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A Monte Carlo Study of the Criticality of the 3D XY Model

Sindre Vaskinn

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MASTER THESIS

Preface

All integrated master students at Mathematics and Physics NTNU have a 30 ECTS master thesis the 5th year, where the students is to immerse into a subject. The department of physics gives the students great freedom regarding the subject and where the thesis is to be written. I chose to write my thesis at Laboratoire de physique théorique de la matière condensée (LPTMC) at Université de Pierre et Marie Curie (UPMC). The division for Complex Materials has a wide focus of research, including: investigating the properties of soft matter (for example colloids such as clays, polymers or amphiphiles) with neutron scattering, how the properties change in soft matter with external stress (ex. magnetic or thermal), polymers, nano-structured surfaces and modelling of systems (for example traffic or populations).

Motivation

The personal motivation to do this thesis for me is that statistical physics is the field I find most interesting, especially that of phase transitions. In addition I wanted to learn to programme better, especially on a larger scale than I have done earlier. That I could learn a new programming language and learn how to make parallel programs was also a great motivation for me.

Structure of the Thesis

I have chosen to write a thorough introduction, to convince myself and any other person which is not an expert in statistical physics, phase transitions, scaling, renormalization and universality. In the end the XY model will be presented. In part two the results from the simulations will be presented. A summary, conclusion and suggestion to further work will be given. Finally, in the appendix some results that not where included and a summary of the program are added. My suggestion is that if you are well familiarized with phase transitions, renormalization, etc. you can skip the theory part, since nothing new will be presented here and rather start on the Results section. However, for persons new to the field the introduction is a good place to start and probably necessary to understand the rest of the thesis.

<div align="center">

Paris, March 6, 2015

Sindre Vaskinn

</div>

Be the hero of your own movie.
If your life was a movie and it
started now. What would the
hero of your life's movie do right
now. Do that. Do those things.

<div align="right">Joe Rogan</div>

Acknowledgment

I would like to thank my supervisor at UPMC Philippe Sindzingre for giving me the opportunity to do a project in the field I find most interesting, and for the opportunity to learn parallel programming, and a new programming language (fortran) which is widely used in the scientific community.

The LPTMC who welcomed me twice (Erasmus year and master thesis) and gave me the opportunity to learn more statistical physics.

From NTNU student advisor Peder Brenne was of great help with administrative task which made the bureaucracy almost funny. In addition, he was always in a good mood and willing to help.

I also would like to thank Jon Andreas Støvneng, my advisor at NTNU that agreed to be my advisor on short notice and helped with the administrative tasks.

I would also like to thank Pink Floyd for making the best working music. It has been with throughout the studies and for countless hours spent on this thesis.

Finally, I would like to thank everyone who has supported me over the years, teachers, friends, family, without you the days that pass wouldn't be the same.

Summary

In this master thesis the criticality of the 3D XY model with cubic anisotropy has been examined by the means of Monte Carlo simulation. The 3D XY model is a special case of the $O(n)$ spin-vector model which describe numerous phenomena's. Here, n is the number of vector dimensions and for the XY model $n = 2$. The $O(n)$-model is invariant for global rotations. This means that it is arbitrary which direction in the symmetry breaking occurs. In real system one should always expect perturbations from a perfect system, here it is done by adding a cubic anisotropy (order $p = 4$) then the symmetry of the Hamiltonian is lowered and it will be advantageous for the spins to be ordered in directions 90° apart. This symmetry is called C_4, which is a part of the cyclic group, and it restricts the symmetry breaking to one of these four directions.

The criticality of this model is when the spins suddenly align as the temperature is lowered to a critical temperature. Sufficiently close to the critical temperature quantities like the magnetization, which is the sum of spins, will show a power law growth characterised by critical exponents specified by the class of universality of the transition. The critical exponents can be obtained by finite-size scaling. By applying renormalization theory on the critical region one can show that some of parameters in the Hamiltonian are: relevant and effect the scaling, irrelevant and does not effect the scaling and dangerously irrelevant meaning that they only affect some of the critical exponents. Previous Monte Carlo and renormalization calculus show that anisotropy which is relevant for $p < 4$ becomes dangerously irrelevant for $p \geq 4$. The question of interest is what kind of effect the dangerously irrelevant parameter in the Hamiltonian has on the scaling. This is interesting because the effect of dangerously irrelevant parameters is hardly studied and anisotropy arise in many crystal systems because of the lattice geometry.

The results are obtained by Monte Carlo simulations and the critical slowing down close to the phase transition is solved by the method of parallel tempering. This method was chosen because it is simple to implement in a parallel code.

The Binder cumulant for different quantities and the peak of the magnetic susceptibility was used support a critical temperature $T_c = 2.2019$ k for no field applied and no anisotropy. The known critical exponents for the no field and no anisotropy was used. The scaling made a good collapse, meaning that the right T_c and the correct critical exponents where used. The scaling did not take into account a magnetic field and therefore a good collapse of curves where not obtained in this case. When the cubic anisotropy was

added the critical exponent for the magnetic susceptibility and the cubic order parameter changed, while the other exponents where unchanged. This supports the view that cubic anisotropy is dangerously irrelevant for the 3D XY model. The scaling of the magnetic susceptibility showed a possible new kind of scaling, a scaling which is different on the two sides of the transition. Although a more accurate determination of the critical exponent in the ordered phase require more extensive simulations. It appears that this exponent is larger than the exponent in the disordered phase, where one recovered the isotropic exponent. The difference in the critical exponents has been predicted to increase with p and an investigation of the hexagonal anisotropy $p = 6$ has been started.

Sammendrag

I denne master oppgaven er 3D XY modellen med kubisk anisotropi under-søkt ved hjelp av Monte Carlo simulering. 3D XY modellen er et spesial tilfelle av $O(n)$ spin-vector modellen som beskriver mange fenomener. Her er n antall vektor dimensjoner og for $n = 2$ får enn XY modellen. $O(n)$-modellen er symmetrisk for globale rotasjoner. Dette betyr at det er vilkårlig hvilken rettning symmetry brudd skjer. I reelle systemer må enn alltid regne med perturbasjoner fra et perfekt system. Her blir det gjort ved å legge til anisotropy h_p av kubisk orden $p = 4$ til systemet så symmetrien i Hamil-tonien blir senket. Dette gir systemet en C_4 symmetri som er en del av den sykliske symmetri gruppen og det vil begrense symmetri bruddet til 4 rettninger.

Kritikalitet av denne modellen er når de fleste spinnene plutselig retter seg i en bestemt rettning når temperaturen er senket til en kritisk tem-peratur T_c. Tilstrekkelig nært denne kritiske området er kvantiteter som magnetiseringens (som er summen av spin) beskrevet av potens lover som er karakterisert av eksponenter som tilhører phase overgangens universalitets klasse. De tilhørende eksponentene kalles kritiske exponenter og de kan bestemmes ved hjelp av finite size scaling. Ved å bruke renormaliserings teori på det kritiske området kan man man vise at noen parametre i Hamil-tonen er: relevant og påvirker skaleringen, irrelevant og påvirker ikke ska-leringen, eller farlig irrelevant og kan påvirke deler av skaleringen. Tidligere Monte Carlo simuleringer og renormalisering beregning viser at anisotropi er relevant for $p > 4$ og dermed blir farlig irrelevant for $p \geq 4$ for 3D XY modellen. Så spørsmålet er hvilken effekt har anisotropien påskaleringen. Dette spørsmålet er interessant for anisotropi er tilstede i mange systemer på grunn av krystall strukturen.

Resultatene er oppnådd ved hjelp av Monte Carlo simuleringer hvor par-allel temperering er brukt for å hindre kritisk nedbremsing. Denne metoden ble valgt for den er lett og implementere i en parallel kode.

Binder kumulanten for forskellige kvantiteter og maksimumet til den magnetiske susceptibiliteten ble brukt for å bekrefte en kritisk temperatur $T_c = 2.2019$ uten magnetisk felt og anisotropi. De kjente kritiske eksponen-tene ble brukt. Skaleringen ga en god kollaps av kurver som betyr at den riktige T_c og de riktige kritiske eksponentene ble brukt. Skaleringen tok ikke hensyn til et magnetisk felt så det ble som forventet ingen kollaps da. Når kubisk anisotropi ble lagt til ble de kritiske eksponentene for kubiske ordens parameteren og den magnetiske susceptibiliteten endret, mens de andre ek-sponentene forble de samme. Skaleringen av den magnetiske susceptibiliteten

viste en ny skalering, nemlig en hvor eksponenten er avhengig av hvilken side av den kritiske temperaturen den er på. Det ser ut som at eksponenten er større i den uordnede fasen enn i den ordnede, hvor en finner den isotropiske eksponenten. Forskjellen i de kritiske exponentene er forventet å øke med p og en undersøkelse av $p = 6$ har blitt startet.

Contents

Chapter 1

Introduction

In nature there is an abundance of phase transitions, where the phases can be very different and the transitions abrupt. For instance in a set of magnetic moments the set favours alignment at a sufficiently low temperature because they are correlated at infinite distances. At high high temperatures the entropy will make the set favour an unordered alignment, because of the short length correlation. The transition from an unordered set to an alignment in is what is called a spontaneous symmetry breaking. If the set is sufficiently large the transition will be abrupt. In the thermodynamical limit phase transition is characterised by a abrupt change in a derivative of a physical quantity, e.g. the heat capacity. This abrupt change happen at a temperature called the critical temperature T_c. It is useful to define a reduced temperature $t = \frac{T - T_c}{T_c}$. So that above the phase transition $t > 0$ and under $t < 0$. The exponential growth of a phase can be observed in other quantities in other materials as well. Close to T_c thermodynamic quantities follow power law behaviour. This phenomena are widely studied in physics because it is interesting and useful to predict how material properties change with temperature (or some other parameter), and because they are notoriously difficult to solve.

The $O(n)$-model is a simple spin vector model on a lattice and it is defined as $H = -J \sum_{i,j} \vec{S}_i \cdot \vec{S}_j$. Here, n is the dimension of the spin vector $\vec{S}_i$ on sites i, j and with unit length $|\vec{S}_i| = 1$, J is the coupling and one sum over neighbouring spins. By letting $N = 2$ one obtain the XY model and in reality one do expect some extra terms due to a non-perfect system. Here a magnetic field $\vec{h}$ and anisotropic perturbation h_p of order p ($p = 4$ for cubic perturbation) will be added. The Hamiltonian for the model is as following:

$$H = -J \sum_{i,j} \vec{S}_i \cdot \vec{S}_j - h \sum_j \cdot \vec{S}_j - h_p \sum_i \cos(p\theta_i). \qquad (1.1)$$

Here J is the coupling and it is only for the nearest neighbours. The effect of the magnetic term, where h is the magnetic field strength and it is equal over the whole of the lattice. If a field is applied the spins $\vec{S}_i$ will try to order them self after this field. The third term in the Hamiltonian is the anisotropy and h_p its strength. The anisotropy may arise naturally in magnetic systems due to the underlying lattice structure of the material [1]. The p denotes the order of the anisotropy. So $p = 4$ is cubic anisotropy, $p = 6$ is hexagonal anisotropy, etc.. If a magnetic field is not present, this term will make it more advantageous for spins to point in p different directions, i.e. $p = 4$ then there are 4 directions where it is the lowest energy with respect to the anisotropic term for $t > 0$.

