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XY model

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Introduction

1.1 Lattice models for phase transitions

A very successful and general set of models in statistical mechanics is the one in which the components of a system are located on an array of lattice sites, with every component interacting only with the closest ones (*nearest-neighbour interaction*). This kind of models turns out to describe well enough a very broad range of phase transitions including ferromagnetism transitions, gas-liquid and gas-solid transitions, superconductive transitions and so on. [1]

The case considered in this dissertation will be the *ferromagnetic* transitions.

Being defined on a lattice entails a discretization of space, a caveat that fits very well if the system under study is a metal whose atoms are almost locked in a crystalline structure. The crystalline nature of metals allows to introduce another semplification in this kind of models: considering the atoms as harmonic oscillators swinging around the equilibrium point, their kinetic energy can be neglected and only their magnetic interactions has to be considered. It has to be said that this kind of facilitation turns out to be adequate also for other kinds of transitions and for materials very different from metals.

1.2 Hamiltonian of ferromagnetic lattice systems

Being interested only in the magnetic interactions of atoms means that they can be considered as magnetic dipoles having a magnetic moment μ. Every magnetic dipole in the N lattice sites will have a magnitude $\mu = g\mu_B\sqrt{J(J+1)}$, with g being the Landè factor, μ_B the Bohr magneton and J being the total angolar momentum quantum number. The total number of possible orientations of the magnetic momenta in space is given by the multiplicity of J: $(2J+1)$. This magnetic dipoles will interact witch each other and will interact with an eventual external field $\mathbf{B}$.

[1] The foregoing discussion is heavily based on Pathria (1972) section 12.3

The net magnetization of the system $\overline{M}$ will depend on both the temperature T and the field B ($\overline{M} \equiv \overline{M}(T, B)$). Studying the *spontaneous magnetization* $\overline{M}(T, 0)$ of the system, a *critical temperature* T_c can be defined as the threshold temperature for $\overline{M}(T_c, 0) \neq 0$ for $T < T_c$: above T_c the thermal agitation will be too big to allow a spontaneous magnetization to manifest, then at T_c the system will perform a *ferromagnetic transition.*

Detailed studies beyond the scope of this dissertation have shown that ferromagnetic properties arise when $J = \frac{1}{2}$ and so it can be assumed that this kind of phenomena are due to electrons' spin. Then the magnetic moment can be rewritten as $\mu = 2\mu_B\sqrt{s(s+1)}$, where $g = 2$ is the Landè factor for electrons and s is the spin of the electron.

From quantum mechanics considerations (see Bransden, Joachain, and Plivier 2003) it can be shown that the interaction energy between two electrons can be expressed as $K_{ij} \pm J_{ij}$ with i and j being the two indices indicating two neighbouring electrons. The plus and minus sign are determined based on S, the total spin of the the two electron: the plus corresponding to the case $S = 0$ and the minus to one with $S = 1$, where only J_{ij} depends on the spins' configuration.

Then the energy difference between the "parallel" spin configuration and the "antiparallel" spin configuration is

$$\Delta E = E_{\uparrow\uparrow} - E_{\uparrow\downarrow} = -2J_{ij}$$

Defining the scalar product operator of the spin of the two electron as

$$\mathbf{s}_j \cdot \mathbf{s}_i = \frac{1}{2}S(S+1) - s(s+1)$$

is easy to show that the interaction energy between the spins can be written as

$$E_{ij} = \text{const.} - 2J_{ij}(\mathbf{s}_i \cdot \mathbf{s}_j)$$

The exact value of the constant is irrilevant since any constant can be added to the potential energy. Still from quantum mechanical considerations it can be seen that J_{ij} falls very rapidly when the distance beetwen the two spins increases, supporting our initial caveat of regarding only the neirest-neighbours interactions.

