Simulation studies of gauge theories for superconductivity

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Abstract

Several models of superconductors are examined by means of Monte Carlo simulations. The objective is to investigate a compact gauge theory using a global order parameter, which is done by successively modifying Hamiltonians with known characteristics. Not observing a transition in the real space compact gauge theory, the dual representation is simulated. This representation results in a critical temperature $T_c \approx 2.365$, in agreement with previous results. The critical exponents $\nu$ and $\alpha$ are calculated using the third moment of energy, resulting in $\nu \approx 0.64$ and $\alpha \approx 0.19$ respectively. The exponents are believed to be those of the Ising universality class, wherefore the obtained value of $\alpha$ seems inconsistent with the expected $\alpha = 0.11$, as well as the hyperscaling relation. However, due to difficulties in the determination of $\alpha$, simulations on larger systems might well yield the expected value of the exponent. Lastly, the problem in finding a transition in the gauge theory in real space might be explained by the inability of the order parameter to capture the essential physics.
Acknowledgements

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Chapter 1

Introduction

There are many models describing many different types of superconductors. One such model is the \( U(1) \) compact gauge theory, valid in systems with Hamiltonians that are both invariant under transformations with complex scalars as well as having the property of being confined to a compact subspace of \( \mathbb{R} \). Practical applications of such models are of interest in strongly correlated fermion systems.

From the relatively well known XY model it is possible to formulate a \( \mathbb{Z}_2 \) lattice gauge theory by introducing the Villain approximation and transforming the Hamiltonian to the dual space. In this representation the Hamiltonian can be written in terms of flux lines and monopoles. The dual space is also characterized by an inverted temperature scale compared to the real space model.

Simulations of several models have been carried out, first on descriptions with well known qualities, then on the compact gauge theory both in real and dual space. From Elitzur’s theorem \([1]\) we know that no local order parameter can be used to find a transition in systems with gauge symmetry. In this thesis I use a global order parameter \( m \) in real space simulations of the gauge theory, but find that no transition was observed. However in the dual, Coulomb Gas representation, a transition was easily found and studied using a similar order parameter. In this description it was possible to determine important quantities such as the critical temperature and critical exponents \( \alpha, \nu \) and \( \beta \). Due to inaccuracies, the obtained estimation of \( \alpha \) is somewhat different to the expected value for the \( \mathbb{Z}_2 \) gauge theory. As to the difficulties to find a transition in the real space simulations of the gauge theory, it is evident that its fluctuations are far from well understood at the present.

The thesis is divided into the following chapters:

Chapter 2 introduces some important concepts from the field of statistical mechanics such as the canonical ensemble, scaling theory and order parameters. Some general properties of superconductors are also presented.

In Chapter 3, the different models simulated are introduced by the means of formulating and explaining their respective Hamiltonians. Since the Villain approximation plays such a large part in many of the introduced models, it is studied...
in some detail.

Chapter 4 deals with the process of simulating the models and calculating important thermodynamic quantities. Monte Carlo simulation and the thermal exchange algorithm are two main methods to this end. The third moment of the energy is defined in connection with finding critical exponents.

Chapter 5 presents the results of the main simulations of each model and compares them with previously published results.

The thesis concludes with Chapter 6 with a discussion on future steps that might be taken.
Chapter 2

Theoretical Background

2.1 Introductory Notes on Statistical Mechanics

Statistical mechanics gives a microscopic basis for describing macroscopic properties belonging to the classical field of thermodynamics, such as heat capacity and the free energy. Such a microscopic description is based on statistics and probabilities, hence the name of the field suggesting the fusion of the macroscopic with the microscopic world. A classical macroscopic description, based on pure Hamiltonian mechanics, fails at the atomic level due to the increasing importance of a quantum mechanical description. A pure microscopic description of a system of particles would very rapidly cease to be practical as the number of particles under description increases, even if the physics is approximated as far as possible.

The fundamental object in the statistical mechanical description is the quantum state, which has a classical probability assigned to it, so as to describe how “typical” it is to find that particular state given the necessary parameters. The simplest assumption of the probability densities of the states is that of an identical distribution, i.e. $p_i = \frac{1}{W}$, where $W$ is the number of possible quantum states, this leads to the so called microcanonical ensemble. While this ensemble has proven to be successful in certain areas (especially in paving the way for more complex descriptions!), the major drawback is that it requires the energy of all states to be constant. In all physical cases (where the absolute temperature is nonzero), the energy fluctuates throughout the medium (from now on called the system) by exchange of energy with the environment. A more relevant description of the system is achieved using the canonical ensemble.

In the canonical ensemble, particles are essentially allowed an infinite spectrum of energy levels, with probabilities given by the Boltzmann distribution. Here the probability for a certain state with energy $\mathcal{H}_i$ associated to it depends on its relation to the temperature $T$. This is the “global” temperature, interpreted as the equilibrium temperature of a system that is thermally isolated from its surroundings.
The probability assigned to a state $i$ is defined as:

$$p_i = \frac{e^{-\mathcal{H}_i/kT}}{\sum_j e^{-\mathcal{H}_j/kT}}. \quad (2.1)$$

The parameter $k$ is Boltzmann’s constant. For a given temperature, states occur depending on their energies in such a way that for very low temperatures only the low energy states have a significant probability of being occupied. For higher temperatures, higher energies are more permissible at the same time as the denominator in Eq. (2.1) tends to grow, as low energy states continue to contribute to its value.

### 2.2 Partition Function

In connection with the canonical ensemble it is important to mention the *partition function* $Z$, which is usually interpreted as the link between the quantum state-based description and thermodynamics. Classically, the partition function is defined as:

$$Z = \text{Tr}[e^{-\beta\mathcal{H}}],$$

where $\beta \equiv \frac{1}{kT}$ and $\mathcal{H}$ is the complete Hamiltonian of the system. Thus, in the simple setting above, $Z$ corresponds to the denominator in Eq. (2.1). It is straightforward to show (see for instance Ref. [2]) that the free energy $F$ in the canonical ensemble is given by

$$F = -kT \ln(Z). \quad (2.2)$$

Using thermodynamic differential expressions for the free energies it is then possible to define quantities such as the entropy, pressure, heat capacity and other response functions in terms of $Z$.

In practical cases, $Z$ is far too complicated calculate explicitly as the number of accessible states increases rapidly with temperature.
2.3 Ensemble Averages and Ergodicity

It is often impossible to describe the full dynamics of a system, and one then instead has to be content with calculating averages. In light of the Boltzmann distribution, such an average of an operator $\hat{A}$ in the canonical ensemble be written:

$$\langle \hat{A} \rangle = \frac{1}{Z} Tr[\hat{A} e^{-\beta H}].$$

This type of average is called ensemble average, as it uses probabilities associated with a specific ensemble to calculate averages.