In this model the magnetization which is the sum of spins $\vec{M} = \sum_i \vec{S}_i$ is a quantity in where one can observe this exponential growth $m = \frac{M}{N} = |t|^\beta$ sufficiently close to the transition. Where N is the number of spins. By doing finite size scaling it is possible to obtain the critical exponents and the critical temperature. Renormalization theory developed by Kenneth G. Wilson and others gives an explanation to how scaling works and it will be discussed briefly here along with universality, which states that any system that shares the same universal symmetry will have the same critical exponents at the transition. In this thesis the 3D XY model with cubic anisotropy will be studied in the vicinity of the phase transition. This is a simple spin-vector model and it is one of many models which lie in the 3D XY universality class. By using the renormalization theory on the critical region one can show that some of parameters in the Hamiltonian can be renormalized away while others cannot. These parameters are classified as relevant and effect the scaling, irrelevant and does not effect the scaling and dangerously irrelevant meaning that they only effect some of the critical exponents.

When $t > 0$, $h = 0$ and $h_p = 0$ the the 3D XY model is O_2-symmetric, which means that the spin-vectors has equal probability to point in any direction in the XY plane for $t > 0$. However, when $t \approx 0$ the system choose one random direction that the spontaneous symmetry breaking will occur. When continuous symmetry spontaneously break and they are followed by the appearance Goldstone (zero energy) mode and the system have obtained long range correlation. It is interesting to note that rotating one spin will excite the energy, but will conserve the minimum energy. The symmetry can also be broken by adding a magnetic field, then it will be advantageous for

the spins to be arranged after the field. One may also add an anisotropy to the system, this will give the system C_p-symmetry. The order parameter which allows to observe the symmetry breaking for the anisotropic case is defined as:

$$m_p = \langle \frac{(m_x + im_y)^p + (m_x - im_y)^p}{|m|^{p-1}} \rangle. \tag{1.2}$$

The reason this model is interesting is because for $p \geq 4$ the anisotropy is dangerously irrelevant and relevant for $p < 4$ [2]. Which means that the anisotropy will affect one or more critical exponents, since it cannot be renormalized away, even at the transition. The effect the dangerously irrelevant parameter has on the scaling of the 3D XY model with cubic anisotropy has hardly been studied and it is the focus of this master thesis.

Chapter 2

Theory

This section which quantities are being measured will be explained, along with what a phase transition is, and how they are related to critical exponents and universality. In addition a simple and naive view of renormalization theory and finite size scaling will be given.

2.1 A Short Introduction to Statistical Physics

The partition function describes the statistical properties of a system in thermodynamic equilibrium. If one assumes that the system is in contact with an environment with a temperature T, in a volume V and with a discrete number of states, this system is called the canonical ensemble. In principle one can extract a large amount of information from the partition function, like the probability and moments. It is defined as

$$Z = \sum_\mu e^{-\beta E_\mu}. \tag{2.1}$$

Where, μ denotes different states, E_μ is the energy of state μ, and β is equal to

$$\beta = \frac{1}{k_b T}. \tag{2.2}$$

Here T is the temperature and k_b is the Boltzmann's constant. The probability P_μ to be in a state is given by

$$P_\mu = \frac{1}{Z} e^{-\beta E_\mu}. \tag{2.3}$$

The mean (first moment) value of a parameter of the Hamiltonian is related to the probability by the equation

$$\langle X \rangle = \sum_\mu X_\mu P_\mu = \frac{1}{Z} \sum_\mu X_\mu e^{-\beta E_\mu}. \tag{2.4}$$

Where, X is the parameter which is being calculated the mean for. Similarly, the second moment of a parameter is defined as

$$\langle X^2 \rangle = \frac{1}{Z} \sum_\mu X_\mu^2 e^{-\beta E_\mu}. \tag{2.5}$$

The standard deviation σ_X, which is a measure of how much a quantity is fluctuating around a mean, is given by

$$\sigma_X^2 = \langle (X - \langle X \rangle)^2 \rangle = \langle X^2 \rangle - \langle X \rangle^2. \tag{2.6}$$

Now, with the above equations one may calculate the mean energy and the variance of the energy. The energy $U = \langle E \rangle$ is given by

$$U = \langle E \rangle = \frac{1}{Z} \sum_\mu E_\mu e^{-\beta E_\mu} = \frac{-1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\partial \log Z}{\partial \beta}. \tag{2.7}$$

The second moment of the energy is defined as follow:

$$\langle E^2 \rangle = \frac{1}{Z} \sum_\mu E_s^2 e^{-\beta E_\mu} = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2}. \tag{2.8}$$

The variance of the energy is given by

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2} - \left[\frac{1}{Z} \frac{\partial Z}{\partial \beta} \right]^2 = \frac{\partial^2 \log Z}{\partial \beta^2}. \tag{2.9}$$

Another quantity of interest, which is closely related to the variance of the energy is the specific heat capacity, which is the amount of heat required to change the temperature of some matter. The specific capacity heat per spin is given by the following equation

$$c = \frac{1}{N} \frac{\partial U}{\partial T} = \frac{-k_b \beta^2}{N} \frac{\partial U}{\partial \beta} = \frac{k_b \beta^2}{N} \frac{\partial^2 \log Z}{\partial \beta^2} = \frac{k_b}{N} [\beta \sigma_E]^2. \tag{2.10}$$

Where, N is the number of spins. In addition one knows from thermodynamics that the specific heat capacity is also related to the entropy,

$$C = T\frac{\partial S}{\partial T} = -\beta\frac{\partial S}{\partial \beta}. \tag{2.11}$$

Where, S is the entropy of the system, or in words the number of possible arrangements of the system. One can get an expression for the entropy by using eq. (2.11) and eq. (2.10) and integrating up the expression with respect to β, this results in

$$S = -k_b\beta\frac{\partial \log Z}{\partial \beta} + k_b \log Z. \tag{2.12}$$

The integration constant for S is set to zero because the entropy tends to zero as the temperature tends to zero. It is also useful to define the (Helmholtz) free energy which is the amount of energy that can be converted to work at constant temperature and volume,

$$F = U - TS = -\beta^{-1}\log Z. \tag{2.13}$$

If one consider a system of spins $\vec{S}_i$ and are interested in the magnetization $\vec{h}$, and magnetic susceptibility χ. It is necessary to add a magnetic field term to the Hamiltonian, resulting in the following partition function

$$Z = \sum_\mu e^{-\beta\left(E_\mu - \vec{h}\sum_i \vec{S}_i\right)} = \sum_\mu e^{-\beta\left(E_\mu - \vec{h}\cdot\vec{s}\right)}. \tag{2.14}$$

Where $\vec{s} = \sum_{i=1}^N \vec{S}_i$, is the sum of spins. To get the magnetization one do

$$\vec{M} = \langle\sum_{i=1}^N \vec{S}_i\rangle = \frac{\sum_\mu \vec{s}e^{-\beta\left(E_\mu - \vec{h}\cdot\vec{s}\right)}}{Z} = \frac{1}{\beta}\frac{\partial \log Z}{\partial\vec{h}} = -\frac{\partial F}{\partial\vec{h}}. \tag{2.15}$$

Here, i is the site on the lattice and if one are interested in a specific direction then

$$M_\alpha = \langle\sum_{i=1}^N \vec{S}_{i,\alpha}\rangle = \frac{\sum_\mu \vec{s}e^{-\beta(E_\mu - h_\alpha\cdot s_\alpha)}}{Z} = \frac{1}{\beta}\frac{\partial \log Z}{\partial h_\alpha} = -\frac{\partial F}{\partial h_\alpha}. \tag{2.16}$$

Where, α is the direction.

The magnetization per spin is simply

$$\vec{m} = \frac{\vec{M}}{N}, \tag{2.17}$$

and similarly the magnetization per spin in a certain direction is

$$m_\alpha = \frac{M_\alpha}{N}.$$ (2.18)

The magnetic susceptibility per spin, which is a dimensionless parameter that tells you how much a material is magnetized when a magnetic field is applied. It is defined as

$$\chi_{\alpha,\gamma} = \frac{1}{N}\frac{\partial M_\alpha}{\partial h_\gamma} = \frac{1}{N\beta}\frac{\partial^2 \log Z}{\partial h_\alpha \partial h_\gamma} = \frac{\beta}{N}\Big(\frac{1}{Z}\sum_\mu s_{\mu,\alpha}s_{\mu,\gamma}e^{-\beta(E_\mu - h_\alpha \cdot s_{\mu,i} - h_\gamma \cdot s_{\mu,\gamma})}$$

$$- \left[\frac{\sum_\mu s_{\mu,\alpha}e^{-\beta(E_\mu - \alpha \cdot s_{\mu,\alpha})}}{Z}\right]\left[\frac{\sum_\nu \sum_l s_{\nu,\gamma}e^{-\beta(E_\nu - h_\gamma \cdot s_{\nu,\gamma})}}{Z}\right]\Big)$$

$$= \frac{\beta}{N}\left[\langle M_\alpha M_\gamma \rangle - \langle M_\alpha \rangle \langle M_\gamma \rangle\right].$$ (2.19)

Because of symmetry in the 3D XY model there are only two susceptibilities, one longitudinal magnetic susceptibility per spin χ_L which is pointed along the magnetic field and one transverse magnetic susceptibility per spin χ_T which is perpendicular to the magnetic field. The two susceptibilities are defined as:

$$\chi_L = \frac{1}{N}\frac{\partial M}{\partial h} = \frac{1}{N}\langle (S^{||})^2 \rangle - \langle S^{||} \rangle^2,$$ (2.20)

and

$$\chi_T = \frac{1}{N}\frac{M}{h} = \frac{1}{N}\langle (S^\perp)^2 \rangle.$$ (2.21)

Here, $S^\perp$ and $S^{||}$ are the spins perpendicular and along the direction of the applied magnetic field. Here, M is the magnetization along the direction of the field. For $t > 0$ there is no way to distinguish the two. When $t < 0$ and a field is present it is possible to distinguish them by two methods. One is to apply a field so that one know the direction of the average magnetization. Since $\chi_T \sim \frac{1}{h}$ and $\chi_L \sim \frac{1}{h^{\frac{1}{2}}}$ [3] it is possible to distinguish them.

Finally, one have the correlation length ξ which is related to the correlation function G

$$G(i,j) = \langle \vec{S}_i \cdot \vec{S}_j \rangle - \langle \vec{S}_i \rangle \langle \vec{S}_j \rangle \sim \exp\left(\frac{-|\vec{r}_i - \vec{r}_j|}{\xi}\right).$$ (2.22)

Here $\vec{r_i} - \vec{r_j}$ is the distance between two spins. The correlation function gives a measure of how dependent two point are to each other. So if $G \sim 1$ the change of one point will change the other in a similar way, while if $G \sim 0$ there is no connection between the points. By taking the Fourier transform of eq. (2.22) with transformation

$$\vec{S_j}(\vec{q}) = \sum_{j=1}^{N} e^{i\vec{q}\cdot\vec{r_j}}\vec{S_j}. \tag{2.23}$$

Where, $\vec{q}$ is the reciprocal length. The resulting reciprocal correlation function for long wave lengths is given by [4]

$$\tilde{G}(\vec{q}) \sim \frac{1}{\frac{1}{\xi^2} + \vec{q}^2}. \tag{2.24}$$

Where, the tilde denotes that is the reciprocal correlation function.

