University of Ottawa

PHY5355 Term Paper

Critical Behaviour in a 2-Dimensional Ising Ferromagnet

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Abstract

We will investigate the ferromagnetic phase transition in the 2D square-lattice Ising model with nearest neighbour interactions using a simple Metropolis Monte Carlo single spin-flip scheme combined with finite size scaling, as well as the Wolff algorithm for more detailed statistics. The investigation of the basic model will focus on determation of the temperature scaling critical exponents for the phase transition. Finally, the model will be generalized to systems containing imnpurities. In particular, we will inject a sub-population of antiferromagnetic bonds into the lattice in order to simulate the effects of frustration in the system, loosely guided by some analytical work in the field which shows additional low temperature phases in frustrated spin systems.

1 Theory

1.1 The 2D Ising Model

The Ising model describes a conceptually simple platform for modelling spin systems with local interactions and is thus generally used in the study of magnetic materials, though the framework can be applied to a number of other problems within the same universality class [refs]. In the case considered here, the basic model consists of a 2D square lattice, with a particle at each lattice site which can take one of two possible spin states, denoted throughout as ± 1, which interacts with its nearest neighbours and and external magnetic field B through a simple Hamiltonian

$$E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - \mu B \sum_i \sigma_i \tag{1}$$

where $\langle \cdot \rangle$ denotes nearest neighbours and σ_i denotes the spin at site i. J is the nearest neighbour interaction energy, and μ the magnetic moment of the particles, taken here to be homogeneous and uniform throughout the material. This can easily be generalized to more complex interactions, for example by taking J to be site-dependent, or random, as will be considered later. In a ferromagnet, characterized by $J > 0$, spins prefer to align with neighbours, a local interaction which has long-range, macroscopic consequences. At zero external field, as the temperature of the system is lowered, the energy between neighbouring spins comes to dominate thermal fluctuations and local interactions between spins cause the spontaneous formation of magnetic domains, areas of aligned spins. Since the state of minimal energy is one in which all spins are aligned, we find that there is a phase transition at a temperature $T = T_c$ at which point the system switched abruptly from an average magnetization of zero to a near completely magnetized system. The full analytical solution of the model has been carried out[4], though that particular piece of mathematical wizardry will be used here only as a useful basis of comparison for our simulation results. In particular, Onsager's original solution predicts a critical temperature for phase transition between a low temperature ferromagnetic phase and a higher temperature paramagnetic phase of $T_C = \frac{2J}{k_B \ln\left(1+\sqrt{2}\right)}$.

1.2 The Metropolis Algorithm

The Metropolis algorithm is a general class of Monte Carlo methods for simulating stochastic phenomena in statistical mechanics. In its most basic form, implemented here, a single spin site on the lattice is chosen at random and the energy change involved in flipping it, according to equation 1, is computed. The spin is then flipped with a probability determined by the statistical constraints of detailed balance[2], which requires that the system reach a time-invaria equilibrium state. Since the selection probabilities for a particular state change are equal by virtue of involving a randomly chosen spin, detailed balance simply requires that the acceptance probability for a change P, weighted by the appropriate Boltzmann factor, are equal in the forward and reverse directions, that is

$$e^{-\beta E} P_{flip} = e^{-\beta E'} P_{unflip} \tag{2}$$

where E and E' denote energies of the current and possible next state respectively, and β is the Boltzmann factor. We then have the freedom to choose one of the selection probabilities, which we do following the example of[2] to obtain the so-called Metropolis-Hastings Algorithm: if the energy change is negative, the spin is flipped, and if it is positive, it is flipped with the probability required by equation 2, that is,

$$P_{flip} = \begin{cases} 1 & \Delta E < 0 \\ e^{-\beta \Delta E} & \Delta E > 0 \end{cases} \tag{3}$$

with $\Delta E = E' - E$. It is remarkable that this simple equation contains within it the entirety of the dynamics involved in the simulation of a 2D ferromagnetic.

In order to simplify analysis and interpretation of our results, we first rewrite our system in unitless variables. Dividing equation 1 by J and defining $H = \mu B J^{-1}$ and $E' = E J^{-1}$ to be the unitless external field and energy respectively, we obtain the simple equation

$$E' = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i \tag{4}$$

Where energies are now measured in units of the characteristic energy of the system, nearest neighbour interaction strength. Additionally, we will define

$$T' = \frac{k_B T}{J} \tag{5}$$

to be the unitless temperature of the system. Since all of the dynamics of the problem come about through the Boltzmann factor $\beta = k_B T = J T'$ in equation 3, it is clear that what matters for our system is the product JT', not the independent values of J and T' separately. We can thus fix $J = 1$ and sweep our system over temperature without any loss of generality. Henceforth, we will drop the prime notations with the understanding that T and E are measured as discussed here.