In practical cases such as computer simulation, averages take a different form. The system is observed a finite number of times, $N$, and values of the observable $A$ are recorded as a discrete time series $\{A_1, A_2, ..., A_N\}$. The observed time average of $A$ is then calculated as:

$$\bar{A} = \frac{1}{N} \sum_{i=1}^{N} A_i.$$

It is not always clear that the two averages coincide, even in the limit of an infinite number of observations. However, the ergodic hypothesis states that in the limit of infinite observations, time and ensemble averages are identical. It should be stated that not all systems satisfy ergodicity (for instance some hard spheres systems, see Ref. [3]), but it is usually a very reasonable assumption, used henceforth in the thesis.

2.4 Phase Transitions and Order Parameters

Phase transitions are central phenomena in statistical mechanics. Not only are they observed in the transitions between phases of, for example water in everyday life, they are also exhibited in magnetic materials, structural transitions in the crystal structures of solids, and in superconductors. What most transitions have in common is that for some critical temperature, $T_c$, and/or critical magnetic field, $H_c$, certain quantities change abruptly, allowing for the change from one phase to another. The textbook example of this is the change in the heat capacity while boiling (or freezing) water.

Order Parameters

These parameters are defined to be zero on one side of the transition and finite on the other (often approaching a constant asymptotically). This property makes order parameters very useful in describing the transition itself. One example of an order parameter is the average magnetization, $m$, in a ferromagnet. At low temperatures, the magnetic spins are “frozen” close to the ground state due to the Boltzmann statistics and therefore exhibit a high values of $m$ (when $m = 1$ the system is completely magnetized). As the magnet is heated, the spins have more
freedom and tend to position themselves randomly, thus decreasing the average magnetization which approaches zero as \( T \rightarrow \infty \) for sufficiently large systems. In the example of magnetization, a global symmetry, in this case, rotation symmetry is broken at the critical point.

Phase transitions are labelled in two categories; first and second order transitions.

**First Order Transitions**

First order phase transitions are characterized by a discontinuous order parameter at the phase transition, whose value jumps between those of the two phases. Another property is that the two (or more) phases coexist at \( T_c \). The classic example is water, where the molecules need to climb an energy threshold set by the latent heat. Due to the underlying statistics of the molecules, some molecules will during the transition be able to cross the energy barrier (in either way of course) faster than others.

**Second Order Transitions**

Second order phase transitions are characterized by a continuous order parameter at the phase transition. Some examples here are certain magnetic materials, liquid crystal transitions, as well as transitions in high temperature superconductors. Even if this type of transition is continuous, it is still possible to find a critical temperature at which the transition occurs using an appropriate order parameter.

Thermodynamic averages such as the heat capacity and susceptibility jump at a first order transition, but typically show power law singularities at a second order transition.

### 2.5 Scaling Theory

Computer simulations must be performed on small systems. Often, lattices of length \( L \sim 10 \) up to \( L \sim 100 \) are being simulated. A change in the behaviour of order parameters, and often other quantities that are not strictly order parameters, near the critical temperature is then observed while varying the system size. It is important to attempt extrapolation to macroscopic sizes, referred to as the *thermodynamic limit*, \( L \rightarrow \infty \). In this limit, transitions are characterised by a singular behaviour at \( T_c \). In the finite size case, thermodynamic quantities form continuous curves around \( T = T_c \), systematically diverging as \( L \) increases. Diverging quantities typically follow power laws near the critical temperature.

The most basic quantity that behaves singularly around \( T = T_c \) is the *correlation length*, basically describing how large the sub-cluster of correlated spins is. The correlation length is short in both the ordered and disordered phases. At a second order phase transition the system has fluctuations of all sizes, i.e. the typical size
2.6. **FINITE-SIZE SCALING**

of fluctuations, whose linear dimension is the correlation length $\xi$, diverge at the transition.

The diverging correlation length is given by the following power law:

$$\xi \sim |T - T_c|^{-\nu},$$

(2.3)

where $\nu$ is called the correlation length exponent.

Now consider the Ginzburg-Landau-Wilson Hamiltonian

$$\mathcal{H}(s_i) = \sum_i (a_1 s_i^2 + a_2 s_i^4 + a_3 s_i^6 + ...) + \sum_{<i,j>} b_1 (s_i - s_j)^2 + ...,$$

(2.4)

where $<i,j>$ denotes summation over all nearest neighbour spins $s_i$ and $s_j$. It is possible to obtain a scaling relation of the free energy functional $f_s$ under scaling in the parameters $\{a_1, a_2, a_3, b_1, ...\}$ using renormalization group (RG) theory. One makes use of the fact that the partition function should be invariant under all scale transformations of the system near $T = T_c$. From RG results and Eq. (2.2) we get that the free energy should transform as:

$$f_s(a_1, a_2, a_3, b_1, ...) \sim \lambda^{-d} f_s(a_1 \lambda^{y_1}, a_2 \lambda^{y_2}, a_3 \lambda^{y_3}, b_1 \lambda^{y_4}, ...)$$

(2.5)

under a scale transformation with scale factor $\lambda > 1$ ($d$ is the dimensionality of the system). The critical exponents $y_i$ may be identified, depending on the interpretation of the coefficients $a_i$ and $b_i$. Thermodynamic quantities are obtained as derivatives of the free energy. In this way, several scaling laws may be derived, which is of great importance in identifying unknown exponents.

From a practical point of view, knowing how a parameter scales at the critical point is a powerful tool in examining its behaviour at $T_c$. Simulation of the quantities at different lattice sizes, using the scaling relations immediately give estimates of the critical exponents, which is repeatedly done in this thesis.

### 2.6 Finite-Size Scaling

Allowing for finite-size effects in scaling laws is often used in simulations. Since the RG procedure is purely local, scaling relations for finite systems have the same form as those for infinite systems. With a slight change of notation, assuming the free energy to depend on the reduced temperature $t = T - T_c$, the reduced magnetic field $h = H - H_c$, the system size $L$ and other factors,

$$f_s(t, h, ..., L^{-1}) \sim l^{-d} f_s(l^{y_1} t, l^{y_2} h, ..., lL^{-1})$$

(2.6)

for an arbitrary resizing parameter $l > 1$.