2.2 Phase Transitions

In nature there is an abundance of phase transitions and they are popular amoung physicist because important how material properties change and because they are notoriously difficult to solve. The most famous example is the 2D Ising model which Lars Onsager [5] solved by a mathematical tour de force. In a broad sense it is a transition of a substance from one phase to another upon varying some external condition (e.g. temperature, pressure, etc.). Here, a phase is also a broad term, which could denote the magnetisation, crystallinity, etc., of a substance. In this thesis however the term phase transition will be restricted to mean the transition from an unordered magnetic phase (spins point in arbitrary direction) at high temperature to the abrupt ordering (most spins point in the same direction) at the lower, critical temperature. The phase will stay ordered as one continue to lower the temperature from the critical temperature, it will also be considered a phase transition if the process goes the other direction, i.e. ordered to unordered. One of the hallmarks of phase transition is symmetry breaking of some order parameter, and this is exactly what happens when the magnetization choose a direction to be ordered in when the temperature is lowered to the critical temperature or below.

Those transitions who have discontinuities in their first derivative of one or more of the thermodynamic potentials (such as internal energy, Helmholtz free energy, etc.) are called *first order transitions* [6]. Examples of such
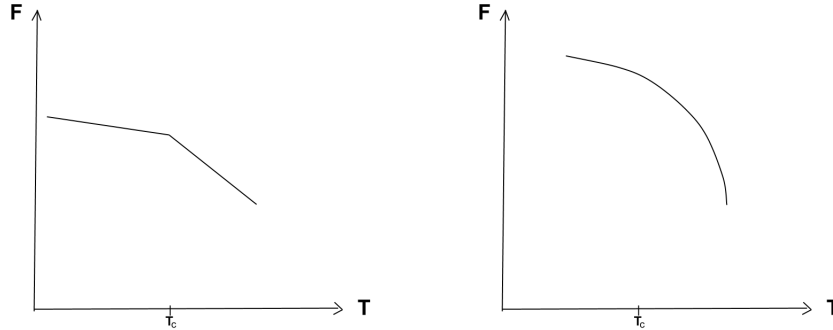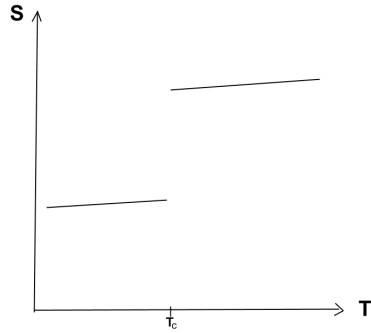
(a) The free energy plotted vs the temperature for a first order phase transition.

(b) The free energy plotted vs the temperature for a continuous (here second order) phase transition.
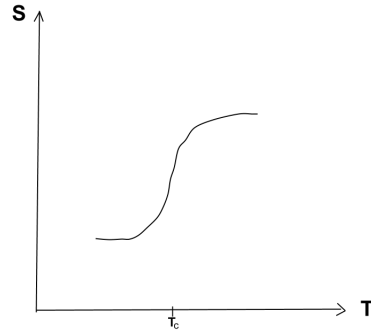
Figure 2.1

transitions are the liquid-solid and liquid-gas transitions for water. On the left hand side of figures 2.1, 2.2 and 2.3 one can see examples of figures for such a transition.

In the transitions where the first derivative of the thermodynamic potential is continuous, while higher order derivatives are discontinuous are called *continuous phase transitions* [6]. Examples of such transitions are superconducting transition. On the right hand side of figures 2.1, 2.2 and 2.3 one can see examples of how quantities vary for a continuous transition. It is this kind of phase transition which is happening in the 3D XY model.

Most problems in physics deal with a large number of degrees of freedom. For example in materials there are more than 10^{23} number of electrons and without simplifications it would be impossible to calculate, lets say the wave function. Normally, one can simplify problems greatly by assuming that some density of the system (e.g. energy) is independent of system size at equal temperature and pressure. This is correct down to a system size at certain length, called the correlation length ξ. This does not change the properties of the material [7]. When the ξ is small one can use series expansion, perturbation, etc. to calculate the relevant properties (even though one normally has to do further approximations). However, as one approaches the phase transition the ξ increase, and eventually at the critical point it diverges. This means that the methods mentioned above will not work and this brings us to renormalization theory and the next section.
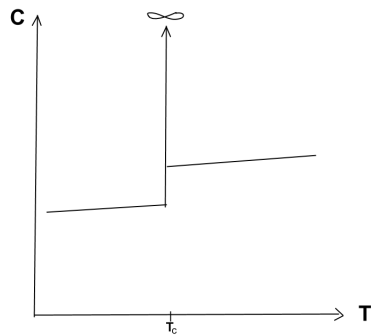
(a) The entropy $S = -\frac{\partial F}{\partial T}$ plotted vs the temperature for a first order phase transition. Here one see the discontinuity in the first derivative of F.
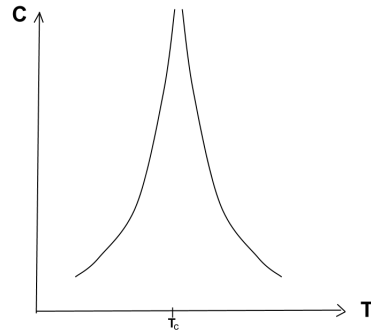
(b) The entropy $S = -\frac{\partial F}{\partial T}$ plotted vs the temperature for a continuous (here second order) phase transition.

Figure 2.2

(a) The heat capacity $C = -T\frac{\partial^2 F}{\partial T^2}$ plotted vs the temperature for a first order phase transition. Because of the discontinuity in the first derivative the second derivative is diverging at T_c.

(b) The heat capacity $C = -T\frac{\partial^2 F}{\partial T^2}$ plotted vs the temperature for a first continuous (here second order) phase transition. The heat capacity is diverging at T_c.

Figure 2.3

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2.3 Renormalization theory

The renormalization theory (RG) was developed in the 1960s by Kenneth G. Wilson, although many other contributed such as L. P. Kadanoff and M. E. Fisher, to mention some. The theory is widely used in phase transitions [7] and in almost all field theories [8]. A thourough review of the RG is beyond the scope of this report. The interested reader is referred to the authors Wilson, Delamotte and Fisher [6, 7, 8] for great reviews and introductions to the subject. The goal of RG to calculate critical exponents and it can show which details which are important and which are not. Is useful in the vicinity of the phase transition because the data is here unknown. Fluctuations of large length scale govern the critical behaviour and renormalization theory can show which parameters matter for the model. The two main task for renormalization theory is therefore:

- Simplifying a task by reducing the number of degrees of freedom.

- Explain how qualitative features arise, i.e. scaling laws and critical exponents.

Universality is closely related to renormalization and scaling. The universality hypothesis states that two different physical systems can show the same behaviour close to the critical point if they share the same essential symmetry [9, 10]. Where essential symmetry are the spatial dimensions, symmetry of the Hamiltonian, number of components of the order parameter and the range of microscopic interactions. Two different systems in the same universality class will share the mentioned essential symmetry, in addition to having the same critical exponents. For instance will the liquid-gas phase transition for different liquids have the same critical exponents, independent of the chemical composition of the liquid.

Suppose the original system is a spin-system with lattice spacing L_0. In order to reduce the degrees of freedom one can rescale the spacing to $2L_0$ and thereby forbidding fluctuations which is smaller than $2L_0$. This process can be done repeatedly, until the separation is of the order of the correlation length ξ. The simplification in renormalization theory is that the interactions $\mathcal{H}_1$, $\mathcal{H}_2$, ...,$\mathcal{H}_n$ are only coupled directly to nearby interactions [6] so that

$$\tau\left(\mathcal{H}_0\right) = \mathcal{H}_1, \qquad \tau\left(\mathcal{H}_1\right) = \mathcal{H}_2, \qquad \tau\left(\mathcal{H}_2\right) = \mathcal{H}_3, \qquad \text{etc..} \qquad (2.25)$$

Where τ is a transformation operation. A fixed point as reached when the transformation τ as no further effect on the effective interaction $\mathcal{H}$,
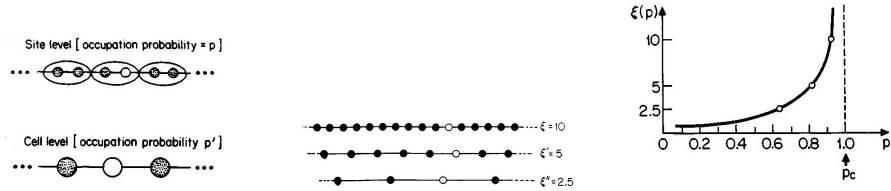
(a) A figure taken from [11] which show how the chain is merged together, when $L \to 2L$.

(b) Another figure taken from [11] which show how the chain is affected by the transformation.

(c) A figure taken from [11] which shows a plot of the correlation length ξ vs the occupation probability p.

Figure 2.4

$$\tau\left(\mathcal{H}^*\right) = \mathcal{H}^*. \tag{2.26}$$

The correlation length is now $\xi \sim 2^n L_0$ and one has a finite number of degrees of freedom which hopefully can be solved by some further approximation.

The most intuitive example the author has found is the problem of a 1D-percolation and it is greatly presented in [11] by E. H. Stanley. The problem is as following: Suppose on have a 1D chain where each site has an occupation fraction p, see fig. (2.4a). The question is then: is the chain broken? In the same figure one can see how the effect of the renormalization (or merging of sites). The "renormalized" occupation parameter p' can be written as

$$p' = \tau_b(p). \tag{2.27}$$

Where $\tau_b(p)$ is the renormalization transformation. For the one dimensional case the $\tau_b(p) = p^b$ and eq. (2.27) becomes

$$p' = p^b. \tag{2.28}$$

Where $b = 2$ for the Kadanoff cells as in this example. So if one start at $p = 0.9$ then $p' = p^2 = 0.81$ and so on. This results in the figure (2.5a) and the two fixed points $p* = [0, 1]$. Where one recognise $p* = 1$ as an unstable fixed point and $p* = 0$ as a stable fixed point. Therefore one see by doing renormalization one can show that the occupation probability p leads to two

13
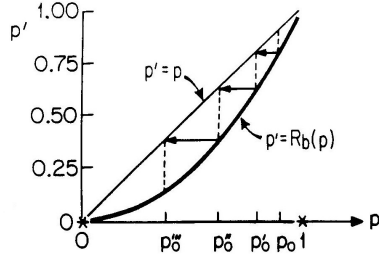
(a) The figure is taken from [11] and is showing how the renormalized occupation parameter p' goes as a function of the occupation parameter p. Here it is clear that it is two fixed points, namely $p* = [0, 1]$.
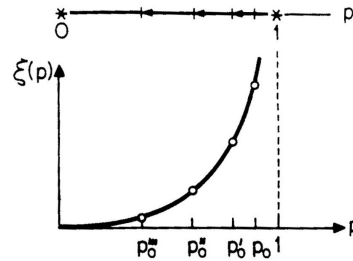
(b) The figure is taken from [11] and is showing how the correlation length is changing with the renomalized occupation parameter p'.

