt{2}J \approx -1.414J, \tag{1.30}$$

$$\frac{s_c}{k_B} = \log\left(\sqrt{2}e^{2G/\pi}\right) - \sqrt{2}\frac{J}{k_B T} \approx 0.306 \tag{1.31}$$

with G Catalan's constant.[4]

[2] This is the limit in which the number of particles on the lattice tends to infinity.

[3] We use lowercase letters to denote the thermodynamic properties of a single spin on the lattice and uppercase letters when refering to the entire lattice. Taking as an example the internal energy, $U/N = u$ with N the number of spins on the lattice.

[4] $G = 1^{-2} - 3^{-2} + 5^{-2} - 7^{-2} + \ldots \approx 0.916$

1.2.1 Thermodynamic Properties of the Two-Dimensional Ising Model

From the free energy it is relatively simple to determine the specific heat per spin and the internal energy per spin by taking the appropriate derivatives of the free energy[15]. We work with the isotropic case where $|J_1| = |J_2| = J$ and $z_1 = z_2 = z = \tanh(\beta J)$, corresponding to eq. (1.18). Then the expression for the free energy becomes

$$\begin{aligned} F = -\frac{1}{\beta}\Bigg[&\log\Big(2\cosh^2(\beta J)\Big) + \log\Big(1+z^2\Big) \\ &+ \frac{1}{2\pi^2}\int_0^{\pi} \mathrm{d}\theta_1 \int_0^{\pi} \mathrm{d}\theta_2 \log\Big(1 - \frac{1}{2}k\Big\{\cos(\theta_1)+\cos(\theta_2)\Big\}\Big)\Bigg], \end{aligned} \tag{1.32}$$

with

$$k = \frac{4z(1-z^2)}{(1+z^2)^2} = \frac{2\sinh(2\beta J)}{\cosh^2(2\beta J)}. \tag{1.33}$$

Performing the substitutions $\omega_1 = \frac{1}{2}(\theta_1+\theta_2)$ and $\omega_2 = \frac{1}{2}(\theta_1-\theta_2)$ and integrating over ω_1 the free energy becomes

$$F = -\frac{1}{\beta}\left[\log(2\cosh(2\beta J)) + \frac{1}{\pi^2}\int_0^{\frac{\pi}{2}} \mathrm{d}\omega_1 \int_0^{\frac{\pi}{2}} \mathrm{d}\omega_2 \log(1 - k\cos(\omega_1)\cos(\omega_2))\right] \tag{1.34}$$

$$= -\frac{1}{\beta}\left[\log\Big(\sqrt{2}\cosh(2\beta J)\Big) + \frac{1}{\pi}\int_0^{\frac{\pi}{2}} \mathrm{d}\omega \log\left(1 + \Big\{1 - k^2\cos^2(\omega)\Big\}^{\frac{1}{2}}\right)\right] \tag{1.35}$$

We will take derivatives from this expression to determine expressions for thermodynamic properties. The internal energy per spin is

$$u = \frac{\partial \beta F}{\partial \beta} \tag{1.36}$$

$$= -2J\tanh(2\beta J) + k\frac{\mathrm{d}k}{\mathrm{d}\beta}\frac{1}{\pi}\int_0^{\frac{\pi}{2}} \mathrm{d}\omega \frac{\sin^2(\omega)}{\Delta(1+\Delta)} \tag{1.37}$$

with

$$\Delta = \Big(1 - k^2\sin^2(\omega)\Big)^{\frac{1}{2}}. \tag{1.38}$$

Note that the argument of the integral in eq. (1.36) can be rewritten as

$$\frac{\sin^2(\omega)}{\Delta(1+\Delta)} = \frac{(1-\Delta)\sin^2(\omega)}{\Delta(1-\Delta^2)} = \frac{1}{k^2}\left(\frac{1}{\Delta} - 1\right), \tag{1.39}$$

from which it follows that

$$u = -2J\tanh(2\beta J) + \frac{1}{\pi}\frac{1}{k}\frac{\mathrm{d}k}{\mathrm{d}\beta}\left[K(k) - \frac{\pi}{2}\right]. \tag{1.40}$$

Here $K(k)$ is the complete elliptic integral of the first kind

$$K(k) = \int_0^{\frac{\pi}{2}} \frac{\mathrm{d}\phi}{\Big(1 - k^2\sin^2(\phi)\Big)^{\frac{1}{2}}}. \tag{1.41}$$

Taking the derivative of k

$$\frac{1}{k}\frac{\mathrm{d}k}{\mathrm{d}\beta} = \frac{2J}{\tanh(2\beta J)}(1 - 2\tanh^2(2\beta J)), \tag{1.42}$$

the internal energy per spin becomes (see fig. 1.2 for a plot)

$$u = \frac{-J}{\tanh(2\beta J)}\left[1 + \frac{2}{\pi}\left\{2\tanh^2(2\beta J) - 1\right\}K(k)\right]. \tag{1.43}$$