Scaling laws of important quantities are defined in table 2.1. Since we know how the correlation length scales, we can deduce the scaling relation $|T - T_c| = |t| \sim \xi^{-1/\nu}$. In the case of an infinite system, $\xi \to \infty$ at criticality, while for a finite
CHAPTER 2. THEORETICAL BACKGROUND

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<th>XY 3d</th>
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<td>t</td>
<td>^{-\nu}$</td>
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<td>$C$</td>
<td>$</td>
<td>t</td>
<td>^{-\alpha}$</td>
<td>$\alpha$</td>
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Table 2.1: Scaling relations of quantities together with their characteristic exponents and their accepted values for the Ising and XY models.

system the divergence of $\xi$ is cut off by the finite system size $L$ at $T = T_c$.

This means that we can form quantities such as $mL^{\beta/\nu}$ that scale with a critical exponent equal to zero near $T_c$, i.e. it is independent of the system size $L$. In this manner it is then possible to determine $T_c$ by plotting the length-invariant quantity against $TL^{1/\nu}$ for different lengths, as they will collapse to a common curve.

2.7 Introduction to Superconductors

Superconductors have been known since the year 1911, when H. K. Onnes measured the resistance of a small sample of mercury under extreme cooling.

He found the resistance curve to be a smooth curve until it suddenly seemed to vanish completely—he had observed the (first order) phase transition of mercury turning into a superconductor, a state allowing electricity to pass with negligible resistance. A plot of the transition is provided in Fig. 2.1.

![Figure 2.1: Onnes' original resistance plot (\(\Omega\)) versus temperature (\(K\)).](image)

Intense study led to the classification of superconductors into two groups known as type I and type II superconductors. The former exhibit the Meissner effect, showing expulsion of external magnetic fields $H < H_c$ in the superconducting phase. Type II superconductors also exhibit the Meissner effect for $H < H_{c1}$, but in the
2.8. LANDAU THEORY OF SUPERCONDUCTIVITY

regime \( H_{c1} < H < H_{c2} \) partial magnetic penetration is allowed while the material may still super-conduct.

Type II superconductors enable the critical temperature to be raised considerably. The term high temperature superconductors, HTS, has been coined pertaining to compounds of type II allowing for critical temperatures around 100 K, which is to be compared with \( T_c = 4.2K \) of mercury\(^1\).

2.8 Landau Theory of Superconductivity

In the ensuing effort to describe the strange phenomenon of superconductivity, the results of BCS theory\(^2\) and Landau’s formulation of the free energy are fundamental. The description is based upon the existence of a complex order parameter, which describes the bound state of the electron pairs formed during the superconducting phase. The order parameter is then the bound-state (BCS) wave function \( \Psi \). It acts as an order parameter, since in the domain \( T > T_c \), \( \Psi = 0 \) as the material ceases to be superconducting.

The expression for the free energy may then be Taylor expanded near \( T = T_c \) to produce the Ginzburg-Landau free energy

\[
F[\Psi] = \int d^dr \left[ \frac{1}{2m^*} \left| i\hbar \nabla + \frac{2e}{c} A \Psi(r) \right|^2 + \alpha(T - T_c) |\Psi(r)|^2 + \frac{\beta}{2} |\Psi|^2 + \frac{(\nabla \times A)^2}{2\mu_0} \right]. \tag{2.7}
\]

Here \( m^* \) is the mass of the electron pair known as the Cooper pair, \( A \) is the magnetic vector potential, \( \hbar \) is proportional to Planck’s constant (\( \hbar = \frac{h}{2\pi} \)). Equation (2.7) is to be interpreted as the sum of kinetic, superconducting-phase condensation and magnetic energies.

Together with the Landau formula, there are two important temperature-dependent and dimensionless quantities called the coherence length \( \zeta(T) \) and the screening length \( \lambda(T) \).

The wave function \( \Psi \) can be written on polar form:

\[
\Psi = |\Psi|e^{i\theta}. \tag{2.8}
\]

A much more useable order parameter instead of the whole wave function is to take the phase \( \theta \) of \( \Psi \) so as to map the order parameter into the interval \([0, 2\pi]\). It is then possible to use and modify existing models for \( 2\pi \)-periodic parameters.

A useful approximation valid in many problems is obtained by setting the amplitude \(|\Psi|\) = constant. This leaves only phase fluctuations, which is a great simplification.

\(^1\)The highest reached temperature is \( T_c = 138K \) for \( \text{Hg}_0.8\text{Tl}_0.2\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_8\text{.33}[4] \).

\(^2\)After Bardeen, Cooper and Schrieffer.
2.9 Vortices and Flux Quantization

In type II superconductors, magnetism permeates the medium by the means of vortex lines for \( H_{c1} < H < H_{c2} \). Each vortex has a value of the magnetic flux \( \Phi_0 = \frac{\hbar}{2e} \).

The flux carries a vector potential, which is represented by means of the gauge field \( A \), such that the magnetic induction, \( B \) is

\[
B = \nabla \times A \tag{2.9}
\]

\( A \) is a gauge field since it can readily undergo a gauge transformation

\[
A_i(x) \rightarrow A_i(x) + \partial_i \theta(x) \tag{2.10}
\]

where \( x \) denotes a lattice point, leaving \( B \) invariant under the transformation.

Furthermore, due to the angular nature of the order parameter \( \theta \), we have for the vortex that

\[
\Delta \theta = \oint_l d\theta = \oint_l dr \cdot \nabla \theta(r) = 2\pi n \tag{2.11}
\]

for some integer \( n \).

Quantum mechanically, the current flowing in the superconducting phase is given by

\[
j = -\frac{e}{2m} \left[ \Psi^\dagger (-i\hbar \nabla + \frac{2e}{c} A) \Psi + ((-i\hbar \nabla + \frac{2e}{c} A) \Psi)^\dagger \Psi \right]. \tag{2.12}
\]

Using the order parameter field, Eq. (2.8) and letting \( c = 1 \), we immediately get the expression of the current to be

\[
j = - \left[ \frac{2e^2}{m} A + \frac{e\hbar}{m} \nabla \theta \right] |\Psi|^2. \tag{2.13}
\]

Deep inside the superconductor, where the magnetic flux through each of the vortex lines is shielded by the current given by Eq. (2.13), no current is induced by the vector potential \( A \). Thus we have

\[
0 = \int j \cdot dr \iff \frac{2e^2}{m} \int_l A \cdot dr = \int_l \frac{e\hbar}{m} \nabla \theta \cdot dr. \tag{2.14}
\]