1.3 n-vector models

In statistical mechanics the formalization of the ideas presented in the previous sections for ferromagnetic lattice models is the so called n-vector model. A n-vector model is a system of interacting spins on a crystalline lattice as the ones described above. This formalization was developed by Stanley (see Stanley 1968)

who was able to show that most of the critical properties of this kind of systems depends only on the dimension of the lattice and on the dimensionality of the spins in the system.

Fromalized in a mathematical way we have a n-vector model when we can describe a system composed of n-dimensional spins as unit-length vectors, located on the sites of d dimensional lattice.

The evolution of the system is described by the hamiltonian

$$H = -J \sum_{n.n.} \mathbf{s}_i \cdot \mathbf{s}_j \tag{1.1}$$

where the meaning of the symbols follows directly from the one used in the previous sections and the subscript $n.n.$ means the summation goes over only on the nearest-neighbour spins.

Equation 1.1 shows that *ferromagnetic* phenomena are possible when $J > 0$ since the configuration $\uparrow\uparrow$ is energetically favorable in respect to the $\uparrow\downarrow$ configuration; if $J < 0$ *antiferromagnetic* phenomena could arise.

Obviously in the presence of an external field the hamiltonian will be modified in the following way

$$H = -J \sum_{n.n.} \mathbf{s}_i \cdot \mathbf{s}_j - h \sum_{i} \mathbf{s}_i \tag{1.2}$$

where now J is the same as in equation 1.1 divided by $k_B T$ and $h = \mu B / k_B T$, where B is the magnitude of the external magnetic field. As a consequence of the presence of the field, magnetization properties will also depend on the field itself.

1.3.1 Ising Model

The Ising model was the first of the ferromagnetic lattice models invented, much before Stanley's formalization, in 1920 by professor Wilhelm Lenz who gave it as problem to his student Ernst Ising. [2]

The Ising model is basically the n-vector model for $n = 1$: the spins are considered as a one dimesional vector that can take only two values: up and down. This is the simplest physically important case ($n = 0$ being of importance merely from a mathematical point of view) and was solved analytically in the $d = 1$ case by Ising in 1924. He showed no transitions can occur in such a model, but it was the ground zero for the development of much more complicated models for higher dimensions.

In the following years the case for $d = 2$ was also solved and transitions were shown to be possible. Analytical solutions for higher dimension are still to be found, if there are some, and are definitely outside of the scope of this dissertation.

[2] check `https://en.wikipedia.org/wiki/Ising_model`

1.3.2 Heisenberg Model

The Heisenberg model is the n-vector model for $n = 3$ and require a quantum mechanical approach and is obviously the closest one also to a description of reality. Being more complex as a model makes it a tremendously more difficult problem to tackle and it requires a mathematical and quantum mechanics formalization called Potts models [3] that integrates also the n-vector models.

The Heisenberg model has multiple apllications in quantum mechanics and it is one of the most studied models of magnetism. [4]

[3] check `https://en.wikipedia.org/wiki/Potts_model`

[4] For a detailed view of Heisenberg model see Nolting and Ramakanth (2009)

XY model

2.1 Definition

The $n = 2$ n-vector model is the one of interest in this dissertation and it is the so called *XY model*. Its name is due to the fact that the spin is imagined as a two dimensional vector lying on the xy plane. Introduced in the 1950s, this model was actually used to describe quantum lattice gas and superfluid transitions, then in the late 1960s it was adopted to model ferromagnets.

As in any n-vector model properties of the system are detrmined also by the dimensionality of the lattice considered to describe the system. In the 1 dimensional case there exists an exact solution in the absence of an external field. Being exactly solvable means an exact form for the partition function can be found and thermodinamical properties can be derived theoretically. When periodic boundaries conditions are applied, using the statistical mechanics *transfer-matrix method*, first introduced by Kramers and Winnier in the study of the Ising model in 1941[1], the partition function can be written in a very simple form as

$$Z = 2\pi I_0(\beta J) \tag{2.1}$$

where $I_0(x)$ is the first modified Bessel function and $\beta = 1/k_B T$. From equation 2.1 thermodinamical quantities can be exactly derived. In figure 2.1 below is plotted the specific heat per spin. [2]

The most physically interesting cases are the 2 dimensional and the 3 dimensional one and they will be discussed in details in the following sections.