For the specific heat per spin we take the derivative of the internal energy per spin with respect to the temperature

$$c = \frac{\partial u}{\partial T} = \frac{-1}{k_B T^2}\frac{\partial u}{\partial \beta} \tag{1.44a}$$

$$\begin{aligned} &= \frac{J}{k_B T^2}\left[\frac{-2J}{\cosh^2(2\beta J)}\left\{1 + \frac{2}{\pi}\left(2\tanh^2(2\beta J) - 1\right)K(k)\right\}\right] \\ &+ \frac{16}{\pi}\frac{J}{\tanh^2 2\beta J}K(k) + \frac{2}{\pi}\frac{\left(2\tanh^2(2\beta J) - 1\right)}{\tanh(2\beta J)}\frac{\mathrm{d}k}{\mathrm{d}\beta}\frac{\mathrm{d}K(k)}{\mathrm{d}k}. \end{aligned} \tag{1.44b}$$

For the derivative of the elliptic integral we use the identity[15]

$$\frac{\mathrm{d}K(k)}{\mathrm{d}k} = \frac{1}{kk'^2}\left[E(k) - k'^2 K(k)\right], \tag{1.45}$$

where $E(k)$ is the complete elliptic integral of the second kind

$$E(k) = \int_0^{\frac{\pi}{2}} \mathrm{d}\phi \left(1 - k^2\sin^2(\phi)\right)^{\frac{1}{2}}, \tag{1.46}$$

and $k'^2 = 1 - k^2$. Using eq. (1.42) and eq. (1.46) the expression for the specific heat per spin becomes (see fig. 1.2 for a plot)

$$c = k_B\left[\frac{\beta J}{\tanh(2\beta J)}\right]^2 \frac{2}{\pi}\left[2K(k) - 2E(k) - \left(1 - k'\right)\left\{\frac{\pi}{2} + k'K(k)\right\}\right]. \tag{1.47}$$

1.2.2 The Ising Model around T_c

Given that we would like to know how the Ising model behaves around T_c, we need to expand the expressions for the internal energy and the heat capacity around this temperature. When $T \approx T_c$ the argument k as defined in eq. (1.33) of the elliptic integrals in the definitions eq. (1.43) and eq. (1.47) becomes approximatly 1. More precisily

$$k \approx 1 - 4\beta_c^2 J^2(\frac{T}{T_c} - 1)^2, \tag{1.48}$$

$$k' \approx 2\sqrt{2}\beta_c J(\frac{T}{T_c} - 1) \tag{1.49}$$

with $\beta_c = \frac{1}{k_B T_c}$. It is obvious that for $k = 1$ $E(k) = 1$ whereas $K(1)$ diverges since the integral becomes

$$\int_0^{\frac{\pi}{2}} \frac{1}{\cos\theta}\,\mathrm{d}\theta \to \infty \tag{1.50}$$

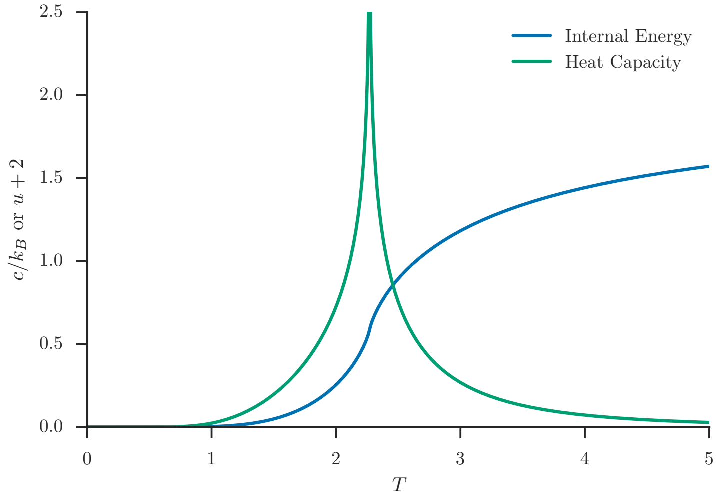

Figure 1.2: The internal energy per site and the specific heat per site of the two-dimensional Ising model in zero-field. Notice the divergence of the specfic heat around $T = T_c \approx 2.269$, which is cutoff in this graph due to the limited resolution.

Nevertheless an approximation around $k = 1$ yields $K(k) \approx \log\left(\frac{4}{k'}\right)$.