Stokes' theorem then gives

\[
\frac{2e^2}{m} \int_l A \cdot dr = \frac{2e^2}{m} \int_S (\nabla \times A) \cdot dS = \frac{2e^2}{m} \int_S B \cdot dS = \Phi \frac{2e^2}{m} \tag{2.15}
\]

Hence,

\[
\Phi \frac{2e^2}{m} = \frac{e\hbar}{m} 2\pi n, \tag{2.16}
\]

and thus the magnetic flux \( \Phi \) is quantized by means of the relation \( \Phi = n\Phi_0 \).
Chapter 3

Theoretical Models

3.1 XY Model

A simple model with which one might describe the superconducting phase is the XY model, originally studied by Lieb et al. [5] The XY-model has been shown to successfully model the superfluid phase transition of $^4$He. [6]

The XY Hamiltonian takes the form

\[ H_{XY} = -J \sum_{<i,j>} \cos(\theta_i - \theta_j - A_{ij}) - \lambda_0^2 (\nabla \times A)^2. \]  (3.1)

Here $\lambda_0$ is the bare screening length (essentially a material property), $\theta_i$ henceforth denotes the phase of the superconducting wave function at the lattice point $i$, $A_{ij} = \Phi_0 \int_i^j \mathbf{dr} \cdot \mathbf{A}$, where $\mathbf{A}$ is the vector potential between the sites $i$ and $j$. $J = \frac{\hbar^2}{2m^*} |\Phi|^2$ is the coupling constant describing the Cooper pairs (for more information on various interpretations of $J$, see Ref. [7] Ch. 32).

Note that here the discrete version of the circulation of the angle, Eq. (2.11) is

\[ \Delta \theta = \sum_i \Delta \theta_i = 2\pi n, \]  (3.2)

where $n = 0, \pm 1, \ldots$ is the vorticity and the sum is to be performed as a closed loop over the lattice.

The presence of the vector potential gives rise to so called frustration, since the ground state is not able to simultaneously minimize all terms in $H$. The ground state here invariably consists of some spins creating vortices to cancel the effect from $\mathbf{A}$. In the mixed state, the lowest energy state is an Abrikosov lattice, where penetrating magnetic flux form a triangular vortex lattice.
3.2 Villain Approximation

Taking the cosine, as in Eq. (3.1) is only one method of ensuring \(2\pi\)-periodicity, but there exists a more preferable way to enforce the periodicity condition while retaining the essential physics of the problem. The procedure is called the Villain approximation, after J. Villain [8].

Consider a general coupling \(U(\theta)\) in stead of the cosine expression in Eq.(3.1). The Fourier transform of \(\exp(U(\theta))\) is then:

\[
e^{U(\theta)} = \sum_{k=-\infty}^{\infty} e^{ik\theta+U(k)}
\]  

(3.3)

where the Fourier coefficients are defined as

\[
e^{U(s)} = \frac{1}{2\pi} \int_{0}^{2\pi} d\theta e^{-is\theta+U(\theta)}.
\]  

(3.4)

Poisson’s summation formula for the sum over \(s\) of a function \(f(s)\) states that

\[
\sum_{s=-\infty}^{\infty} f(s) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{+\infty} d\phi f(\phi)e^{-2\pi m\phi}.
\]

Using the summation formula on Eq. (3.3) we get:

\[
e^{U(\theta)} = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{+\infty} d\phi e^{U(\phi)+i\phi\theta-2\pi m\phi}.
\]  

(3.5)

We can then rewrite Eq. (3.5) by identifying a coefficient \(U_0\) such that

\[
e^{U_0(\theta)} = \int_{-\infty}^{+\infty} d\phi e^{U(\phi)+i\phi\theta}.
\]

Thus it is possible to write

\[
e^{U(\theta)} = \sum_{m=-\infty}^{\infty} e^{U_0(\theta-2\pi m)}.
\]  

(3.6)

The result is that Eq. (3.6) describes a \(2\pi\)-periodic coupling which is independent of the behaviour of \(U_0\). Of course, since \(e^{U(\theta)}\) is periodic, so is \(U(\theta)\). Furthermore, Villain made the choice of \(U_0(\theta) = -\beta V \theta^2 / 2\). In this way, \(e^{U(\theta)}\) will have a Gaussian shape with peaks centred at \(2\pi m\) for \(m \in \mathbb{Z}\).

It is possible to show (see the excellent treatment on the subject in Ref. [9]) that for all values of \(\beta\), the Boltzmann weight in the cosine interaction can be approximated with the Villain function in the following manner:

\[
e^{\beta \cos(\phi)} \approx R_V(\beta) \sum_{m=-\infty}^{\infty} e^{-\beta V (\phi-2\pi m)^2/2}
\]  

(3.7)
3.3. VILLAIN MODEL WITH MAGNETIC FIELD ENERGY

The expansion in the case $\beta \to \infty$ will be important (as this corresponds to the approximation at low temperatures), which allows us to set $\beta V = \beta$ and $R V = e^{\beta [9]}$.

It is convenient to define the Villain potential by taking the logarithm of Eq. (3.7). This means that the Villain function is dependent on the temperature $T = \frac{1}{\beta}$, having the consequence of changing the Gaussian behaviour of $V(\theta) \equiv e^{-U(\theta)/T}$: for $T \to 0$ the peaks become more sharp and $V(\theta) \to \infty$, whereas for $T \to \infty$ $V(\theta) \to 0$. For all $T \in (0, \infty)$, the coupling is $2\pi$-periodic.

As a final note it might be added that the sum in Eq. (3.6) normally converges very rapidly, so that summation of only a handful of terms near $U_0(0)$ gives a very good approximation to the true value of the sum. Since there is a dependence on temperature as well however, high temperatures make it necessary to sum over more terms to compute the sum accurately.

3.3 Villain Model with Magnetic Field Energy

An inherent property of the now much studied Type II superconductors is that the screening length is larger than the coherence length. In the limit $\lambda \gg \xi_0$, the system behaves as a London Superconductor.

The Lattice London Superconductor, LLS is described by the Hamiltonian [10]:

$$H_{LLS} = \sum_{i\mu} \left\{ U(\theta_{i+\hat{\mu}} - \theta_i - A_{i\mu}) + \frac{1}{2} J \lambda_0^2 [\partial \times A]_{i\mu}^2 \right\}, \quad (3.8)$$

where the sum is performed over the lattice sites $i$ and directions $\mu = x, y, z$ (in the three-dimensional case, which is studied here). The term $\theta_{i+\hat{\mu}}$ is to be interpreted as the phase of the nearest neighbour to $\theta_i$ in the direction $\hat{\mu} = \{e_x, e_y, e_z\}$. The kinetic energy term $U(\phi)$ is defined through the the Villain function

$$e^{-U(\phi)/T} = \sum_{m=-\infty}^{\infty} e^{-J(\phi - 2\pi m)^2/(2T)}, \quad (3.9)$$

The Hamiltonian (3.8) is thus a variant of the XY Hamiltonian, Eq. (3.1), where the cosine interaction has been replaced by the Villain function. The only difference between the XY model and the Villain model potentials is that the latter is temperature dependent. Thus the LLS should have the same or very similar characteristics, such as critical exponents.