2.2 2D case

Phase transitions are classified based on discontinuities of derivatives of the free energy, e.g. a ferromagnetic transition is a second-order phase transition because

[1] see Kramers and Wannier 1941

[2] source `https://upload.wikimedia.org/wikipedia/commons/6/68/1D_XY_Specific_Heat.svg`

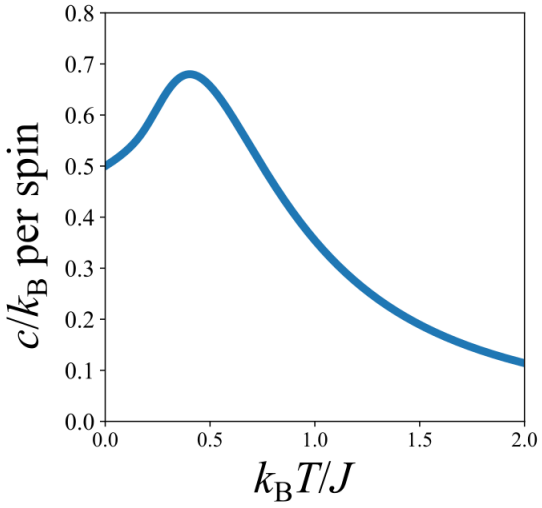

Figure 2.1: Exact specific heat of 1D XY model

it is the magnetic susceptibility, the second derivative of the free energy with respect of the magnitude of the external field, to be discontinous at the critical temperature while the magnetization, the first derivative, is continous.

The 2D case for the XY model is very peculiar because it can be shown to exhibit an *infinite-order* phase transition called a Kosterlitz-Thouless transition after the physicists that have studied it first. [3]

The Kosterlitz-Thouless transition consists in a transition beetwen a quasi-ordered phase under the critical temperature with a correlation function with a powerlaw decrease with distance and a disordered phase over the critical temperature with a correlation decreasing exponentially with the distance. These kind of order and disorder states can be shown by identifing vortices in the system. Kosterlitz and Thouless gave the following thermodinamical argument to show the existence of such a transition. In the ground state at low temperatures all spins are in the same orentation and adding a single vortex will change the entropy of the system by an amount $\Delta S = k_B \ln(L^2/a^2)$ where L is the system size, while a is the radius of the vortex core. The change in internal energy of the system will be instead $\Delta E = \pi J \ln(L/a)$. Then the amount of change of free enrgy will be:

$$\Delta F = \Delta E - T\Delta S = (\pi J - 2k_B T)\ln(L/a)$$

At high temperatures (for $\Delta F < 0$) in the thermodinamic limit the system will favor the formation of vortices, while viceversa at low temperatures any vortex

[3] see Kosterlitz and Thouless 1973. Thouless and Kosterlitz were awarded the Nobel Prize in Physics in 2016 "for theoretical discoveries of topological phase transitions and topological phases of matter." `https://www.nobelprize.org/prizes/physics/2016/summary/`

will try to annihilate with an antivortex to lower the system energy. The critical temperature will be the one for which $\Delta F = 0$, so $T_c = \pi J/2k_B$.