While the model is conceptually very simple, there are a number of potential hurdles that we must anticipate before attempting to extract values from it. Firstly, this algorithm has very poor asymptotic scaling with system size. In all of the simulations int this paper, we start the lattice by randomly assigning a spin to each lattice site. Because short range interactions will cause spins to preferentially align with nearest neighours regardless of temperature, this is clearly not an equilibrium state. Before any information can be extracted from the system, it must be allowed to thermalize by iteratively choosing random spins and applying equation 3. Secondly, because it is a single spin-flip algorithm, we must flip a very large number of spins before the particular microstate in which we find the system is actually independent of the last state we considered. We will address both problems following the example of [2]: near criticality, the performance of the algorithm slows down because fluctuations of the magnetization and become comparable to the size of the system, whereas each spin flip makes only a very small change to the overall system properties. Fluctuations near the critical point are comparable to a random walk over the magnetization, so we expect an independent microstate to exist after we have traversed the entire range of possible values, corresponding to N^2 spin-flips. At any temperature other than the critical point, this is not really an issue, and so less than N^2 flips are necessary between independent outputs.

Some numerical experiments with the time required to reach an equilibrium state suggest that taking N^2 flips is actually overkill anywhere away from criticality. To be on the safe side, and since going over the limit needed to achieve a statistically independent microstate will do no harm, any simulation results in this paper are taken after at least N^2 thermalization steps between including any particular microstates in the ensemble. Combined with a need to calculate many microstates in order to achieve any sort of accuracy about the ensemble, this puts fairly heavy restrictions on the system sizes that are accessible to a desktop computer. Nevertheless, we will see that we can extract useful information while working within these limitations.

1.3 The Wolff Algorithm

While the Metropolis algorithm has the advantage of being conceptually very simple, it suffers from performance issues because it only flips a single spin at a time. This becomes especially pronounced near the critical point, where fluctuations are large compared to the changes introduced by flipping a single spin. The Wolff algorithm is an example of a cluster algorithm wherein entire groups of spins are flipped at once, greatly increasing performance by moving very quickly through phase space. First, a random spin is chosen as the seed for a cluster. Its nearest neighbours of the same spin are added to the cluster with probability $1-\exp\left(-\frac{2}{T}\right)$ and the process is repeated on the new members of the cluster. When the cluster stops growing, all of its constituent spins are flipped at once. That this scheme satisfies detailed balance is demonstrated elsewhere[2]. In this way, large portions of the system flip at once, and phase space can be sampled very efficiently. Independent microstates are achieved after only a handful of cluster flip operations, and so high quality statistics can be generated in a fraction

of the time that the Metropolos algorithm would require.

Unfortuantely, the Wolff algorithm is poorly suited to simulating the effects of an external field. The unconditional flipping of clusters generated as described above is dependent on the fact that in the absence of an external field, spins that are entirely within the cluster experience no energy change when the cluster is flipped. With an external field present, the cluster is built the same way, but is only flipped with Boltzmann probability determined by the energy change against the external field. At low temperatures especially, clusters can be on the order of the system size and so even a small external field is enough to cause an overwhelming majority of spin flips to be rejected, resulting in drastic slowing down of the algorithm.

1.4 Thermodynamic Results

The natural framework in which to study the Ising model is the Gibb's ensemble: we fix temperature and the external magnetic field and allow the system to achieve a state of minimal energy. This ensemble also has the advantage that we may calculate specific heat capacity C_V and specific magnetic susceptibility $\chi_{|M|}$ of our ferromagnet in terms of fluctuations in the energy E and magnetization $|M|$ respectively. Note that because in the absence of an external field the two possible directions for magnetization are entirely equivalent, it is more natural to use the absolute value of magnetization. Simple calculations using the Gibbs ensemble in the case of fixed temperature and external field give

$$C_V(T) = \frac{1}{NT^2}\left(\langle E^2\rangle - \langle E\rangle^2\right) \tag{6}$$

$$\chi_{|M|}(T) = \frac{1}{NT}\left(\langle M^2\rangle - \langle |M|\rangle^2\right) \tag{7}$$