Figure 2.5

possibilities. Namely, a stable point where the chain is broken and a unstable point where the chain is connected.

When a Hamiltonian is renormalized to larger and larger scales close to a critical point there are three types of parameters one can have in the Hamiltonian. Relevant parameters, which increase. Irrelevant parameters, which decrease and therefore only contribute with corrections to scaling. Dangerously-irrelevant parameter however, cannot be neglected since their effect can be felt arbitrarily close to the phase transition [12].

2.4 Critical Exponents

It is a fact that many experimental systems [11] show this exponential decay and growth of phases sufficiently close to the critical temperature, although the term "sufficiently close" varies a lot from system to system [11]. The critical exponents can be extracted by the mean field theory for higher dimensional systems (4 or more for the O(n)-model) or by renormalization for lower [7].

In the 1960s there was a revolution in the understanding of critical exponents, and it is greatly summarized M. E. Fisher [6]. For second order phase transition one can split the free energy density into two functions
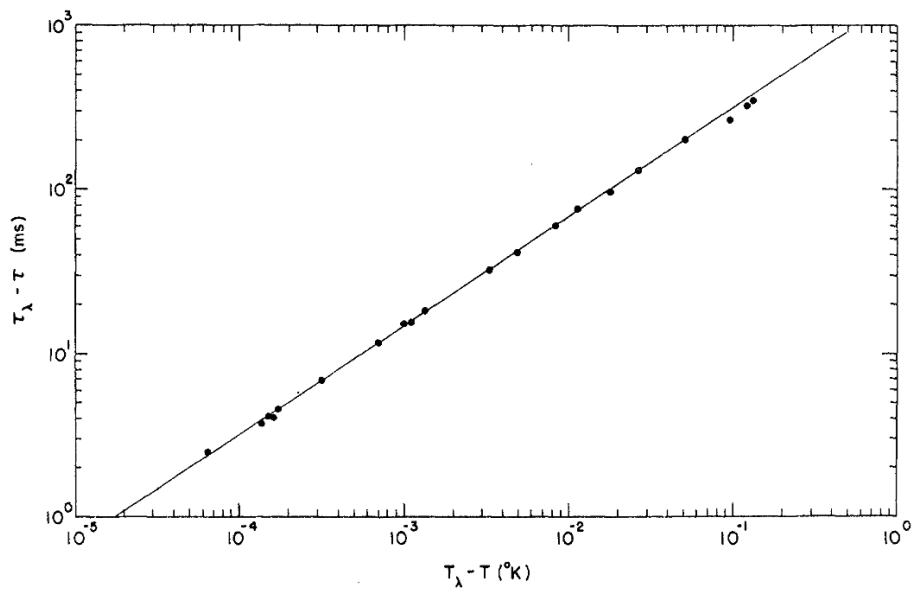
Figure 2.6: A figure from [13], where one see a plot of the density (y-axis) of Helium-4 near the critical temperature, where the x-axis is the temperature. One clearly see the growth of power $\frac{2}{3}$.

$$f = f_r + f_s \tag{2.29}$$

Here, f_r is the regular part of the free energy function and f_s is the singular (diverging) part of the free energy function. The singular function f_s scales as follow

$$f_s = b^{-d} f\left(tb^{y_t}, hb^{y_h}, h_p b^{y_{h_p}}, \frac{L}{b}\right) \tag{2.30}$$

f is now redefined to mean the scaling function for f_s and b is a positive scale factor. Each term in the scaling function is scaled with b to some power. d is the spatial dimension, L is the size of the system, $t = \frac{T-T_c}{T_c}$ is the reduced temperature, h is the strength of the field, h_p is the strength of the anisotropy and y_t, y_h, y_{h_p} are the exponents to the parameters of the system.

Sufficiently close to the phase transition and by letting $b = t^{\frac{-1}{y_t}}$ one may write the free energy function as

$$f_s = t^{\frac{d}{y_t}} f\left(1, ht^{\frac{-y_h}{y_t}}, h_p t^{\frac{-y_{h_p}}{y_t}}, Lt^{\frac{1}{y_t}}\right) \tag{2.31}$$

If one consider a system of zero field and zero anisotropy some physical will have a $(Lt^{\frac{1}{y_t}})^\lambda = x^\lambda$ dependence as one approach the phase transition $(t \to 0)$

$$g(x) \sim x^\lambda \text{ as } x \to 0. \tag{2.32}$$

Here g is just some derivative of the singular free energy density giving some parameter, i.e. the magnetization. λ is the critical exponent for that physical quantity. Note that one cannot simply assume that $g(x)$ is proportional to x^λ, one must always expect higher order terms or non-simple cases of eq. (2.32), see [6] for a further discussion. From eq. (2.32) one can define the critical exponent λ as

$$\lambda = \lim_{x \to 0} \frac{\log |g(x)|}{\log |x|}. \tag{2.33}$$

Sufficiently close to the phase transition physical quantities show an exponential dependence as in figure 2.6. The critical exponents for the magnetization can be obtained by using equation 2.31 and 2.15 and letting $t \to 0$

$$m \sim \frac{\partial F}{\partial h} \sim |t|^{\frac{d-y_h}{y_t}} \sim |t|^\beta \tag{2.34}$$

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Similarly the exponents can be obtained for the heat capacity c, the magnetic susceptibility χ and the correlation length ξ

$$\xi \sim |t|^{-\nu}, \tag{2.35a}$$

$$c \sim |t|^{-\alpha}, \tag{2.35b}$$

$$\chi \sim |t|^{-\gamma}. \tag{2.35c}$$

2.5 Finite Size Scaling

Finite size scaling is a method of finding numerical constants and the transition temperature by using different system sizes. The physical quantity are dependent on the system size, the critical exponent and a scaling function. By using the correct critical exponents on the scaling of different system sizes the plots should collapse on one single line for sufficiently large system sizes sufficiently close to the transition.

2.5.1 The Scaling Relations

It is possible to relate the different critical exponents to each other. This can be done by starting with the free energy density without anisotropy. The explanation given here follow [14]. The scaling hypothesis states that the singular part of the free energy density is a homogeneous function near a second-order phase transition [14, 15]. Now one can write the equation 2.31 where the finite size effect is not considered as

$$f_r(t, h, h_p = 0) = t^{\frac{d}{y_t}} f\left(1, ht^{\frac{-y_h}{y_t}}, 0, 0\right) \tag{2.36}$$

Now by using equation (2.36) with the definitions of M, C, ξ, M, G and ξ one can get a relations between the different critical exponents (α, β, γ, δ, d, η, ν). Since they all can be derived from the free energy density f. From the magnetization per spin one get

$$m = \frac{1}{k_b T} \frac{\partial f_r}{\partial h}\Big|_{h=0} \sim |t|^{\frac{d-y_h}{y_t}} \Rightarrow \beta = \frac{d - y_h}{y_t}. \tag{2.37a}$$

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Where, h is the applied magnetic field. While the specific heat per spin give the relation

$$c = \frac{\partial^2 f_r}{\partial t^2}\Big|_{h=0} \sim |t|^{\frac{d}{y_t}-2} \Rightarrow \alpha = \frac{d}{y_t} - 2, \qquad (2.37b)$$

and the magnetic susceptibility gives

$$\chi = \frac{1}{k_b T}\frac{\partial m}{\partial h}\Big|_{h=0} = \frac{1}{(k_b T)^2}\frac{\partial^2 f}{\partial h^2}\Big|_{h=0} \sim |t|^{\frac{d-2y_h}{y_t}} \Rightarrow \gamma = \frac{d-2y_h}{y_t}. \qquad (2.37c)$$

At the isotherm M should remain finite even as $t \to 0$, this will give exponents for the magnetization per spin at the critical isotherm

$$m = \frac{1}{k_b T}\frac{\partial f_r}{\partial h} = |t|^{\frac{d-y_h}{y_h}} m'\left(|t|^{-\frac{y_h}{y_t}} h\right) \sim |t|^{\frac{d-y_h}{y_h}} \frac{h^{\frac{d-y_h}{y_h}}}{|t|^{\frac{d-y_h}{y_t y_h}}} = h^{\frac{d-y_h}{y_h}} \Rightarrow \delta = \frac{y_h}{d-y_h}.$$
$$(2.37d)$$

The correlation function has a homogeneous form $G(r) = b^{-2(d-y_h)}G\left(\frac{r}{b}, b_t^y t\right)$ and by letting $b = r$ and $t = 0$ one get

$$G \sim r^{d-2-\eta} \Rightarrow \eta = d + 2 - 2y_h \qquad (2.37e)$$

Finally, the correlation length has the following relation

$$\xi \sim |t|^{-\frac{1}{y_t}} \Rightarrow \nu = \frac{1}{y_t}. \qquad (2.37f)$$

Where $m'(x) \sim x^{\frac{d}{y_h}-1}$ is used in eq. (2.37d). From eqs. (2.37) one can obtain the following scaling relations

$$\alpha + 2\beta + \gamma = 2 \qquad \text{Rushbrook's Identity} \qquad (2.38a)$$

$$\delta - 1 = \frac{\gamma}{\beta} \qquad \text{Widom's Identity} \qquad (2.38b)$$

$$2 - \alpha = d\nu \qquad \text{Josephson's Identity (Hyperscaling Relation)} \qquad (2.38c)$$

$$\gamma = \nu(2 - \eta) \qquad (2.38d)$$

Here the exponents y_h and y_t are cancelled and since there are 6 equations and 8 exponents this means that there are only two independent exponents.

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2.5.2 Finite Size Scaling

Numerical simulations is a powerful tool which can give insight to problems which are very hard or even impossible to solve analytically. However, because of the finite size of the processing time and memory one cannot simulate infinite systems (the thermodynamic limit). Therefore there will be a difference between simulated finite systems and infinite systems. For instance in a second order phase transition the magnetic susceptibility diverges for an infinite system. For a finite system however the peak is dependent on the system size, larger system sizes gives steeper and taller peaks, see figure 3.4a. So the question is: how can one extract the exponents for the thermodynamic limit with a finite size simulation?