In Equation (3.8), the lattice circulation $[\partial \times A]_{i\mu}$ is to be evaluated. This is done by defining the lattice forward difference operator $\partial_{i,k}$ situated on site $i$ taking the difference in direction $k$ through:

$$[\partial \times A]_i = \epsilon_{jkl} \partial_{i,k} A_{i,l} \cdot \hat{e}_j = \epsilon_{jkl} (A_{i+k,l} - A_{i,l}) \cdot \hat{e}_j, \quad (3.10)$$
where the index \( i \) denotes the lattice coordinate and thus the index \( i + \hat{k} \) is interpreted as the nearest lattice neighbour in direction \( k \). The component of Eq. (3.10) in the \( \mu \)-direction is then

\[
[\partial \times A]_{i\mu} = \epsilon_{\mu kl}(A_{i+\hat{k},l} - A_{i,l}).
\]

Using the properties of the permutation symbol \( \epsilon_{\mu kl} \) we can immediately sum over the free indices \( k \) and \( l \) using \( \mu, \nu, \sigma \) (being cyclic permutations of \( x, y, z \)):

\[
[\partial \times A]_{i\mu} = A_{i,\nu} + A_{i+\hat{\nu},\sigma} - A_{i+\hat{\sigma},\nu} - A_{i,\sigma}.
\]  

Equation (3.11) has the simple geometric interpretation of an elementary plaquette in the \( \nu - \sigma \) plane with circulation starting and ending at the coordinate \( i \) and normal pointing in the \( \mu \)-direction. At the same time, Eq. (3.11) is also to be interpreted as a measure of flux quanta through the plaquette.

There is also a constraint to be made, the gauge must be fixed. The Landau gauge \( \nabla \cdot A = 0 \) is used, in this context this means that:

\[
[\partial \cdot A]_i = 0 \iff A_{i+\hat{k},k} = A_{i,k}.
\]  

A sketch of the three elementary plaquettes surrounding a lattice point \( P = (i, j, k) \), where \( \{i, j, k\} = 1, \ldots, L \), is provided in Fig. 3.1 below. It is evident that each node is free of divergence if the gauge-fixing condition of Eq. (3.12) is implemented over the entire lattice. The vector potential is defined to originate from a lattice point so that it points in a positive direction only. Hence the point \( P \) has the potentials \( A(i, j, k, 1) \), \( A(i, j, k, 2) \), and \( A(i, j, k, 3) \) associated to it in a 3d lattice.
3.4 Compact Gauge Theory

The compact gauge theory is formulated through the following Hamiltonian \([11]\) with \(U(1)\) symmetry:

\[
H = -J \sum_{\mu} \left\{ \cos(\theta_i + \hat{\mu} - \theta_i + g A_{\mu}) + \frac{1}{g} \cos[\vartheta \times A]_{\mu} \right\}.
\] (3.13)

This equation is similar to the LLS, yet its physical behaviour is radically different due to the cosine of the magnetic field \(B\). The major consequence is the fact that the Hamiltonian allows magnetic monopoles with charge \(2\pi\) to exist, contradicting the Maxwell law \(\nabla \cdot (\nabla \times A) = 0\). Equation (3.13) is also characterized by a charge variable, \(q\), here we let \(q = 2\) so as to describe a superconductor consisting of Cooper pairs.

3.5 Clock Model

There is also a duality transformation from Eq. (3.13) to a model with a discrete, \(Z_q\), symmetry. The transformation is accomplished by making repeated use of the
Villain approximation, which allows the contribution of spin-wave excitations to the partition function to be factored out. Detailed information on this process can be found in Refs. [11], [12] and [13]. The Hamiltonian for the dual model, also called the clock model, reads[11]:

\[
H = \frac{1}{K\lambda} \left\{ \sum_{\mu} [1 - \cos(\theta_{i+\mu} - \theta_i)] + \frac{1}{q^2\lambda^2} \sum_i [1 - \cos(q\theta_i)] \right\}. \tag{3.14}
\]

The constant \( K \) is related to the coupling constant by \( K = (2\pi)^2 J \), and \( \lambda \) is the screening length.

The value of \( q \) is very important as it determines the symmetry of the model. For \( q = 2 \) this model should then have similar characteristics compared to the Ising model, since this also has \( \mathbb{Z}_2 \) symmetry, represented by spins being allowed to point either “up” or “down”. Even if the critical temperature of the clock model will be different, the same critical exponents are expected by universality.
Chapter 4

Simulation Methods

4.1 Monte Carlo Method

In order to obtain averages of statistical mechanical quantities (such as the magnetization of the system), one often has to calculate complicated integrals of the type

$$\langle A \rangle = \frac{1}{Z} \int_{\Omega} dx A(x) e^{-\beta \mathcal{H}(x)}, \quad (4.1)$$

where $A$ is the quantity whose average is of interest, $\Omega$ is the space in which the (dummy) index $x$ lives, $\mathcal{H}$ is the system Hamiltonian, $Z$ is the partition function defined in Ch. 2 above (this is just a reformulation of the ensemble average described in Sec. 2.3). In computer simulation all quantities are usually discretized, which leads to the following discrete time averaging formula:

$$\langle A \rangle \approx \frac{\sum_{\nu=1}^{M} A(x_{\nu}) e^{-\beta \mathcal{H}(x_{\nu})}}{\sum_{\nu=1}^{M} e^{-\beta \mathcal{H}(x_{\nu})}}, \quad (4.2)$$

For sufficiently large $M$, this quantity should approximate Eq. (4.1) if ergodicity holds. To obtain an efficient algorithm that converges towards Eq. (4.1) for a reasonably large value of $M$, it is very advantageous to generate states $x$ distributed according to the Boltzmann distribution $P(x) = \frac{1}{Z} e^{-\beta \mathcal{H}(x)}$ itself. This turns Eq. (4.2) into an arithmetic average of the form:

$$\bar{A} = \frac{1}{M} \sum_{\nu=1}^{M} A(x_{\nu}).$$

The process of sampling states according to the target Boltzmann distribution is the basis of Monte Carlo, MC, simulation.
4.2 Markov chains and detailed balance

In order to generate Boltzmann distributed states, the general method is to use Markov chains. A stochastic process \( \{X_t; t = 1, 2, \ldots\} \) is a Markov Chain if:

\[
P(X_{t+1} = x_{t+1} | X_1 = x_1, X_2 = x_2, \ldots, X_t = x_t) = P(X_{t+1} = x_{t+1} | X_t = x_t)
\]  
for all \( t \) and states \( x_1, x_2, \ldots, x_{n+1} \).