At T_c the internal energy per spin u does not diverge and has the value

$$u(T_c) = \frac{-J}{\tanh(2\beta_c J)} = -\sqrt{2}J. \tag{1.51}$$

The heat capacity per spin c does diverge. Using the previous expansions

$$\frac{c(T)}{k_B} \approx \frac{8}{\pi}\left(\beta_c J\right)^2 \left[\log\left(\frac{4}{k'}\right)\right] \tag{1.52}$$

$$= \frac{2}{\pi}\log\left(1+\sqrt{2}\right)^2 \left[-\log\left|\frac{T}{T_c} - 1\right| - 1 - \frac{\pi}{4} - \log\left(\frac{\sqrt{2}}{4}\log\left(1+\sqrt{2}\right)\right)\right] \tag{1.53}$$

and we see c diverging logarithmically as $T \to T_c$. This means that the critical exponents $\alpha = 0$ for the two-dimensional Ising model. When Onsager first solved the model, it also highlighted the first instance of universality. Onsager considered the general case where the interaction energy in the x- and y-directions differed, but the logarithmic divergence depended only on the critical temperature, and not on the ratio J_1 J_2.[3] Note that the sharp phase transition as described here only occurs when the lattice is of infinite extent. When we do not operate in the thermodynamic limit the partition function of the Ising model is analytic for all T and has a maximum but no divergence at T_c.[18]

1.2.3 Magnetization of the Ising Model

Onsager also calculated the magnetization of the Ising model. On the square lattice with $T < T_c$ and $J_1, J_2 > 0$ the magnetization squared is equal to the spin-spin correlation function

$$M^2 = \lim_{N\to\infty} \langle \sigma_{00}\sigma_{0,N}\rangle = \lim N \to \infty \langle \sigma_{00}\sigma_{N,N}\rangle. \tag{1.54}$$

Determining the correlation function is non-trivial, but the result is

$$M^2 = \lim_{N\to\infty} \langle \sigma_{00}\sigma_{0,N} \rangle = \left[\frac{(1-\alpha_1^2)(1-\alpha_2^2)}{(1-\alpha_1\alpha_2)^2}, \right]^{1/4} \tag{1.55}$$

with

$$\alpha_1 = \frac{z_1(1-|z_2|)}{1+|z_2|}, \alpha_2 = \frac{1}{z_1}\frac{1-|z_2|}{1+|z_2|}, \tag{1.56}$$

where we use z_1 and z_2 as defined in eq. (1.23). The magnetization is then (see fig. 1.1 for a plot)

$$M = \left[1 - \left\{\sinh(2\beta J_1)\sinh(2\beta J_2)\right\}^{-2}\right]^{1/4}. \tag{1.57}$$

When we approach the critical temperature from below we can expand around T_c and get

$$M \propto \left[4\beta_c \left\{ \frac{J_1}{\tanh(2\beta_c J_1)} + \frac{J_2}{\tanh(2\beta_c J_2)} \right\} \left\{ 1 - \frac{T}{T_c} \right\} \right]^{1/8}. \tag{1.58}$$

Comparing with eq. (1.10) we see that $\beta = 1/8$.[23]

Finally the magnetic susceptibility can be shown to diverge as $\chi \propto |T - T_c|^{-7/4}$, giving $\gamma = 7/4$. With the earlier result $\alpha = 0$, we can use the scaling laws (section 1.1.2) to determine that $\delta = 15$, $\eta = 1/4$ and $\nu = 1$.[6]

1.3 The Potts Model

The Potts model was first defined by Potts in 1953 as a generalization of the Ising model on the suggestion of Domb, his supervisor.[19] Domb suggested that that to generalize, we can consider the spins of the model to be confined to a plane, with each spin pointing in one of q equally spaced directions, separated by an angle $\theta_n = 2\pi n/q$, with $n = 0, 1, \dots q-1$. The nearest neighbour interaction depend only on the angle between those neighbours. The hamiltonian for this system is

$$H = -\sum_{\langle i,j \rangle} J(\theta_{ij}), \tag{1.59}$$

with $J(\theta)$ a 2π-peridic function and $\theta_{ij} = \theta_i - \theta_j$ the angle between two spins. Domb suggested to use $J(\theta_{ij}) = -\epsilon_1 \cos(\theta_{ij})$. This is now known as the planar Potts model.[23]

Making use of a duality relation which showed that the partition function at a low temperature T was equal to that at a high temperature T^*, $(Z(T) = Z(T^*))$ Potts found the critical temperature for $q = 2, 3, 4$, by assuming that there is exactly one temperature for which $T = T^*$. This method was first used by Kramers and Wannier in 1941[13], to determine the critical temperature of the two-dimensional Ising model three years before Onsager's exact solution.

Potts also gave a formula for the critical temperature of a system with a different interaction strength: $J(\theta_{ij}) = -\epsilon_2\delta(\sigma_i, \sigma_j)$, where δ is the Kronecker delta. For this system he established that for all q the transition ocurres at[19]

$$\frac{x_0}{x_1} = 1 + \sqrt{q}, \tag{1.60}$$

with

$$x_0 = e^{-J_0/k_BT} \qquad \text{for spins in like orientations,} \tag{1.61}$$

$$x_1 = e^{-J_1/k_BT} \qquad \text{for spins in unlike orientations.} \tag{1.62}$$