The simplest case for scaling is when $h = 0$ and $h_p = 0$. Then the simulated quantities differ from the thermodynamic exponents with something which is dependent on the system size and the temperature it is reasonable to introduce a scaling function g_X which has the following properties

$$g_X(x) \to const. \ as \ x \to \infty. \tag{2.39a}$$

$$g_X(x) \sim x^{\frac{Y}{\nu}} \ as \ x \to 0. \tag{2.39b}$$

Where Y denotes the critical exponent for the quantity X, e.g. for $X = M$ then $Y = \beta$. In the finite case the expression for the exponents in equations (2.35) will now have an extra part, namely the scaling function. One see that when one approach the critical temperature $(t \to 0)$ the scaling function has a exponential dependence, and when one goes infinitely far away from the critical temperature $(t \to \infty)$ the scaling function becomes simply a constant. The expression for the finite size magnetic susceptibility then become

$$\chi = |t|^\gamma \chi_0 \left(\frac{L}{\xi} \right) = \xi^{\frac{\gamma}{\nu}} \chi_0 \left(L|t|^{\frac{1}{\nu}} \right). \tag{2.40}$$

Here $\chi_0 \left(\frac{L}{\xi} \right)$ gives the finite size effect, and it has a cut-off when $\xi > L$ so that the magnetic susceptibility does not diverge. The form of equation 2.40 is not the one used in practice, because of the $|t|^{\frac{1}{\nu}}$ dependence. Therefore it is normal to define a new dimensionless function $\tilde{\chi}$

$$\tilde{\chi} \left(|t|L^{\frac{1}{\nu}} \right) = \left(|t|L^{\frac{1}{\nu}} \right)^\gamma \chi_0 \left(|t|^\nu L \right), \tag{2.41}$$

so that the equation for χ now can be written as

$$\chi = L^{\frac{\gamma}{\nu}} \tilde{\chi} \left(|t|L^{\frac{1}{\nu}} \right). \tag{2.42}$$

Now, one may write the new equations for the scaling as

$$m = L^{-\frac{\beta}{\nu}} g_M \left(tL^{\frac{1}{\nu}} \right), \tag{2.43a}$$

$$\chi = L^{\frac{\gamma}{\nu}} g_\chi \left(tL^{\frac{1}{\nu}} \right), \tag{2.43b}$$

$$c = L^{\frac{\alpha}{\nu}} g_C \left(tL^{\frac{1}{\nu}} \right). \tag{2.43c}$$

Where, g_χ is the dimensionless scaling function $\tilde{\chi}$. The scaling for m and c can be obtained in exactly the same manner as for χ. The important point about these functions is that the curves will collapse into each other for different system sizes if one are sufficiently close to the T_c and the values for the exponents are correct, see figure 3.9. Therefore it is possible to use a curve fitting program and extract the critical exponents. This sounds easy enough, however in practice this can be pretty hard. Especially since one do not know the T_c in general, and one need sufficiently large system sizes and the scaling could be dependent on several exponents. A possible way to extract the T_c is to use the Binder Cumulant which is defined as

$$U_L(X) = 1 - \frac{\langle X^4 \rangle_L}{3 \langle X^2 \rangle_L^2}. \tag{2.44}$$

Here X is a parameter such as the magnetization per spin m, energy E, etc.. At the T_c the Binder Cumulant is not dependent on the lattice size, and therefore if one plot the Binder Cumulant vs T one can easily see crossing point and hence the critical temperature $T_c \approx 2.2$ in fig. 3.7.

$$\frac{\langle M^4 \rangle_L}{\langle M^2 \rangle_L^2} = \frac{L^{\frac{-4\beta}{\nu}} g_{M^4} \left(tL^{\frac{1}{\nu}} \right)}{\left(L^{\frac{-2\beta}{\nu}} g_{M^2} \left(tL^{\frac{1}{\nu}} \right) \right)^2} = \frac{g_{M^4} \left(tL^{\frac{1}{\nu}} \right)}{g_{M^2} \left(tL^{\frac{1}{\nu}} \right)^2} \tag{2.45}$$

Because of equation 2.39b the equation (2.45) goes to the same constant value for different system sizes L at the critical temperature. This is because the equation (2.45) is only dependent on $tL^{\frac{1}{\nu}}$, and for $t = 0$ all the system sizes should take the same constant value. The Binder Cumulant is therefore a good quantity to obtain the critical temperature and critical exponent ν from. Another possibility is to use the location of the peak of the magnetic susceptibility, but normally the Binder Cumulant is better to use.

Now if one want to scale the magnetic susceptibility with a magnetic field and an anisotropy the scaling is not as simple as in 2.42 and one have to add additional terms to the scaling function and the results is a scaling dependent on several parameters and this makes the plots much more difficult to fit.

$$\chi = L^{\frac{\gamma}{\nu}} \tilde{\chi} \left(h L^{y_h}, h_p L^{y_{h_p}}, |t| L^{\frac{1}{\nu}} \right), \tag{2.46}$$

or with the parameters from equation 2.37 and $y_{h_p} = \frac{1}{\nu_p}$

$$\chi = L^{\frac{\gamma}{\nu}} \tilde{\chi} \left(h L^{\frac{d+2-\eta}{2}}, h_p L^{\frac{1}{\nu_p}}, |t| L^{\frac{1}{\nu}} \right). \tag{2.47}$$

One interesting fact is that the anisotropy does not effect the scaling for all the parameters except for the order parameter m_p and the magnetic susceptibility χ when $t > 0$. As will be shown in the next section and is supported by the results.

One may express the f_s with the critical exponents similar to equation 2.47 as

$$f_s = L^{-d} f \left(h L^{d-\frac{\beta}{\nu}}, h_p L^{\frac{1}{\nu_p}}, |t| L^{\frac{1}{\nu}} \right). \tag{2.48}$$

2.5.3 Scaling with Dangerously Irrelevant Parameters

The anisotropy in the Hamiltonian eq. (1.1) for the 3D XY model makes the scaling somewhat different from eq. (2.43). This is because the scaling is dangerously irrelevant for the parameters. Which means that the effect of the anisotropy cannot be renormalized away and there will be an effect on the scaling function, in [16] its proposed the scaling is normal for all but the order parameter, and it has the following scaling

$$m_p = L^{\frac{-\beta}{\nu}} g_{M_p} \left(|t| L^{\frac{-1}{y_{h_p}}} \right) = L^{\frac{-\beta}{\nu}} g_{M_p} \left(|t| L^{\frac{1}{\nu_p}} \right). \tag{2.49}$$

Here one see that ν is replaced in the scaling function by the new exponent ν_p, which is an effect of the anisotropy. Equation (2.49) can also be derived from conventional scaling arguments from the following equation [16]

$$P \left(\vec{h}; L, t, a \right) = L^{\frac{\beta}{2\nu}} \hat{P} \left(|t| L^{d-\frac{\beta}{\nu}} \vec{h}, h_p L^{\frac{1}{\nu_p}} \right). \tag{2.50}$$

Here $P \left(\vec{h} \right)$ is the order parameter distribution, h_p is the strength of the anisotropy, $\hat{P}$ is the scaling function and $\frac{1}{\nu_p} > 0$ is the dimension of the anisotropy. See [17] for a derivation of the scaling relation with a renormalization group approach.

Chapter 3

Results and Discussion

In this section the results obtained by the simulations of the model presented in the introduction section. A short summary of results by others is also presented. The summary of the code can be found in the Appendix A. In the figures following below the L denote a $L \times L \times L$ lattice.

3.1   Summary of Previous Work

There is done a lot of work on the 3D XY universality class. In this section relatively new work will be summarized. Normally such simulations are run over large time scales in order to get accurate results. For this master thesis there has been obtained results supporting [18] and with more time accurate results could have been obtained.

3.2   The Magnetization

For an infinite system with $h = 0$ and $t < 0$, one expect that most spins point in the same direction and hence that the magnetization is over zero. At the critical temperature the systems goes abruptly to zero as in fig. 3.1a, and above the critical temperature all the spins point in random directions and hence the magnetization is zero. For the case of an applied magnetic field the plot is somewhat similar (see figure 3.1b). The main differences is that the abrupt change is soften and moved to a higher temperature and the magnetization is not zero above the critical temperature, but rather slowly closing in as the temperature is increased.

For a finite system in zero field one expect that the abrupt transition at T_c get smeared out (not abrupt with respect to the temperature) and

Table 3.1: Estimates of the critical exponents for the 3D XY universality class without anisotropy. The symbol * indicates that the results are obtained by the scaling relations in eq. (2.38a). The different methods used are: MC = Monte Carlo, HT = High temperature expansion , IHT = Improved HT, FT = Field Theory and 4He = Experimental result.

p=0					
Refrence	Method	γ	ν	η	α
[18]	MC + IHT	1.3177(5)	0.67155(27)	0.0380(4)	-0.0146(8)*
[18]	MC	1.3177(10)	0.6716(5)	0.0380(5)	-0.0148(15)*
[19]	HT				-0.014(9), -0.022(6)
[20]	FT	1.3169(20)	0.6703(15)	0.0354(25)	-0.011(4)
[20]	FT	1.3110(70)	0.6680(35)	0.0380(50)	-0.004(11)
[21]	4He		0.67019(13)*		-0.01056(38)
[22]	T_c= 2.2019				

Table 3.2: Estimates of the critical parameters for anisotropic cases.

Reference	Method	parameter
[16]	MC with cluster	$\nu_4 = 0.72$
Reference	Method	parameter
[1]	MC with cluster	$\nu_6 = 0.75$

that it is not zero above T_c, but rather closing in on zero as T increases. In figure 3.2 one see plots of different lattice sizes. One note that as the as the lattice size decrease the plots become more and more different to that of the $L \to \infty$. This is what is called finite size effects see [23] for a introduction to Monte Carlo simulations where finite size effects are described, along with finite size scaling.

Finally, in figure 3.3 one can see the effect of both finite size scaling and the applied magnetic field. One note that the difference of the plot without field has a smaller difference from that with a field as the system size is decreased, i.e. the smaller the system size the more similar is the field and non-field cases. The critical temperature is increased and the transition is more smooth.
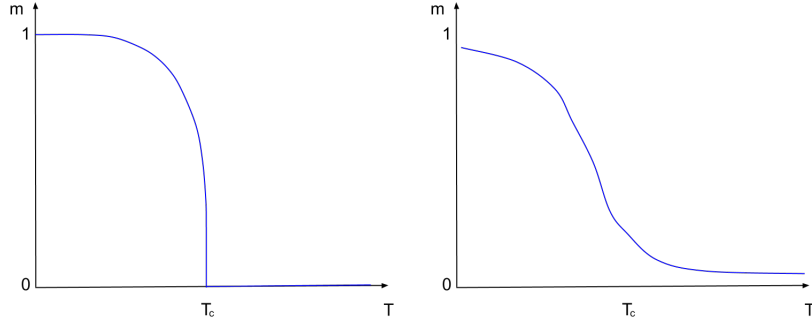
(a) The theoretically expected shape of the magnetization for an infinite system with zero external field.

(b) The theoretically expected shape of the magnetization for an infinite system with an external field.
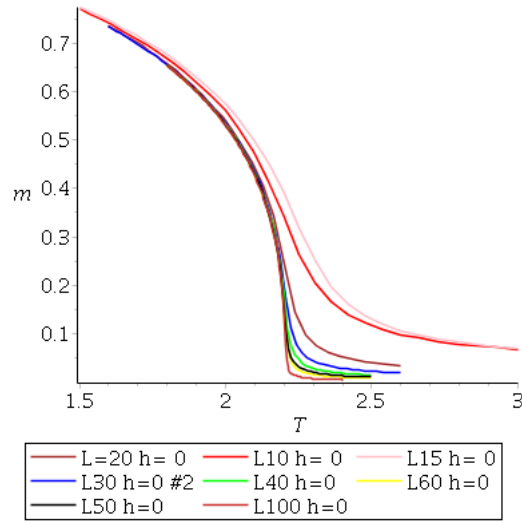
Figure 3.1

Figure 3.2: The magnetization for the cubic anisotropic case when no magnetic field is applied. It is easy to see that as the system size increases the system critical behaviour becomes more and more similar to that of the $L \to \infty$.