In words, the conditional probability of a process at time \( t+1 \) taking the specific value \( x_{t+1} \) is dependent only on the realization at time \( t \).

The next step is to introduce the transition probability, which is the probability of the process taking the value \( y \) at time \( t \) given the fact that it had the value \( x \) at time \( t-1 \):

\[
w_{xy} = P(X_t = y | X_{t-1} = x).
\]  

In order for the transition to take place, a specific change must be proposed as well as accepted.

The transition probability can then be split into two parts, since accepting and proposing is done independently:

\[
w_{xy} = q(x, y) \cdot \alpha(x, y),
\]  

where \( q(x, y) \) is the probability of proposing the change from state \( x \) to \( y \), \( \alpha(x, y) \) is the acceptance probability.

It can be shown (see for instance Ref. [14]) that two conditions are sufficient for the Markov Chain to approach the (Boltzmann) equilibrium distribution \( \pi(x) \propto e^{-\beta \mathcal{H}(x)} \):

(a) The Markov chain is ergodic, which in this context means that we can reach an arbitrary state \( y \) from any other state \( x \) by means of a finite number of transitions. More formally we the condition can be written as:

\[
\exists \ N < \infty \ s.t. \ w_{xy}^{(N)} \equiv P(X_N = y | X_0 = x) \neq 0
\]  

For any states \( x, y \).

(b) Time reversibility holds. This is also called detailed balance, which means that transitions are made in accordance with the equation

\[
\pi(x) \cdot w_{xy} = \pi(y) \cdot w_{yx} \quad \forall x, y.
\]  

If we propose changes according to a distribution which has \( q(x, y) = q(y, x) \), the detailed balance condition means that

\[
\alpha(x, y)e^{-\beta \mathcal{H}(x)} = \alpha(y, x)e^{-\beta \mathcal{H}(y)}
\]  

and thus with the definition \( \Delta \mathcal{H} \equiv \mathcal{H}(y) - \mathcal{H}(x) \) one gets

\[
\frac{\alpha(x, y)}{\alpha(y, x)} = e^{-\beta \Delta \mathcal{H}}.
\]
4.3 Metropolis Algorithm

Equation (4.9) allows for a large number of different acceptance probabilities, the choice first made by Metropolis [15] is

\[ \alpha(x, y) = \min\left(1, e^{-\beta \Delta H}\right). \] (4.10)

Another acceptance probability is called heat bath, given by

\[ \alpha(x, y) = (1 + e^{\beta \Delta H})^{-1} \] (4.11)

It is easily checked that the two probabilities satisfy the detailed balance condition of Eq. (4.9) as well as being confined to [0, 1] for all states.

The single flip Metropolis algorithm implements the acceptance probability given by Eq. (4.10) and weights the proposed changes using a uniformly distributed random number \( r \) using the following algorithm (where \( \phi \) denotes the spin configuration and \( L^d \) the system volume):

1. Start with an initial spin configuration, the ground state for instance.
2. Select a random site to update with a random quantity \( \phi' \in (0, 2\pi) \).
3. Calculate the energy difference \( \Delta H = H(\phi') - H(\phi) \).
4. Generate \( r \) and accept if \( e^{-\beta \Delta H} > r \).
5. If the move is accepted, determine the changes in letting \( \phi' = \phi \), if not accepted, do not change anything.
6. Repeat steps 2–5 until enough trial moves have been made (usually \( L^d \) times).
7. Compute averages.

Performed enough times (usually iterations are of the order of at least \( 10^5 \)), the Metropolis algorithm will result in the system having a distribution very close to the Boltzmann distribution (a proof is provided in [15]). To avoid bias in the averages and heavy initial fluctuations in the system energy due to the selected initial condition, a “warm-up” simulation must precede the computation of averages. Warm-up iterations are usually of the order \( 10^5 \) but depend on how quickly the system approaches thermodynamic equilibrium.

Another technicality is that computers only can generate pseudorandom numbers, which means that the sequence of random numbers has a finite period, but with good random number generators this period far exceeds the number times random numbers have to be generated\(^1\).

When updating phases it is enough to draw the proposed angle from \( U(0, 2\pi) \), but when updating the vector potential \( A_i \in \mathbb{R}, i = x, y, z \) it is vital to ensure

\(^1\)The Marsaglia random number generator used here has a period in excess of \( 2^{60} \).
that there is no restriction on its actual value. Furthermore, in order to preserve the gauge, changes are attempted on a whole elementary plaquette. A sequential update of $A$ is performed using the Metropolis algorithm where $A'_i = A_i + \delta A_i$. The proposed change $\delta A_i$ must be carefully chosen. Too small a $\delta A_i$ results in unnecessarily many steps to approach equilibrium and too large a value of $\delta A_i$ has the same effect since the system is easily (too often) thrown far away from equilibrium. Normally it is sufficient to select $\delta A_i$ from $U(-1,1)$.

4.4 Temperature Exchange Algorithm

In order to speed up the convergence of the simulation, a good method to use is parallel tempering, also known as the temperature exchange method. For low temperatures the acceptance probabilities are small and thus many update attempts are redundant. The idea is to simulate all temperatures in the system (usually around 10-20) simultaneously. Knowing the high temperature realizations, one may thus “heat up” the low temperature states and allow them to cool down before attempting to heat them up again.