For $q = 3$ we find that the critical temperature is $T_c = \frac{1}{\log(1+\sqrt{3})} \approx 0.995$.[10] We call this system the standard Potts model. Throughout the rest of this thesis we will mainly consider this model and will simply refer to it as the Potts model. The planar and standard Potts models are related for $q = 2$ by $\epsilon_2 = 2\epsilon_1$ and for $q = 3$ by $\epsilon_2 = \frac{3}{2}\epsilon_1$. For the Potts model in two dimensions the transition at the critical point is first-order for $q > 4$ and second-order for $q \leq 4$.[2, 23] Potts found that an earlier result by Ashkin and Teller for the discontinuities of the energy and specific heat[1], $\Delta E, \Delta C$, could be generalized to show the relationship between those quantities:

$$\sqrt{q}T\Delta E = \log\left(\frac{x_0}{x_1}\right)\Delta E. \tag{1.63}$$

Therefore transitions with a continuos energy exclude the possibility of a discontinuous heat capacity. This does however not mean that the specific heat needs to be finite at T_c.

At the critical temperature the internal energy is[3, 5]

$$u_{\text{average}} = -\left(1 + \frac{1}{\sqrt{q}}\right)J, \tag{1.64}$$

with

$$u_{\text{average}} = \frac{1}{2}(u_c^+ + u_c^-), \tag{1.65}$$

where $u_c^+ = \lim_{T\to T_c^+}\langle u\rangle$ and for a second order transition $u_c^+ = u_c^-$. For $q = 3$ (a second order transition) $u_{\text{average}} = -(1 + \frac{1}{\sqrt{3}})J \approx -1.577J$.

To properly define when the phase transition occurs we define the order parameter, which here is the magnetization, as

$$m = \frac{1}{N}\left|\sum_i^N e^{i2\pi n_i/q}\right|, \tag{1.66}$$

with the sum running over every site of the lattice, N being the number of sites and n_i being the state of the spin at site i. This is based on the definition of the q-state Potts model as consisting of equally spaced vectors. It has the desired properties of being 1 when all spins on the lattice point in the same direction and being 0 when the spins are equally distributed over the possible states.

The Potts model has not been solved exactly, thus we do not know the exact values of the critical exponents. There are however other systems in the same universality class as the Potts model. For $q = 2$ the model reduces to the Ising model and associated exponents (section 1.2.3). For $q = 3$ the model is conjectured to be equal to absorbed monolayers (two-dimensional model), a system that can be probed experimentally and gives $\alpha = 0.36$[5]. It is also suspected that the hard hexagon model (a two-dimensional lattice model describing a gas of non-overlapping spheres, placed on a triangular lattice so no two molecules are adjacent) is in this universality class. This model is exactly solved and has the critical exponents[3, 23]

$$\alpha = \frac{1}{3}, \quad \beta = \frac{1}{9}, \quad \delta = 14, \quad \nu = \frac{5}{6}, \quad \gamma = \frac{13}{9}, \quad \eta = \frac{4}{15}. \tag{1.67}$$

While no exact solution exists, Den Nijs has put forth conjectures for the values of the exponents.[9] We have

$$2-\alpha=\frac{1}{y_t}, \quad 1+\frac{1}{\delta}=\frac{2}{y_h}, \tag{1.68}$$

with the thermal and magnetic exponents:

$$y_t=\frac{3(1-u)}{2-u}, \quad y_h=\frac{(3-u)(5-u)}{4(2-u)}. \tag{1.69}$$

For $q \leq 4$[23]

$$0 \leq u=\frac{2}{\pi}\arccos\left(\frac{\sqrt{q}}{2}\right) \leq 1. \tag{1.70}$$

The critical exponents then become[3, 23]:

$$\begin{aligned}
\alpha &= \frac{2(1-2u)}{3(1-u)}, & \delta &= \frac{(3-u)(5-u)}{1-u}, \\
\beta &= \frac{1}{12}(1+u), & \nu &= \frac{2-u}{3(1-u)}, \\
\gamma &= \frac{u^2-4u+7}{6(1+u)}, & \eta &= \frac{1-u^2}{2(2-u)}.
\end{aligned} \tag{1.71}$$

For $q=3$, $u=1/3$, and these equations reproduce eq. (1.67).

Chapter 2

Simulating Lattice Models

2.1 Markov Processes and Monte Carlo Methods

While some success is to be had by using analytical methods to study lattice models and their critical exponents, often the partition function can not exactly be determined. At that point we can use computer simulation of the models in question to study phase transitions, while having the exactly solved models as a benchmark for these simulations.

We are almost always interested in the value of a thermal average of a quantity:

$$\langle X \rangle = \sum_{\alpha} X_\alpha p_\alpha, \tag{2.1}$$

with $\langle X \rangle$ a thermal average, the sum running over all configurations, each labeled by α, and p_α the Boltzmann probability of state α in equilibrium[6]:

$$p_\alpha = \frac{e^{-\beta E_\alpha}}{\sum_\alpha e^{-\beta E_\alpha}}. \tag{2.2}$$

While for small lattices (e.g. 3 by 3) the number of states is tractable (this number scales as 2^N for the Ising model and q^N for the Potts model), for larger lattices the sum can no longer be performed numerically and some clever way has to be found to sample only important states.