Theoritical and Monte Carlo simulation estimates of the critical temperature have been attempted over the years reaching the well established value of $k_B T_c/J \simeq 0.88$. Monte Carlo simulations allow also to visualize this kind of behaviour using a color map: mapping the spin angles with a colour using a continous and periodic color spectrum like a red-green-blue one, where the angle spans in the interval $[-\pi, \pi)$, the formation of vortex-antivortex pairs can be shown at low temperatures as in figure 2.2. [4]

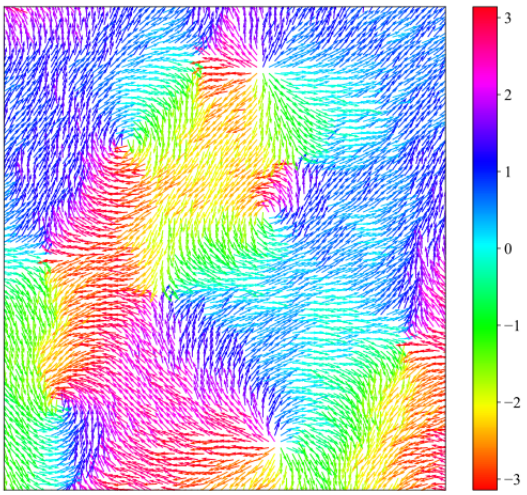

Figure 2.2: Vortex-antivortex formations in 2D XY model at $k_B T/J = 0.4$

2.3 3D case

In the 3D case (and in higher dimensions) the XY model exhibits a ferromagnetic-paramagnetic transition at the critical temperature $k_B T_c/J \simeq 2.22$. From a physical point of view this transition plays a central role in establishing the validity of the model because the values of the so called *critical exponents* can be obtained via theoretical means, with quantum field theory, by experiments and by Monte Carlo simulations.

[4] source `https://upload.wikimedia.org/wikipedia/commons/7/77/XY_Vortices.svg`

Critical exponents are a very useful tool used in phase transition description. They are used to describe the behavior of physical quantities near the critical temperature in a huge variety of different systems. They are used in n-vector model descriptions because it is believed, on strong experimental basis, that they do not depend on the particulars of the physical system under study but only on the following general properties:

- the dimension of the system
- the dimension of the *spins* considered
- the range of interaction

The critical exponents are usually denoted by a greek letter and usually the most important ones are α, β, γ and δ. Their meanings will be explained in the next chapter.

In 3 dimensions critical exponents can be derived analytically in mean field theory [5] and experimentally by studying easy-plane magnets and liquid ^{4}He.

[5] see `https://en.wikipedia.org/wiki/Mean-field_theory`

Montecarlo simulation

The XY model has been studied with various approaches, the one taken in this dissertation is a Monte Carlo simulation that will be implemented to compute physical observables from which it will be attempted to estimate some critical exponents. A brief introduction on theory of Monte Carlo simulations will be followed by a description of this particular implementation and finally the results obtained will be illustrated.

3.1 Theory

The main idea of Monte Carlo simulations is to sample a quantity of interest treating it as a random variable even if in principal this quantity could be obtained deterministically. This kind of probabilistic approach, instead of the deterministic one, become useful when the deterministic evaluation via numerical means becomes impossible. In physics this usually happens when numerical calculations in high dimensions are required, as in evaluation of integrals in multiple dimensions, and the computational cost in time scale as N^2 or in gerenal as a higher power of N, with N being the number of dimensions.

Monte Carlo methods are based on the law of large numbers and on the central limit theorem that states that the expected value of some random variable can be obtained by the sample mean of indipendent samples of the variable. Then the central problem of a Monte Carlo algorithm becomes sampling the variables of interest in a indipendent and representative way.

In phisics and mathematics the algorithm mostly used to accomplish the requirements needed is the so called Markov chain Monte Carlo sampler. The Markov chain [1] is constructed based on the target sample distribution and the sampling of the states, composing the chain, will approach the desired distribution in the limit of an infinite chain.

Finally the algorithm that puts all of these concepts togheter is the Metropolis-

[1] see `https://en.wikipedia.org/wiki/Markov_chain_Monte_Carlo`

Hastings algorithm. [2] This algorithm samples any random variable provided that the probability density function $P(x)$, or a function proportional to it, is known. Being based on a Markov chain implicates every sample is generated based on the sample generated before, then the sample is accepted or not on probabilistic considerations built on $P(x)$. In the case which the new sample proposal is rejected, the old sample value is retained and counted as a new sample on which the values of observables will be computed again.