3.3 The Magnetic Susceptibility

As for the magnetization, one get an effect on the magnetic susceptibility from the finite lattice size and if one add a field. In figure 3.4 one can see
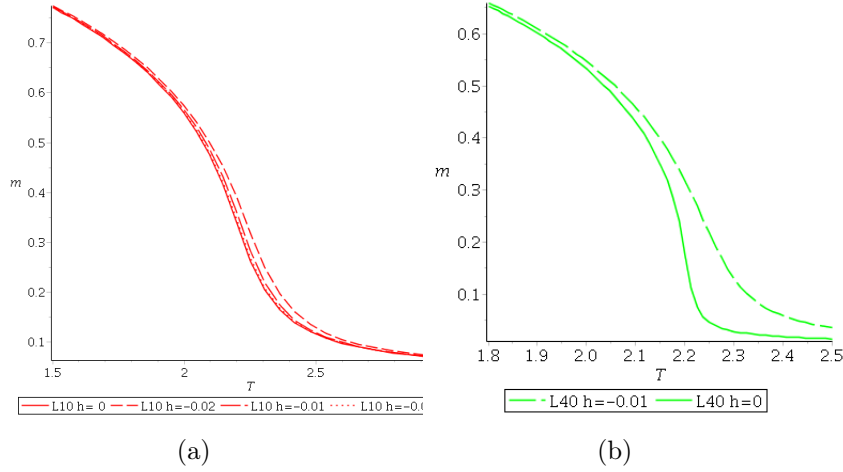
(a)   (b)

Figure 3.3: In figure 3.3a the magnetization in zero field is shown for the system size L=10 and in figure 3.3b for L=40. The effect of adding a field is that the plot is smother and the critical temperature is moved to a higher temperature, this effect becomes more apparent when the system size is large. When $L = 10$ one cannot see the shift when a field is present since all the plots are on top of each other, for $L = 40$ however it is easy to see the shift.

the effect of having different lattice sizes. Clearly as one increase L the peak of the magnetic susceptibility also increases and gets narrower. One see from figure that when going from $L = 30$ to $L = 40, 50, 100$ the peak increases with approximately a factor of 1.8, 2.5 and 10. By letting $L \Rightarrow \infty$ one expect that the peak diverges, as we expect from a second order phase transition. In figure 3.5 one can see how applying a magnetic field effect the magnetization per spin. One clearly see that when the field is increasing the peak is decreasing, expanding and the centre of the peak is shifted to an higher temperature.

The observant reader might ask how the magnetic susceptibility is calculated. The way it is done in the program is by doing an average over the spins $\bar{m} = (\sqrt{\sum_i \vec{S}_i})^2$ and then using this to quantity to calculate an approximate magnetic susceptibility which is a melange of χ_L and χ_T and it is $\bar{\chi} = \frac{\langle \bar{m}^2 \rangle - \langle \bar{m} \rangle^2}{NT}$ which is shown in the results.
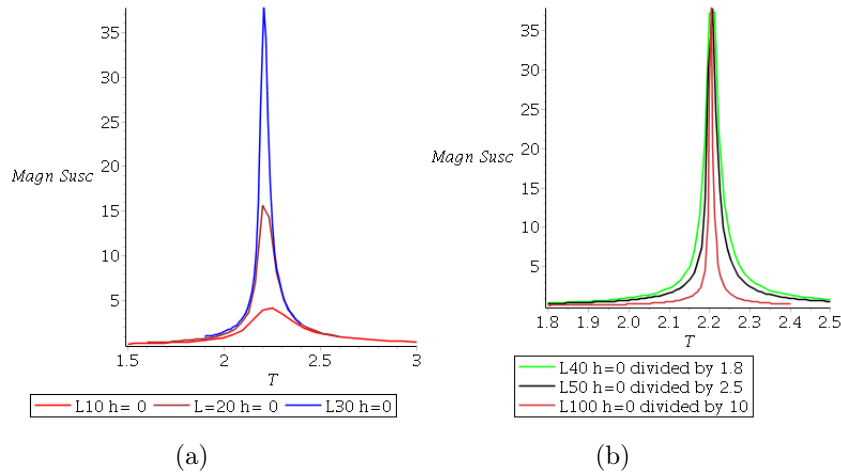
Figure 3.4: Plots of the magnetic susceptibilities when there is no field applied. The peak of the magnetic susceptibility is increased and sharpened as the system size is increased.
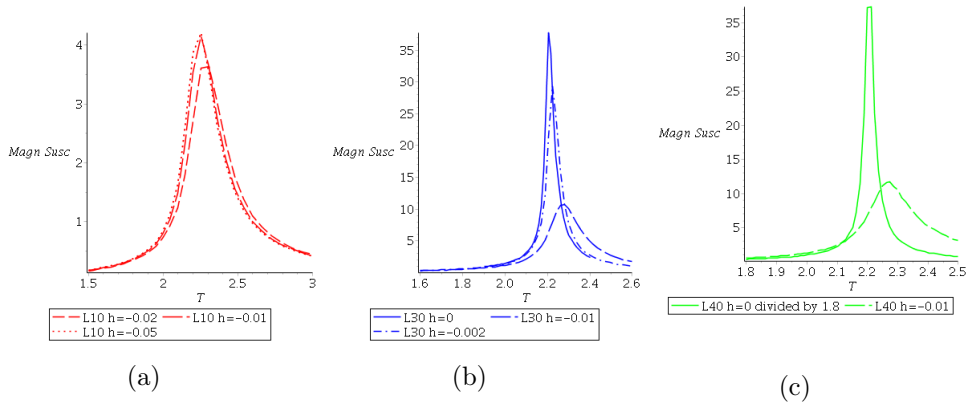

Figure 3.5: The magnetic susceptibility for different system sizes where one vary the applied field. The effect of a field is that the peaks get smaller and wider. Their center are also moved to a higher temperature.

3.4 The Order Parameter

The order parameter is defined in 1.2 and it will tell you what phase the system is in. In figure 3.6a, one can see that for sufficiently large system sizes the order parameter tends to zero when the temperature goes above the critical temperature, just as for the magnetization. When a field is

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added, see figure 3.6c, the effect on the order parameter is similar to that of the magnetization, namely that the order parameter gets a higher transition temperature.
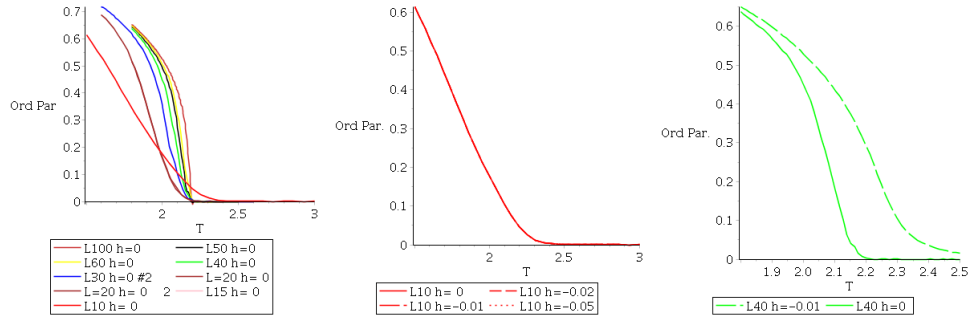
(a) The order parameter m_4 for different system sizes at zero field.

(b) The order parameter m_4 for different fields when $L = 10$.

(c) The order parameter for m_4 for different fields when $L = 40$.

Figure 3.6: The order parameter goes to zero in zero field at $T \approx 2.2$ and smoothed out and shifted to an higher temperature if a field is present.

3.5   The Binder Cumulants

As mentioned in section 2.5.2 the plots of the different system sizes should cross when they are at the T_c for the Binder Cumulant if there is no field and anisotropy present. This can be done for many parameters, such as the magnetization and order parameter. In figures 3.7 and 3.8 these quantities are plotted. For the zero applied field (3.7a and 3.8a) it is clear that the plots cross at a temperature $T_c \approx 2.2$. The result of a field is that the plot is displaced from the non-field plot and the effect gets larger with the system size as before. When a field is applied there is also no crossing of plots for different system sizes for the Bidner Cumulant. This is expected since the scaling that has been used does not take into account the field.

3.6   Finite Size Scaling

By doing scaling with the correct exponents one should be able to get the curves to collapse, at least for sufficiently large system sizes close enough to the critical temperature. In the figure 3.3 the magnetization is scaled as in
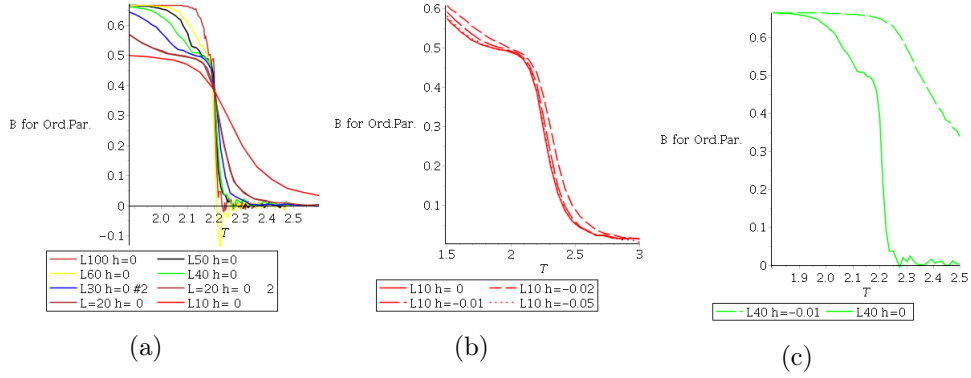
Figure 3.7: The Binder cumulant for the order parameter m_4. For the zero field the crossing is $T \approx 2.2$. If a field is present the Binder cumulant do not cross since one have to take into account the field in the scaling.
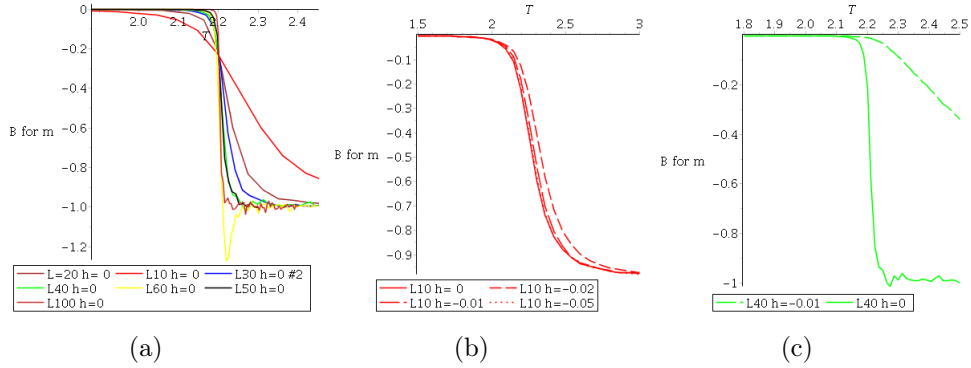

Figure 3.8: The Binder cumulant for the zero field is crossing on $T \approx 2.2$. If a field is present the Binder cumulant do not cross since one have to take into account the field in the scaling.

equation 2.43a. The fit in figure 3.3 is very good sufficiently close to the transition ($|t|L^{\frac{1}{\nu}} < 5$).

Since the fit of the magnetization was good the critical temperature and the critical exponents ν, β and ν_p in the tables 3.1, 3.2 and article [1] are supported by the simulation done here. The effect of an external field is similar to before. Namely, that the plot with field is moved away from the plot without field and the effect becomes more and more apparent as the system size is increased.