Instead, we randomly choose states distributed according to a probability distribution p_α. If we choose M random states the estimator for the quantity X is

$$X_M = \frac{\sum_{i=1}^{M} Q_{\alpha_i} \frac{1}{p_{\alpha_i}} e^{-\beta E_{\alpha_i}}}{\sum_{j=1}^{M} \frac{1}{p_{\alpha_i}} e^{-\beta E_{\alpha_i}}}, \tag{2.3}$$

which becomes $\langle X \rangle$ when $M \to \infty$. We could set $p_{\alpha_i} = 1$ and choose all states with equal probability. However, often only a few states dominate the sums in eq. (2.3). In a large system we will then sample a huge amount of states that contribute almost nothing to the sums.

To resolve this problem we can use the fact that a physical system samples the states available to it according to the Boltzmann probability . We therefore set p_{α_i} equal to eq. (2.2), after which the estimator becomes

$$X_M = \frac{1}{M} \sum_{i=1}^{M} X_{\alpha_i}. \tag{2.4}$$

This way of sampling is called importance sampling. The states that contribute the most are also sampled most often.

To pick states randomly according to the Boltzmann distribution we use a Markov process.

While specific algorithms are described below, the steps of a simulation are broadly the same. Firstly, to be able to change spins we need to prepare the system in a given state at the start of the simulation. Common choices are to prepare the system in a $T = \infty$ state where all spins are randomly aligned, or $T = 0$ where all spins are pointing in one randomly chosen direction.

After every step of the algorithm, measurements are performed. What we can measure are the magnetization and the energy. The magnetization can be

2.1.1 Ergodicity and Detailed Balance

2.2 The Metropolis Algorithm

The Metropolis algorithm, first published by Metropolis *et al.* in 1953 [16], is a simple algorithm that was first used by its creators to study the dynamics of continuously displaceable hard spheres. The algorithm is as follows[6]:

1. Choose a random site on the lattice.
2. Flip the spin on this location and calculate the change in energy ΔE associated with this spin-flip.
3. Calculate the probability of accepting this move:
$$A = \begin{cases} e^{-\beta \Delta E} & \Delta E > 0 \\ 1 & \Delta E \leq 0 \end{cases} \tag{2.5}$$
4. Generate a random variable r in the interval $[0, 1)$.
5. Accept the move if $r \leq A$. Otherwise leave the lattice as it was.

The spin flip may also happen to a non-random spin simply by iterating over the rows and columns of the lattice. When studying only equilibrium dynamics, the two approaches are identical.[14]

2.2.1 Critical Slowing Down

2.3 The Wolff Algorithm

The Wolff algorithm goes as follows:

1. Choose a random site on the lattice i
2. Look at the neighbours of i. If a neighbour j has the same spin as i, add it to the cluster with probability $P = 1 - e^{-2\beta J}$.
3. Repeat step 2 for spin j until no more spins can be added to the cluster.
4. Flip the entire cluster.

If a spin was considered during a previous step but not added to the cluster, this spin may be reconsidered for future steps. Spins that are already part of the cluster are not added again.[17]

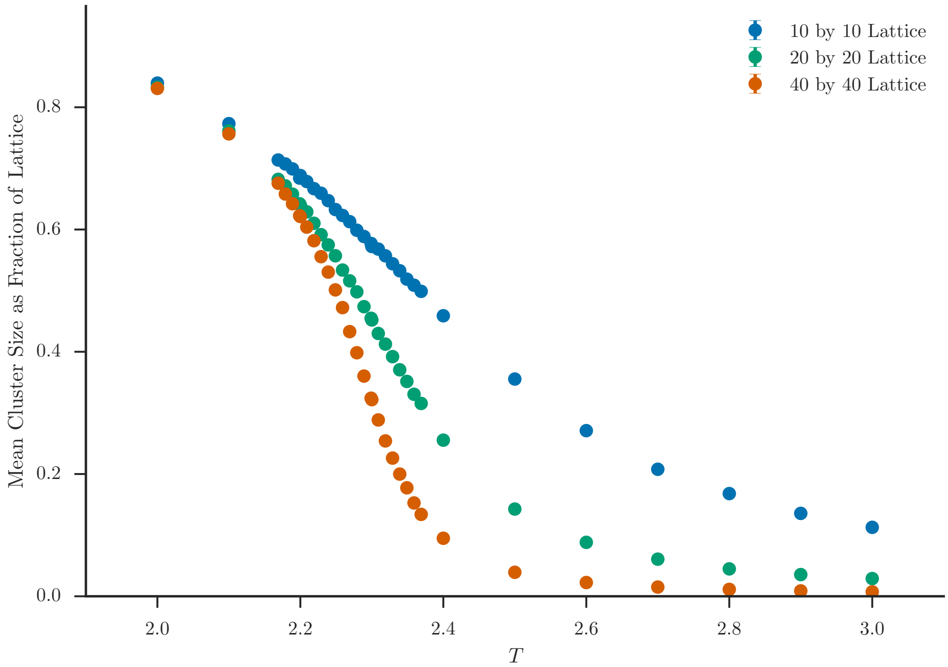

Figure 2.1: The mean size as a fraction of the lattice of clusters generated with the Wolff method. During the simulation the temperature varied from 2 to 3 in steps of 0.1, with a higher resolution from 2.169 to 2.369 in steps of 0.01. The errorbars are too small to see.