In the case of a lattice as in the XY model, starting from a random spins' configuration, the canonical distribution, coming from canonical ensemble theory, is used to determine which configuration utilize to compute observables' values. The canonical distribution is defined as

$$P(\{\sigma_i\}) = \frac{\exp(-\beta H(\{\sigma_i\}))}{Z} \tag{3.1}$$

where $\{\sigma_i\}$ is the spins' configuration and Z is the partition function.

Then in every Metropolis step a new candidate sample is created and the probabilities of the configuration are compared using the ratio between them

$$A = \frac{P(\{\sigma_i\}_{mc})}{P(\{\sigma_i\})} = \exp(-\beta(\ H(\{\sigma_i\}_{mc}) - H(\{\sigma_i\})\ )) \tag{3.2}$$

where the mc suffix means the configuration is the Monte Carlo candidate. Then a random number η with a uniformal probability distribution between 0 and 1 is picked and the candidate is accepted if $A > \eta$ or rejected viceversa.

Obtained the new sample (that could easily be the same as the last one) an observable value is computed on the configuration. At every step the value of the observable is saved, and in the end the average over the step values represents the value desired and the one comparable with experimental results.

The error on values of the observable cannot only be considered as the standard deviation of the values computed after every step as these values are not indipendent: the value from the $n+1$ step follows directly from the value at the n step, therefore there is an intrinsic correlation between these two. To account for this, correlation has to be taken in consideration when estimating the uncertainty of the observable. The correlation of a function f (an observable in this case) is defined as

$$\langle S_L^2 \rangle = \frac{1}{L} \sum_{l=0}^{L} \langle f(x_{i+l}) f(x_i) \rangle \tag{3.3}$$

where S_L^2 is an estimate of the correlation, x_i is the step i of the Markov chain and L is the "maximux" distance in steps in which the correlation is considered significant. Finally the error on $\langle f \rangle$ will be approximated by $\sqrt{S_L^2 - \langle f \rangle^2}$.

[2] Check the original work of the Metropolis spouses and Rosenbluth (Metropolis et al. 1953) that inspired the invention of the Metropolis-Hastings algorithm

3.2 Implementation

The computation of observables values is done in the 3D case, on a cube of side $L = 6$ and periodic boundaries where applied. The atoms in a ferromagnets are definitely much more than $L^3 = 216$, then the cube under study can be imagined as a portion of 216 atoms in the ferromagnet. These atoms will only interact with other atoms of the magnet as if they were in an infinite system composed of repeated cubes of 216 atoms. Then periodic boundaries conditions are applied by making interact the most right atoms with the most left ones, as if an other identical cube was attached on the right of the cube.

Most implementation of the XY model found in higher detailed works usually change one spin at every Monte Carlo step: obviously this garantees a higher precision avoiding higher fluctations on energy values, but it comes with a very big cost in computation. Since the computational power in this case was very limited all of the spin are changed at every step garanteeing a bigger change between a step and an other, decreasing a lot the correlation between a step and the following one. If the one spin strategy would have been implemented it would have taken many steps to obtain a sufficently different configuration to compute observable values on it.

The amount in change of the angle of the spins is determined by a value usually referred as Δ, initialized at $0.1°$. The value of Δ is the main factor which controls the amount of correlation between a step and the next one: if Δ is too big the candidate configuration will be too different from the original one then most of the candidate configurations will be discarded and the correlation between steps will be very high. Something similar happens when Δ is too little: almost every candidate configuration will be accepted, but every configuration will still be very similar from the one before and again the correlation will be very high. Then this kind of correlation can be minimized updating the value of Δ based on the value of the acceptance ratio: if too many steps are accepted it means Δ is little, while in the opposite Δ will be to big.

Since the configurations of interest are the ones in equilibrium, the first 10k steps are used to reach equilibrium and to correct the Δ to reach an acceptance ratio in the interval $[0.35, 0.65]$. After these 10k steps, other 190k steps are performed on which observable values are computed.