For the order parameter the scaling is a bit more complicated, see equa-
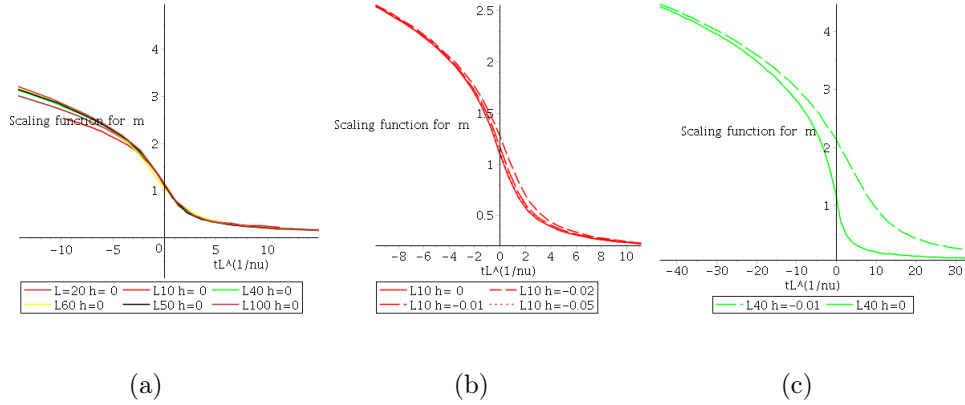
28

(a) (b) (c)

Figure 3.9: The collapse of the rescaled magnetization was good when no field was added. This supports that the anisotropy does not affect the scaling of the magnetization. By adding a field the collapse was not good. This effect get more apparent with larger system sizes.

tion 2.50. The fitting here was not as good as for the magnetization. A reason for this is that the results for the m_4 is fluctuating more, and therefore it is more difficult to make a good fit. This is especially true for $L = 100$, and since larger systems require longer time (more MC runs) to be equilibrated this size should have been run for a longer time.
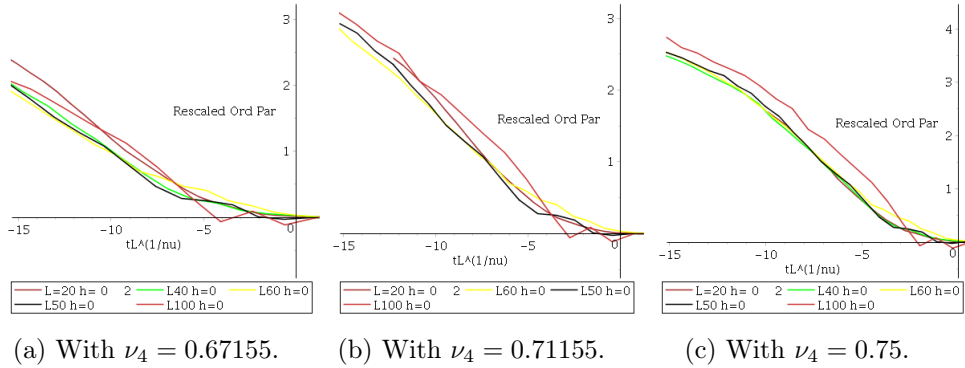

(a) With $\nu_4 = 0.67155$. (b) With $\nu_4 = 0.71155$. (c) With $\nu_4 = 0.75$.

Figure 3.10: The collapse of the order parameter m_4 is promising, meaning that the parameter ν_4 is affecting by the anisotropy. However, more accurate results need to be acquired and a curve collapsing measure has to be programmed because it is hard to say which fit is the best.

The magnetic susceptibility was scaled with equation 2.43b, the results

can be seen in figure 3.11. In the plots there are some system sizes that do not scale well, especially for $L = 40$ and $L = 60$. One should also note that the fit looks better for $\gamma = 1.318$ for $t > 0$. While the fit looked better for $t < 0$ if $\gamma = 1.398$ was used.

(a) $\gamma = 1.318$ gave the best fit for $t > 0$.

(b) $\gamma = 1.328$.

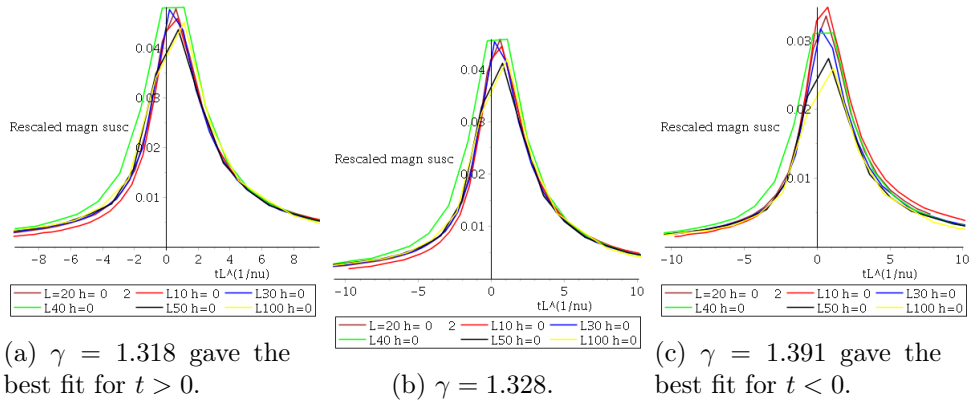(c) $\gamma = 1.391$ gave the best fit for $t < 0$.

Figure 3.11: The rescaled magnetic susceptibility was good encouraging, but more points close to the transition should be simulated to get a more smooth plot. The good fit support that the anisotropy is dangerously irrelevant since it only changes the magnetic susceptibility. Note that the scaling is best with different exponents on the two sides of the transition. This could be a novel kind of critical exponent.

One interesting thing that was noted in the results for the scaled magnetic susceptibility was that it looked like there was two values for the scaling parameter γ. One that govern the behaviour on the left of the transition and one to the right of the transition. Today it is believed that the critical exponent is equal on both sides of the transition. However, from the results obtained here one cannot exclude the possibility that anisotropy might change the exponent as one pass through the transition. If this is the case the scaling will then look like this sufficiently close to the transition

$$
\begin{aligned}
\chi &= |t|^{\gamma_{low}} \ for \ |t| < 0, \\
&= |t|^{\gamma_{high}} \ for \ |t| > 0.
\end{aligned}
\tag{3.1}
$$

For the scaled order parameter m_4 was not nearly as good as for the scaled magnetization. However, if one exclude the $L = 100$ size the fit is quite good and but in order to say something more certain about this scaling further simulation with greater accuracy and more system sizes should be

performed. In appendix B an additional scaling for the order parameter is proposed.

The simulations done here support the thought that anisotropy is dangerously irrelevant for the scaling. It only comes into play for the exponents for the order parameter and magnetic susceptibility. It is interesting to note that the border between relevant and dangerously irrelevant $p = 4$ which is the anisotropy studied here, actually gives the smallest difference in the changed critical exponents. This is completely counter intuitive since one would expect that this gave the biggest difference in the critical exponents, but in fact this gives the smallest change. This makes the simulation hard since one need accurate simulations to see the difference in the critical exponents.

3.7   Further Studies and Work

As mentioned in section 3.1 the time used on simulation in the most accurate papers of the subject, the simulations time are large. So a natural thing to do is to simply run the program with more MC iterations so the results become more accurate. In some figures, especially for large system sizes, it looks like the system has not been properly equilibrated, since the plots have fluctuations (the plot is rugged rather than smooth). See 3.7a for example. A thorough investigation of how well the system reaches equilibrium should therefore be done, see for instance [24].

A natural extension to the program would have been to add a function that can give a more scientific answer to if there is a good collapse of curves when one do the rescaling. There exist a lot of curve fitting algorithms and programs. It was also considered to use, or make a new program, based on Oliver Melchert [25] curve-fitting-program made in Python. Which is a program that can extract the scaling exponents for equations of the shape 2.43 and from there it would be possible to extend this to that of equation 1.1.

The program is fully compatible to do simulation for $p = 6$ anisotropy, and since it exist results for $p = 6$ it would be interesting to do simulation for this as well.

To get a full analysis of the current or future results one would have to add a some error estimation into the curves of the plots and therefore also the critical exponents. This is a bit painful since the scaling is more accurate close to the transition, but still fully possible to implement.

Finally, the most exiting result from these simulation is that cubic anisotropy

might lead to different critical exponents on the two sides of the critical temperature as observed in the rescaled magnetic susceptibility. The results here are not accurate or good enough to say anything certain so this is something that would have to be studied further.

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Appendix A

Summary of Code

A.1 Algorithms

The Metropolis algorithm [26] is a to important part of the program and thesis not to be mentioned. It is also very popular widely used in numerous physical problems and the origin is an interesting story [27]. The algorithm is as following

- Choose the new random state.

- Calculate the energy of the new state.

- If the new energy is lower, accept the swap. If the energy is higher, accept the swap with probability $e^{-\beta(E_{new}-E_{old})}$

The advantage of this algorithm is that is flexible and simple to implement. However, there is on big disadvantage and that is the large autocorrelation time $\tau \sim \xi^z$ [4]. Here, z is the dynamical critical exponent. The problem with MC simulations is when one approach the phase transition the correlation length diverges, this also means that the autocorrelation time diverges. This means that one get stuck in the same state and it take a lot of time to get out of this state. There are several ways to increase the speed of MC simulations, for instance cluster algorithms or parallel tempering. Parallel tempering is used in the program of this thesis and it is as following

- Exchange the lattice at two neighbouring temperatures.

- Calculate the energy of the new state.

- If the energy is lower, accept the swap. If the energy is higher, accept the swap with probability $e^{-\beta(E_{low}-E_{high})}$.

By doing this one speed up the simulation greatly so one can calculate the parameters effectively.

A.2 Random Number Generators

Before the code is given some words on how random numbers are created which is crucial in Monte Carlo simulations. All true random number generators has to be realized through some physical process (e.g.. radiation decay), and these numbers can be stored. Both these ways of getting random numbers are to clumsy and slow for most modern purposes. The way almost all random number are made today is through different simple numerical algorithms which are much faster. The price to pay is that the numbers produced are will start to repeat themselves after some period, they are therefore called pseudo-random. They will just be called random number generators (RNGs) from now.

A good RNG should produce random number (RN) which are uniformly distributed, it should have a long period, it should be fast and it should be repeatable in order to check results, for a nice review on RNG see [28]. For fortran 90, there is no standar RNG, so different compiler will give different results (fortran 95 has the KISS64 RNG as standard). Two good possibilities are the KISS64 and Mersenne Twister, these RNGs have very long periods and they pass tests of randomness [29, 30]. By making some small changes the KISS64 and Mersenne Twister will be fully implemented in the code, so that one can choose to use these or the built-in RNG. This will assure that numerical results can be checked across platforms. This could serve as an extra assurance that the numerical calculations, which heavily rely on RN, are as correct as possible. When using parallel computing and RNGs one has to be extra careful since other phenomenas may occur, the interested reader is referred to [31, 32, 33].