2.3.1 Generalizing Algorithms to the Potts Model

Both the Metropolis and Wolff algorithm can be easily generalized to the q-state Potts model. For the Metropolis algorithm we again pick a random spin s in state i. We then pick a new state j from the remaining $q-1$ possible state for that spin such that $s_i \neq s_j$. After that we proceed as described earlier. Just like for the Ising model the algorithm satisfies the ergodicity and detailed balance conditions. For large q more efficient algorithms exist, but for $q = 3$ Metropolis works fine.

Near phase transitions the Potts model also experiences critical slowing down and cluster algorithms are more appropriate. The generalized Wolff algorithm proceeds exactly the same as in the Ising case, with the only difference being that the probability to add a spin to the cluster has become $P_{add} = 1 - e^{-\beta J}$. We can see where this factor of 2 comes from by considering the $q = 2$ Potts model. The Hamiltonian is still

$$H = -J \sum_{\langle ij \rangle} \delta(\sigma_i, \sigma_j), \tag{2.6}$$

but for the two-state model we can rewrite this as

$$H = -\frac{1}{2} J \sum_{\langle ij \rangle} 2(\delta(\sigma_i, \sigma_j) - \frac{1}{2}) - \sum_{\langle ij \rangle} \frac{1}{2} J. \tag{2.7}$$

These expressions are the same except for a constant, since for $\sigma_i = \sigma_j$ $2(\delta(\sigma_i, \sigma_j) - \frac{1}{2}) = +1$ while it is -1 otherwise. We therefore have an interaction energy $\frac{1}{2}J$ instead of J, explaining the change in the addition probability. This algorithm again satisfies detailed balance and ergodicity.[17]

2.4 Optimizations

When working in a programming language that represents data in continuous blocks of memory such as C, helical boundary condition may improve performance.

2.5 Systemic errors

Chapter 3

Analysis of Monte Carlo Simulations

3.1 Statistics

Now that we have obtained measurements for the energy and magnetization of the Ising and Potts models, we need to find a way to make these measurements statistically uncorrelated, since the state of a lattice after a single algorithm sweep may not be very different compared to the state before. We can calculate the autocorrelation times, but an easier and quicker approach is the Binning method.

3.1.1 Binning

The Binning method creates uncorrelated sequences of data from a given correlated output. Consider an original data set $A_i^{(0)}$ with $i = 1, \dots N$ and N the number of data points in the original set. Iteratively combine two consecutive data points into a bin according to

$$A_i^(l) = \frac{1}{2}\left(A_{2i-1}^{(l-1)} + A_{2i}^{(l-1)}\right) \quad \text{with} \quad i = 1, \dots, N_l = \frac{N}{2^l}, \tag{3.1}$$

with l the current binning step. The average in each bin is less correlated with every step while the mean remains the same. The error on a quantity for a given binning step is

$$\Delta A^{(l)} = \sqrt{\frac{\mathrm{Var}(A^{(l)})}{N_l}}. \tag{3.2}$$

As the binning progresses the error for each step converges to the actual error, meaning that in a plot the errors tend to a plateau (fig. 3.1).

From the binning method we can also determine the autocorrelation time:[8]

$$\tau = \frac{1}{2}\left(\frac{\Delta A^{(l_{max})}}{\Delta A^{(0)}} - 1\right) \tag{3.3}$$