The observables computed here are the specifc heat per spin, the magnetization per spin and are obtained as

$$\frac{C_v}{N} = \frac{\langle U^2 \rangle - \langle U \rangle^2}{N(k_B T)^2}$$

$$\frac{\langle M \rangle}{N} = \frac{1}{N} \big\langle |(\sum_i \cos\theta_i, \sum_i \sin\theta_i)| \big\rangle$$

To compare the values obtained in this work with the ones published before a very simple and rough estimate of the critical exponents α, β and δ is performed. Defining $t \equiv (T - T_c)/T_c$ the critical exponents are defined for magnetic systems as

$$m \sim t^{\beta} \quad (h \to 0, T < T_c)$$

$$m \sim h^{(1/\delta)} \quad (h \to 0, T = T_c)$$

$$C_v \sim t^{-\alpha} \quad \text{for } T > T_c$$

$$C_v \sim (-t)^{-\alpha} \quad \text{for } T < T_c$$

In general m and h are respectively called the *order parameter* and the *ordering field*. Here m corresponds to the magnetization squared, and h corresponds to the magnetic field defined as above. The estimate carried here is rough because is simply a fit of the function defined above. Usually much more sofisticated methods are used such as finite-size scaling methods. [3]

Other critical exponents can be indirectly evalueted using the so called *hyperscale relations*. The one of interest are reported below, where $d = 3$ is the dimension of the system.

$$d\nu = 2 - \alpha = 2\beta + \gamma = \beta(\delta + 1) \tag{3.4}$$

3.3 Results

In the next pages graphs for the squared magnetization and specific heat in respect of temperature are shown. It is easy to see the divergence of the specific heat around the critical temperature $T_c \simeq 2.22$. As said before a rough attempt of estimating the critical temperature and the critical exponents, just by fitting the functions reported above, will be made.