A.3 The Program

The code is programmed in Fortran 90 which is an old (but gold) programming language, which is very efficient and therefore an excellent choice for MC simulations. The initial code was written by prof. Phillipe Sindzingre and it could calculate the magnetization, the magnetic susceptibility and
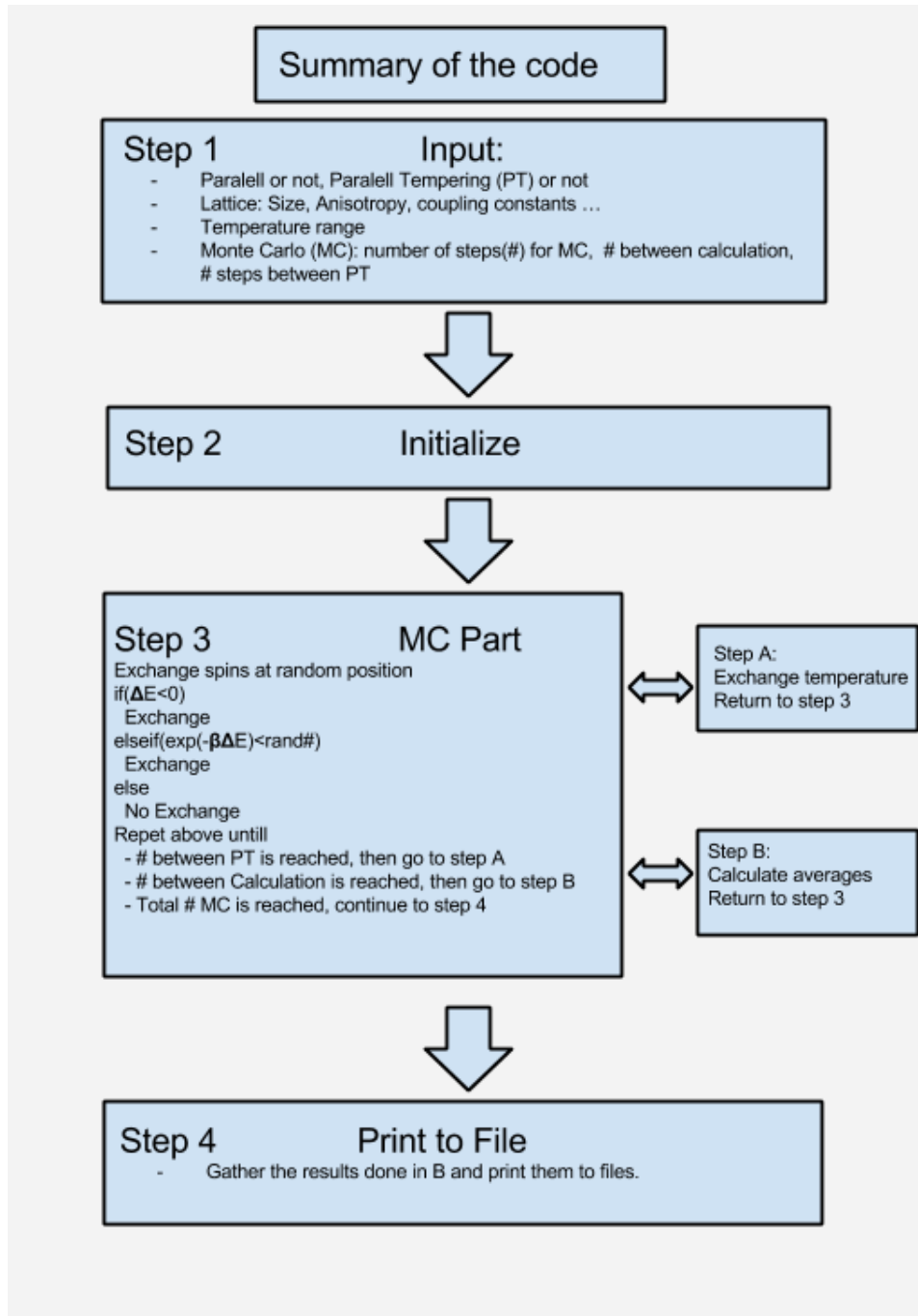
Figure A.1: An overview picture of the code.

different moments for the system. The program was modified further by the author with the help from prof. Sindzingre. The modifications consist of making the program parallel so that it can take advantage of today's parallel computers, adding anisotropy to the 3D XY model and adding calculation of some new quantities.

To add the code here is pointless since the code is distributed over several files with some over 1000 lines. A short summary will instead be given in this section, where an overview picture is given in fig. (A.1). If someone are interested in the code the author or prof. P. Sindzingre can be contacted.

The code starts with gathering inputs from a script or the terminal. Where one define if the code shall be run parallel and with parallel tempering, which temperature range, how large lattice, MC steps, etc. After the input data is read the program will make a table of temperatures and matrix for neighbour interactions and for spin for different temperatures. If the code is run in parallel the temperatures will be scattered to the different processors each with its own spin matrix. The size of the spin varied from 10x10x10 to 100x100x100.

After the initialization is finished the Monte Carlo part starts. It consist of exchanging random spins, and calculating if the energy is lower in the new state. If it is, one swap the spins. If it is not, one take the $e^{-\beta(\Delta E)}$ and if this is smaller than some random number then one also swap. If not one do not swap. This step was repeated 2 000 000 to initiate and 6 000 000 between the samplings. For a discussion on error estimates of correlated data and how equilibrated the simulation is and the interested reader is refereed to [24].

The Monte Carlo step above is repeated until one reach the number where one do the parallel tempering. Meaning that one exchange two nearby temperatures. If the energy is lower for the spin matrix with this new temperature one accept the exchange of temperatures. Else $e^{-\beta(\Delta E)}$ has to be smaller than a random number. Here the temperatures and other relevant information has to be exchanged on the different processors if the code is parallel.

When another number of Monte Carlo simulations are done one calculate some averages. Magnetic susceptibility, magnetization, Binder cumulant, to mention some.

Finally, when the total number of Monte Carlo simulation are done. One gathers the results and prints them in files which can be further studied. The author used Maple to make the figures of the data is this thesis.

In addition of the code mention above, a program which could test the different scaling constant was used. This program maximized the curve col-

lapse and gave a estimate of the scaling constants [25]. The code was made by Oliver Melchert and the idea was to develop this program further or write a own program in Fortran. Unfortunately there was no time to do this, but this would be a natural extension to the program.

Appendix B

Additional Figures

In this part it is added some extra figures, with short explanations, that where not included in the main report. The first figures is the plots of the magnetization per spin in the x- and y-direction. For both plots the quantity is zero over the critical temperature, $T_c \approx 2.2$ and one can see quite large fluctuation in the plots. Why the fluctuations in the x-direction look to be larger than those in the y-direction, are not clear.
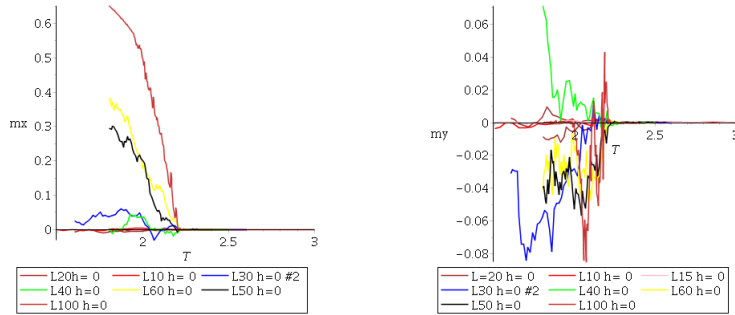

(a) The magnetization per spin in the x-direction.

(b) The magnetization per spin in the y-direction.

Figure B.1: Another example of big fluctuations which imply that the system is not fully equilibrated.

The Binder Cumulant for the magnetization in the x-direction is given in figure B.2 supports the transition temperature of $T_c \approx 2.2$. The effect of an external field is that the plots are moved away from the zero field. In the $L = 40$ case this effect is much larger than in the $L = 10$, similar to those results obtained in the Results section.
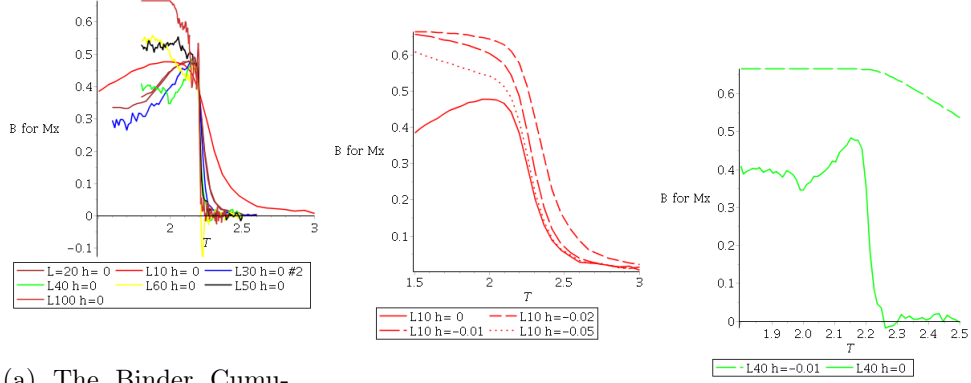
(a) The Binder Cumulant for M_x for different system sizes for zero field.

(b) The Binder Cumulant for M_x for different fields when $L = 10$.

(c) The Binder Cumulant for M_x for different fields when $L = 40$.

Figure B.2

In figure B.3 a different scaling from that in equation 2.50 is shown. This scaling was proposed by Oshikawa in the paper [?]. The scaling is as following

$$\phi_p \sim f\left(c|t|^{\nu_p} L^2\right) \tag{B.1}$$

Here, c is a constant. The plots in figure B.3 looked to follow the same pattern as 3.10. Where the $\nu_4 = 0.67155$ had the best fit and it got worse as ν_4 was increased. The $\nu_4 = 0.67155$ fit also looked better than that of 3.10a for very low values of the horizontal-axis.
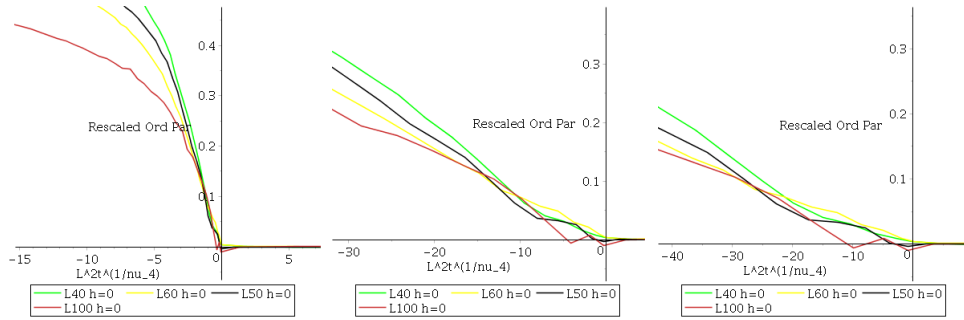
(a) The rescaled order parameter ϕ_4 for different system sizes, that follow the Oshikawa scaling [?]. With $\nu_4 = 0.67155$ and $T_c = 2.2018312$.

(b) The rescaled order parameter ϕ_4 for different system sizes, that follow the Oshikawa scaling [?]. With $\nu_4 = 0.71155$ and $T_c = 2.2018312$.

(c) The rescaled order parameter ϕ_4 for different system sizes, that follow the Oshikawa scaling [?]. With $\nu_4 = 0.75$ and $T_c = 2.2018312$.

Figure B.3

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