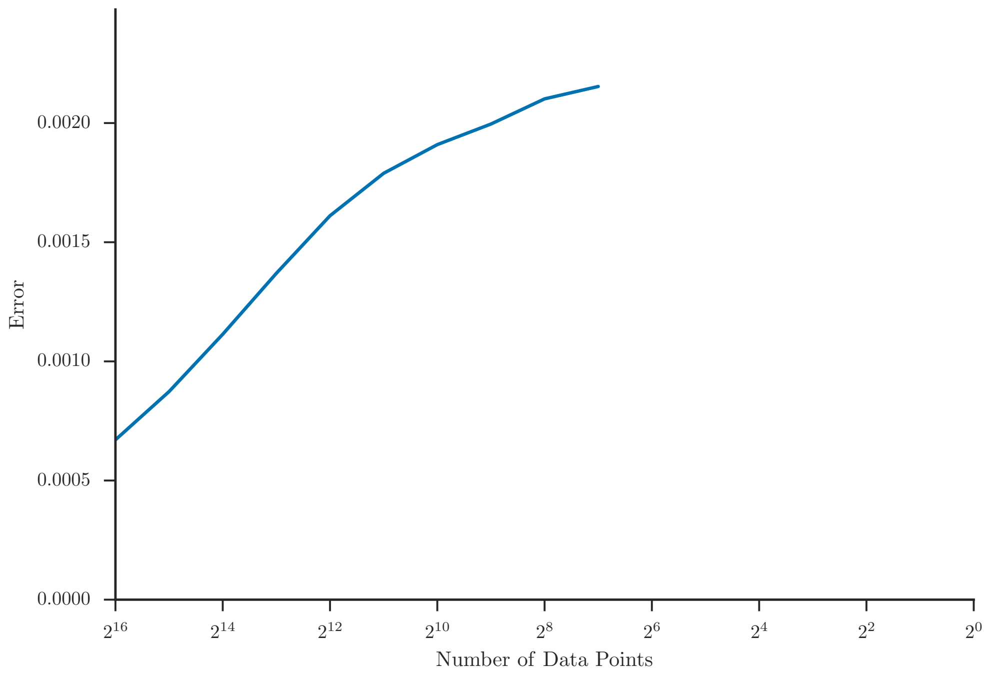

Figure 3.1: The error for the energy per site as a function of the data size. As the binning progresses the error tends to a plateau. A 10 by 10 Ising model was simulated at a temperature of 2, thermalized for 5000 sweeps and then measured for 65536 sweeps.

3.1.2 Bootstrap and Jackknife

Other interesting values we would like to know are functions of measured values. These include the heat capacity c and magnetic susceptibility χ:

$$c = \langle E^2 \rangle, \tag{3.4}$$

$$\chi = \langle m^2 \rangle. \tag{3.5}$$

3.2 The Binder Cumulant

Given these statistically independent measurements, one thing we may like to find is the critical temperature. Unfortunately we can not determine this simply by looking at the order parameter of a system and when it becomes zero, because the finite size of the simulated lattices precludes a sharp phase transition. We can however define the Binder cumulant[4]

$$U_4 = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}, \tag{3.6}$$

which for $L \to \infty$ becomes $2/3$ for $T \to 0$ and 0 for $T \to \infty$.[14] At the critical temperature U_4 has the same value independent of the lattice size. Therefore the critical temperature can be found by plotting the binder cumulant for different lattice sizes and looking for the intersection (as seen in fig. 3.2).

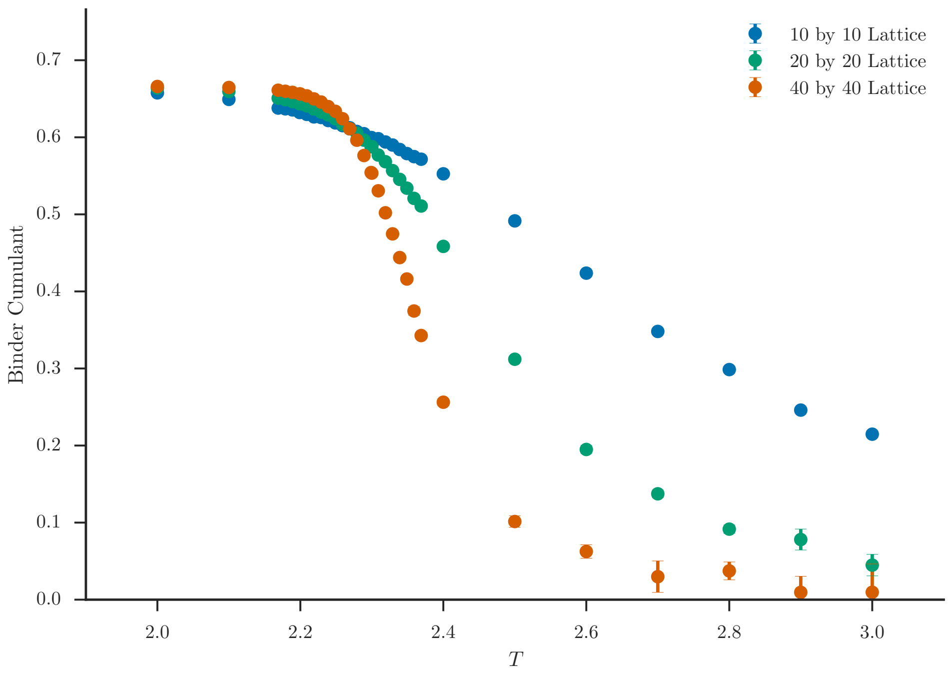

Figure 3.2: The Binder cumulant for the Ising model at three different lattice sizes. The critical point occurs at approximately $T = 2.26$. The values were acquired by simulation the lattice using the Wolff algorithm and running 65536 steps after equilibration. During the simulation the temperature was varied from 2 to 3 in steps of 0.1, with a higher resolution from 2.169 to 2.369 in steps of 0.01. The errorbars are too small to see in this plot.

3.3 Finite Size Scaling

To extract the critical exponents for different models, one way to proceed is to use finites size scaling. The advantage of this method is that T_c does not need to be known in advance, although if a value has already been determined using the Binder cumulant, this can also be used.