The algorithm used here attempts to interchange systems with temperatures $T_i$ and $T_{i+1}$, where $i$ and $i + 1$ denote neighbour indices. The original system is characterized by energies $\{H_i(T_i), H_{i+1}(T_{i+1})\}$, if the temperatures are exchanged the configuration can be written $\{H_i(T_{i+1}), H_{i+1}(T_i)\}$. Exchange acceptance probabilities are given by a modified Metropolis choice. Assuming energies to be temperature dependent, the expression becomes:

$$\alpha(T_i, T_{i+1}) = \exp \left[ -\frac{1}{T_i} (H_{i+1}(T_i) - H_i(T_i)) \right] \exp \left[ -\frac{1}{T_{i+1}} (H_i(T_{i+1}) - H_{i+1}(T_{i+1})) \right].$$

(4.12)

If energies are not dependent on temperature, Eq. (4.12) reduces to

$$\alpha(T_i, T_{i+1}) = \exp \left[ \left( -\frac{1}{T_i} - \frac{1}{T_{i+1}} \right) (H_{i+1} - H_i) \right].$$

(4.13)

The thermal exchange algorithm can be written as follows:

1. Start with the lowest temperature, $i = 0$.

2. Test if $\alpha(T_i, T_{i+1}) > r$, $r \in U(0,1)$.

3. If true, interchange temperatures and all averages associated with the system.

4. Iterate from 2 with $i = i + 1$ until $T_{i+1} = T_{\text{max}}$.

It is necessary to perform the algorithm ‘suitably often’. If interchange is attempted after every MC iteration the simulation is slowed down with no gain in convergence. If attempted too seldom, the algorithm is ineffective. It can be shown (for instance
in Ref. [16]) that the algorithm should be implemented after an amount of iterations at which the energies can be said to be uncorrelated. In the thesis, whenever the algorithm is used, this number is set to be equal to 17.

4.5 Calculation of Averages

In order to analyse the critical point, various moments of either the system energy or magnetization are calculated. The average "magnetization" is calculated as follows:

\[
m = \frac{1}{L^3} \sum_k e^{i\theta_k} = \frac{1}{L^3} \left[ \left( \sum_i \cos(\theta_i) \right)^2 + \left( \sum_i \sin(\theta_i) \right)^2 \right].
\]  

(4.14)

The parameter \(m\) is thus a global order parameter. In this thesis I examine to what extent it is useful in order to describe gauge theories.

Apart from \(m\), the following averages are calculated where \(N = L^3\):

\[
e = \frac{\langle \mathcal{H} \rangle}{N} \tag{4.15}
\]

\[
c = \frac{1}{N} \frac{1}{T^2} \left( \langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 \right) \tag{4.16}
\]

\[
U_L = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2} \tag{4.17}
\]

4.6 Binder Cumulant

The quantity in Eq. (4.17) is called the Binder cumulant. Its scaling relation is

\[
U_L = \tilde{U}_L(L^{1/\nu}(T - T_c)).
\]

This has two important consequences, one of them is the fact that \(T_c\) can be found directly by plotting \(U_L\) against \(T\) for different lengths, since they will assume the same value (within some error) of \(U_L\) at \(T = T_c\).

The Binder cumulant also allows for a rough estimation of \(\nu\) by plotting \(U_L\) against \(L^{1/\nu}(T - T_c)\) for different \(L\) and \(T\), the curves should collapse to a common curve using the correct values of \(T_c\) and \(\nu\).
4.7 Third Moment of the Energy

A useful quantity for finding critical exponents is the third moment of energy, $M_3$, used for similar problems in Ref. [17]. It is calculated through:

$$M_3 = \langle (\mathcal{H} - \langle \mathcal{H} \rangle)^3 \rangle = \frac{1}{L^3} \left( \langle \mathcal{H}^3 \rangle - 3 \langle \mathcal{H} \rangle \langle \mathcal{H}^2 \rangle + 2 \langle \mathcal{H} \rangle^3 \right).$$  (4.18)

![Figure 4.1: General behaviour of $M_3$ together with its scaling relations.](image)

From the scaling of the free energy, we know that the distance between peaks obey the scaling law $y_{\text{peak}} \sim L^{(1+\alpha)/\nu}$, and $x_{\text{peak}} \sim L^{-1/\nu}$. These scalings are marked in the illustration of $M_3$ in Fig. 4.1. From the extrema, one is then able to obtain both $\nu$ and $\alpha$. The major drawback using this method is the lack of precision in finding the exact location of the extrema. Often one has to resort to histogram interpolation to be able to find the points to acceptable precision. In this thesis however, this method proved hard to implement. Instead, a polynomial interpolation near the extrema was used.
Chapter 5

Results

Throughout this chapter, simulations have been performed on cubic lattices using the single flip Monte Carlo method in combination with the temperature exchange method, as described in Ch. 4. Periodic boundary conditions are implemented.

5.1 Villain Model in Absence of Magnetic Field

Letting \( A = 0 \) in the Villain model, the system Hamiltonian reads:

\[
H = \sum_{<ij>} U(\theta_i - \theta_j),
\]

(5.1)

with \( U(\phi) \) given by the Villain function.

MC Simulations of Eq. (5.1) have been performed. 15 runs with averages over \( 10^5 \) sweeps resulted in Fig. 5.1, showing a phase transition near \( T = 3.0 \) using the Binder cumulant. This agrees with previous results, see for instance Ref. [18].

The Villain model under study should have the same critical exponents as the XY model in the corresponding dimension. To check this, finite-size scaling has been performed. Plotting the Binder cumulant against \( L^{1/\nu}(T - T_c) \) choosing \( \nu = 0.67 \) gives a good collapse as is shown in Fig. 5.2(a). Having found an approximate value of \( \nu \), it is then straightforward to obtain the exponent \( \beta \) from the average magnetization, plotting \( m(T, L)L^{\beta/\nu} \) against \( L^{1/\nu}(T - T_c) \). The collapse shown in Fig. 5.2(b) gives \( \beta = 0.32 \), to be compared with the expected \( \beta = 0.35 \).
2.85 2.9 2.95 3 3.05

Figure 5.1: Close-up of the Binder cumulant near $T_c = 3.0$.

(a) Binder cumulant collapse for $\nu = 0.67$  
(b) Magnetization collapse for $\nu = 0.67$, $\beta = 0.32$

Figure 5.2: Scaling collapses for exponents $\nu$ and $\beta$ for the Villain model with no magnetic field contribution.

5.2 Villain Model in Nonzero Magnetic Field

This model is given by the LLS Hamiltonian described in chapter 3. Thus the Hamiltonian reads:

$$\mathcal{H} = \sum_{\mu} \left\{ U(\theta_{i+\mu} - \theta_i - A_{i\mu}) + \frac{1}{2} J^2 \lambda_0^2 |\partial \times A_{i\mu}|^2 \right\},$$

Choosing $\lambda_0 = 0.3 \approx e^{-1}$ for the bare penetration depth, simulations with averages taken over $10^5$ MC sweeps were made. A plot of the Binder cumulant in Fig. 5.3 shows a critical temperature of $T_c \approx 0.80$, in agreement with Ref. [10].
5.2. VILLAIN MODEL IN NONZERO MAGNETIC FIELD

Figure 5.3: Binder cumulant of the Villain model with $A \neq 0$.