[3] see "Introduction to Theory of Finite-Size Scaling" 1988

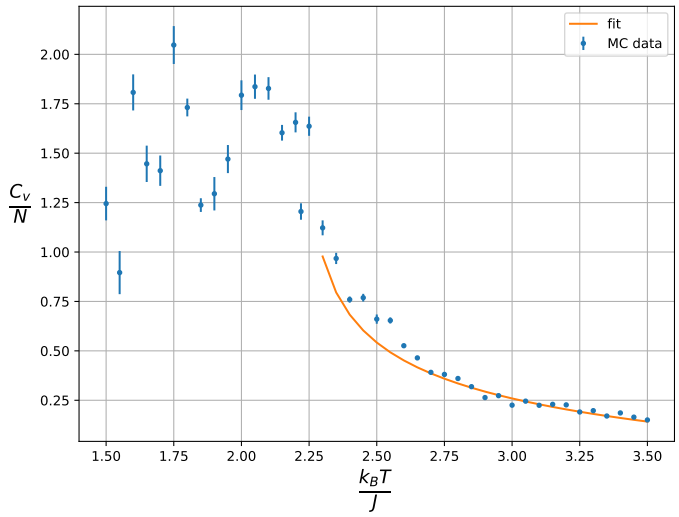

Figure 3.1: $C_v(T)$ for $h = 0$

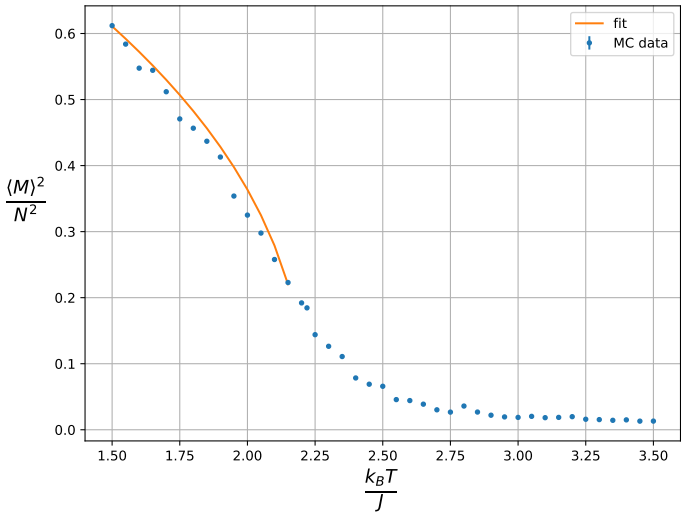

Figure 3.2: $M^2(T)$ for $h = 0$

The roughness of the estimate via simple fit of the functions defining the critical exponents is due to the fact that the Monte Carlo simulations tend to struggle near critcal point where observables' values oscillate excessively, reducing then the effectiveness of the averaging process of the Monte Carlo method.

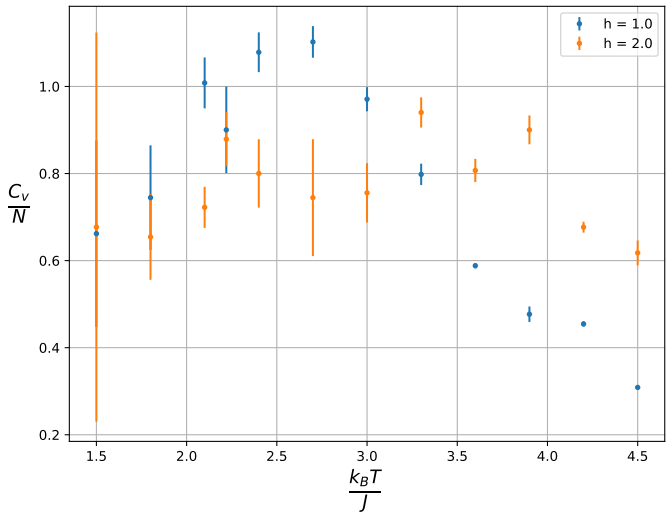

Figure 3.3: $C_v(T)$ for $h \neq 0$

Observable values for the ordering field $h \neq 0$ are reported in the graphs below. The effect of the field is to keep the order in the spin configuration, raising the value of the critical point, as can be seen in figure 3.3, and to keep a considerable magnetization after the transistion, as can be see in figure 3.4.

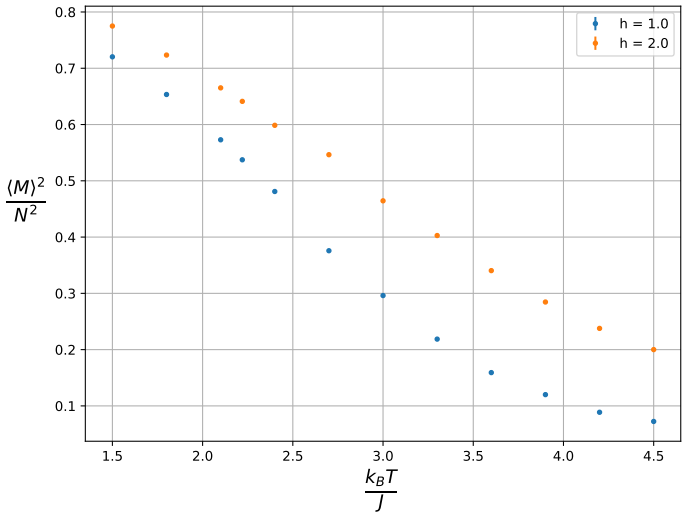

Figure 3.4: $M^2(T)$ for $h \neq 0$

A study of the magnetization at the critical temperature for different values of the ordering field is carried to estimate the critical exponent δ. The results are reported in figure 3.5.