We derive finite size scaling for the magnetic susceptibilty. Close to the critical temperature we have $\chi \propto |t|^{-\gamma}$ with $t = (T - T_c)/T_c$ (eq. (1.9)). We also know that for the correlation length $\xi \propto |t|^{-\nu}$ in this region (eq. (1.8)). Therefore we can write $\chi \propto \xi^{\gamma/\nu}$.

For the specific heat and magnetization similair equations can be derived:

$$\widetilde{c}(L^{1/\nu}t) = L^{-\alpha/\nu}c, \tag{3.7}$$

$$\widetilde{m}(L^{1/\nu}t) = L^{\beta/\nu}m. \tag{3.8}$$

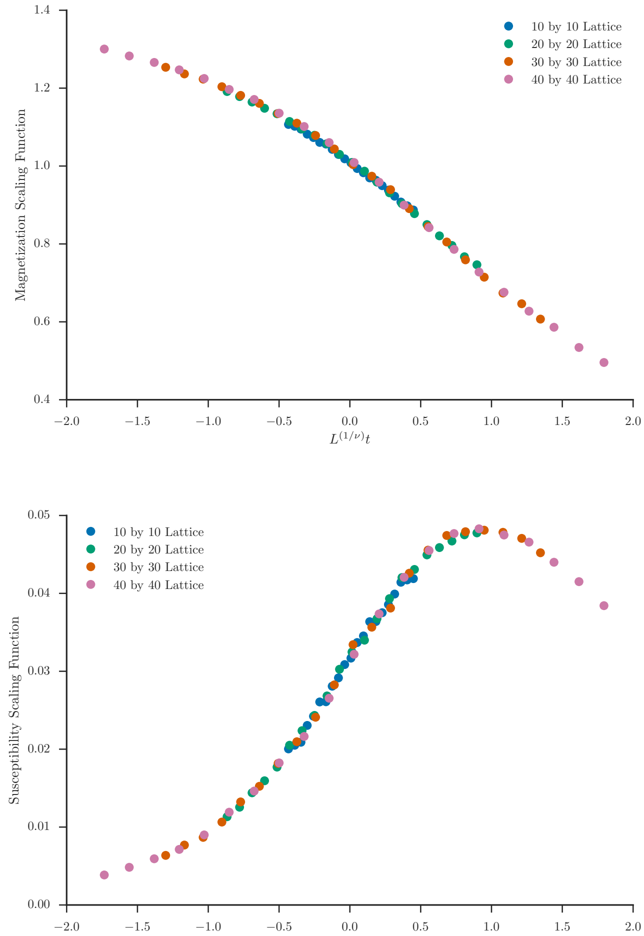

Figure 3.3: Finite size scaling data collapses for the magnetization and the magnetic susceptibility of the Ising model. The exact values for the exponents $\gamma = 7/4$ and $\beta = 1/8$ were used.

Chapter 4

Results

The Binder cumulant intersections were found byThis was also used to find the error Explain

	α	β	γ	η	ν	δ
Den Nijs (1979)[3, 9]	$\frac{1}{3}$	$\frac{1}{9}$	$\frac{13}{9}$	$\frac{4}{15}$	$\frac{5}{6}$	14
Blöte (1981)[7]						
Fan (2007)[10]	0.396(66)	0.108(4)	1.416(62)	0.265(19)	0.816(27)	14.1(1.1)
Ghamei (2001)[11]						
Hu (1980)[12]						
Straley (1973)[21]	0.05(10)	0.103(10)	1.5(1)			

Table 4.1: The critical exponents of the three-state Potts model. The values quoted for Den Nijs are conjectured exact values.

The critical exponent ratio is found by a chi-least-squares test, as suggested by Sandvik[20]

Chapter 5

Conclusions

5.1 Further Work

There are severals way to expand on the work presented here. One way is use renormalization group techniques to calculate the critical exponents. This is the way most papers determine those and has as advantage that the errors on the critical exponents can be better determined.

The Ising and Potts model can also be simulated on different kinds of lattice such as triangular or honeycomb lattices, to verify that the critical exponents (but not the critical temperature) remain the same, thus testing universality.

The autocorrelation times were determined using the data from the binning analysis. The integrated autocorrelation time proved too slow to determine for large datasets. The correlation times could be more accurately investigated and used to establish the occurence of critical slowing down as well as determining the dynamic critical exponents.

It is also possible to go to $q > 4$ and try to determine that the phase transition becomes first order in this case. To that end the latent heat would have to be accurately determined, while also having to deal with phase transitions that are not sharp in finite systems.

The order parameter of the Potts model was in this thesis defined based on the definition of the Potts model. Many papers used a slightly different definition that is does not have the property of being 1 below T_c and 0 above T_c.

Finally the heat-bath algorithm could be used to simulate Potts model with large q more efficiently[17], tying into trying to measure that for $q > 4$ in two-dimensions the transitions is first-order.

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