A scaling collapse of the magnetization is provided in Fig. 5.4, from which one concludes that $\nu = 0.67$ and $\beta = 0.07$, also in agreement with Ref. [10].

Figure 5.4: Collapse for $\nu = 0.67$ and $\beta = 0.07$. 
5.3 Compact Gauge Theory

The compact gauge theory with the following Hamiltonian was studied:

\[ H = -J \sum_{i\mu} \left\{ \cos(\theta_{i+\hat{\mu}} - \theta_i - qA_{i\mu}) + \frac{1}{g} \cos[\theta \times A]_{i\mu} \right\}, \tag{5.3} \]

where in the simulations \( q = 2, J = 1 \) and \( g = 1 \). Quantities such as the magnetization and the Binder cumulant were recorded in 15 observations, each averaging over \( 10^5 \) MC sweeps. Fig. 5.5 shows that even though the cumulant hints at a transition, different lengths do not cross at a point that is easily identified. Larger lengths simulated are found to be unable to improve the picture, longer simulations for each lengths only clarify the fact that the Binder cumulant does not behave as expected.

![Figure 5.5: The Binder cumulant for the compact gauge theory.](image)

5.4 Dual Representation

Using the dual representation of the compact gauge theory, generally believed to be easier to simulate using MC methods, one has the clock-model Hamiltonian in accordance with Ref. [11]

\[ H = \frac{1}{K\lambda} \left\{ \sum_{i\mu} [1 - \cos(q\theta_{i+\hat{\mu}} - \theta_i)] + \frac{1}{q^2\lambda^2} \sum_i [1 - \cos(q\theta_i)] \right\}. \tag{5.4} \]

More than 30 runs were carried out for this model averaging over \( 10^5 \) MC sweeps, letting \( K = \lambda = 1 \) and \( q = 2 \) (as we are describing Cooper pairs). The Binder ratio in Fig. 5.6 crosses at \( T_c \approx 2.365 \), also in very good agreement with Ref. [11].
5.4. DUAL REPRESENTATION

A crude estimation of $\nu$ can be made from the Binder cumulant data plotted in Fig. 5.6. A plot of the collapsed data is presented in Fig. 5.7 giving the estimate $\nu = 0.55$.

Magnetization Data in the Dual Representation

It is possible obtain $\beta$ by the usual procedure of scaling collapses using the average magnetization. The collapse in Fig. 5.8 resulted in the value $\beta = 0.32$ using $\nu = 0.63$. 
CHAPTER 5. RESULTS

Figure 5.8: Average magnetization collapse in the clock model yielding $\beta = 0.32$.

Using the Third Moment of Energy

In the simulations, the quantity $M_3$ was recorded. Many simulations focused on the two extremes of the curve, as it is essential to know their location accurately to be able to deduce the critical exponents $\nu$ and $\alpha$. A plot of the general appearance of $M_3$ is provided in Fig. 5.9, for each system length, the curve for each system size conforms to the appearance sketched in Fig. 4.1.

Figure 5.9: Behaviour of the energy moment $M_3$. 
From the data in Fig. 5.9, the scaling laws for the peak distances should give values of $\nu$ and $\alpha$. The positions of the extrema is located by means of polynomial interpolation in the vicinity of the maxima and minima. The application of scaling laws of critical exponents is transformed to a linear regression problem for the logarithms of the peak distance and the system length. Bootstrap analysis of the fitting error was also performed. The resulting curves are reproduced in Fig. 5.10, giving $\nu = 0.64 \pm 0.015$ and $\alpha = 0.19 \pm 0.03$.

Figure 5.10: Regression data on the peaks of the $M_3$ curve.

The value of $\nu = 0.64 \pm 0.015$ is consistent with the 3d Ising value ($\nu = 0.63$) whereas one should expect $\alpha = 0.11$. Due to the uncertainty in finding the exact position of the $M_3$ peaks however, it is possible that the total error allows for the expected value of $\alpha$. Fig. 5.11 shows the regression line of Fig. 5.10(b) together with a regression dotted line fixing $\alpha = 0.11$. It illustrates the small difference between the obtained and expected value of $\alpha$.

Figure 5.11: Regression line yielding $\alpha = 0.20$, as well as the predicted slope with $\alpha = 0.11$. 
There is also a possibly significant systematic error using the third moment of the energy, due to approximations made in the scaling of the extrema of the $M_3$ curve. This can be motivated as follows: From the scaling relation of the heat capacity

$$c(T = T_c, L) = AL^{\alpha/\nu} + B(T),$$

(5.5)

where $A$ is a constant and $B(T)$ is weakly dependent on the $T$, it is evident that the temperature dependence of $B(T)$ has been neglected when finding the $M_3$ scaling relations. It should thus be more accurate to attempt non-linear regression on Eq. (5.5) to obtain an estimate of $\alpha/\nu$. 
Chapter 6

Conclusion

A large number of models were studied and all except the real space compact gauge theory proved to be readily analysed using the Binder cumulant and the magnetization. Properties of the Villain model such as the critical temperatures in the cases $\mathbf{A} = \mathbf{0}$ and $\mathbf{A} \neq \mathbf{0}$ have been determined together with critical exponents $\nu$ and $\beta$. Failing to observe a transition in the compact gauge theory, the critical behaviour of the dual representation of the compact gauge theory was studied. Simulations on this model were successful in finding a transition using the Binder cumulant method for the critical temperature, together with a third moment of energy analysis for the critical exponents $\nu$ and $\alpha$.

Using $\alpha = 0.11$ as in Fig. 5.11 might provide a slightly better regression for the larger system lengths, as finite size effects due to the small sizes simulated might well have contributed to some of the error in the estimation of $\alpha$. Simulation of larger systems might thus provide a better value of $\alpha$ using the third moment of energy, at the cost of rapidly increasing simulation time.

From the dual representation of the compact gauge theory, we know that a transition does take place. This does not however shed any light on the failure to observe a transition in the real space formulation of the gauge theory. The compactness of the Hamiltonian seems to frustrate the transition in some way, depending on the value of the magnetic vector potential, which it is important to remember can take any value on $\mathbb{R}$. It might be a good idea to use an order parameter which makes use of the compactness as well as the value of the vector potential, in the hope of removing some of the frustrated behaviour at the transition. A possible explanation of the lack of finding a transition is that the value of the Binder cumulant is the same in both sides of the transition. This interesting observation remains to be explained. Further experimentation with different order parameters is clearly needed at this point, if one does not wish to study the dual formulation of the problem.
Bibliography