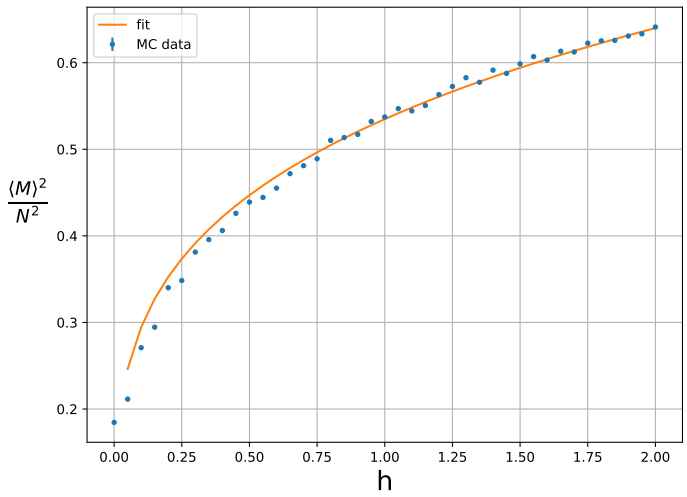

Figure 3.5: $M^2(h)$ for $T = T_c$

A table with the results of the fits and the corrisponding critical exponents is reported below. Theoretical and experimental values for the model are also reported. [4]

Critical exponents

	α	β	δ	γ	ν
Theorical values		0.362 ± 0.012	4.82 ± 0.12	1.39 ± 0.01	0.705 ± 0.005
Experimental values	0.0-0.2	0.3-0.36	4.2-4.8	4.2-4.8	0.62-0.68
Monte Carlo simulation	0.201 ± 0.004	0.438 ± 0.001	3.86 ± 0.09	0.654 ± 0.008	1.08 ± 0.03
χ^2_r	$\simeq 7 \cdot 10^5$	$\simeq 1 \cdot 10^{12}$	$\simeq 3 \cdot 10^{12}$		

The values of α, β and δ have been obtained directly, while γ and ν have been obtained by α, β and δ with the hyperscale realtions in equation 3.4.

By looking at the values of the reduced chi squared it seems obvious that these fit have to be rejected. Such big values are determined both by an underestimate of the errors on observables, mainly in the temperature region near the critical point, and by a not very good choice of the fitting functions. Anyway a kind of agreement, due mainly to the not so precise experimental values, appears beetwen

[4] for tables of theoretical and experimental values see Pathria 1972

experimantal values and the one coming from this work. So it can be said that the macroscopic behaviour and properties of systems which can be described by the 3 dimensional XY model have been shown.

Conclusion

A theorical analisys of the XY model has been given, starting from its generalization the n-vector model, simpler cases have been described such as the Ising model. A detailed theorical study of the 2D and 3D cases for the XY model have been presented. Monte Carlo simulation theory has been breafly described and has been put in practice for the 3D case of the XY model. In the last chapter simulation results have been presented.

The results in the third chapter are not good enough to be compared to other studies: this is probably due to the fact that near the critical point Monte Carlo simulations tends not to perform greatly. They tend up to be stuck in local minima of energy and oscillations in those region of temperature are so high the averaging process of the algorithm perform much worse than it does in other regions. This behaviour is known and there exist a few techniques to avoid this from happening. An example could be the over-relaxation method where the value of a spin is changed with a different one resulting in the same value of energy: the sampler will be oblied to sweep more of the phase space and the likelyhood of being stuck in a local minimum will decrease significantly. To reduce the effects of oscillations, averages on slightly different values of temperature could be taken e.g. the values of observables at $T = 2.2$ could be considered as the average of the values at $T = 2.195$, $T = 2.196$ ... $T = 2.205$.[1]

All of these technique are generally computational expensive and the limited equipment did not allow to use them. Anyway in the previous chapters the macroscopic behaviour of the XY model has been shown, and even if the values of critical exponents are not good enough to be considered as a good estimate, they are good enough to be compared with some experimental values.

[1] for a very detailed work of a Monte Carlo simulation on a GPU for the 3D XY model see Lan, Hsieh, and Kao 2012

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