where we define magnetization as

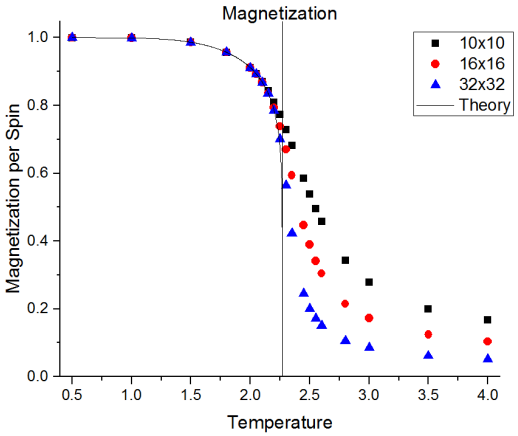
$$M = \sum_{i=1}^{N} \sigma_i \tag{8}$$

2 The Ferromagnetic Transition

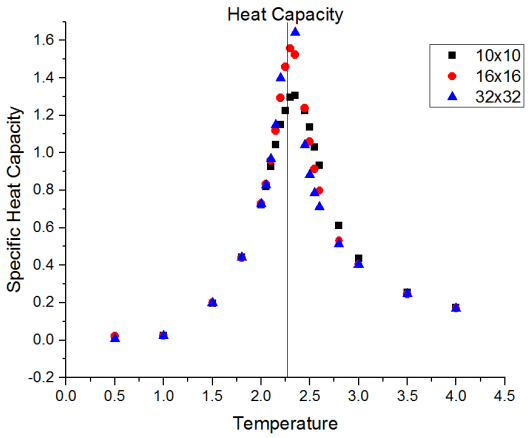
We first consider qualitative trends near the critical point before extracting quantitative information about the nature of the phase transition. Onsager's work[4] predicts a magnetization

$$M(T) = \begin{cases} \left(1 - \sinh\left(\ln\left(1+\sqrt{2}\right)\frac{T_c}{T}\right)^{-4}\right)^{\frac{1}{8}} & T < T_c \\ 0 & T \geq T_c \end{cases} \tag{9}$$

which we see is in increasingly good agreement with our results as system size $L \times L = N$ increases, in figure 1a. We expect a divergence of heat capacity and susceptibility at the critical temperature, that will be quantified shortly, which can be seen in figures 1b and 1c. Obviously a finite system such as this cannot accurately capture an infinite divergence, but we can see



(a)



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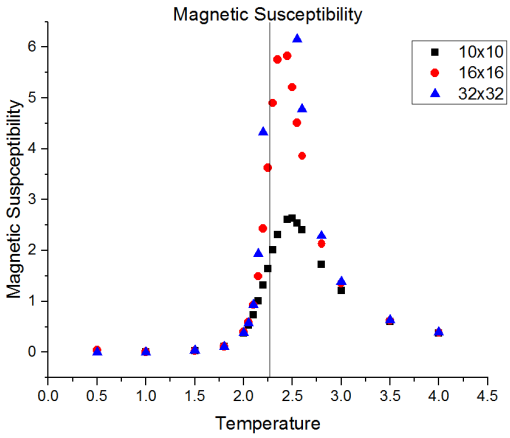


(c)

Figure 1: Qualitative results and comparison to theory for some basic physical quantities. Figure 1a shows average absolute magnetization, while figures 1b and 1c show specific heat capacities and magnetic susceptibilities per lattice site. Vertical lines show the theoretical value of T_c. Each point represents an average over 10^5 independent microstates generated with the Metropolis algorithm.

that the general trend is for increased accuracy as L increases. Note however that the peak for finite system size tends to overshoot the theoretical critical temperature of $T = \frac{2}{\ln\left(1+\sqrt{2}\right)}$.

As is the case with many magnetic systems, the 2D ferromagnet also exhibits hysteresis, retaining magnetization induced by an external field when the temperature is below the transition point. This behaviour can be seen in figure 2, shows shows the result of ramping the externals field from -1 to 1 and back at $T = 1$. This can also be considered from the point of view of energy, where we see the presence of metastable states in a small range around $H = 0$. Above the critical temperature, thermal fluctuations are sufficient to ensure that this behavior disappears.

In order to accurately determine the critical temperature, it is clear that figure 1 is insufficient, since finite size effects need to be taken into account. A more effective method was

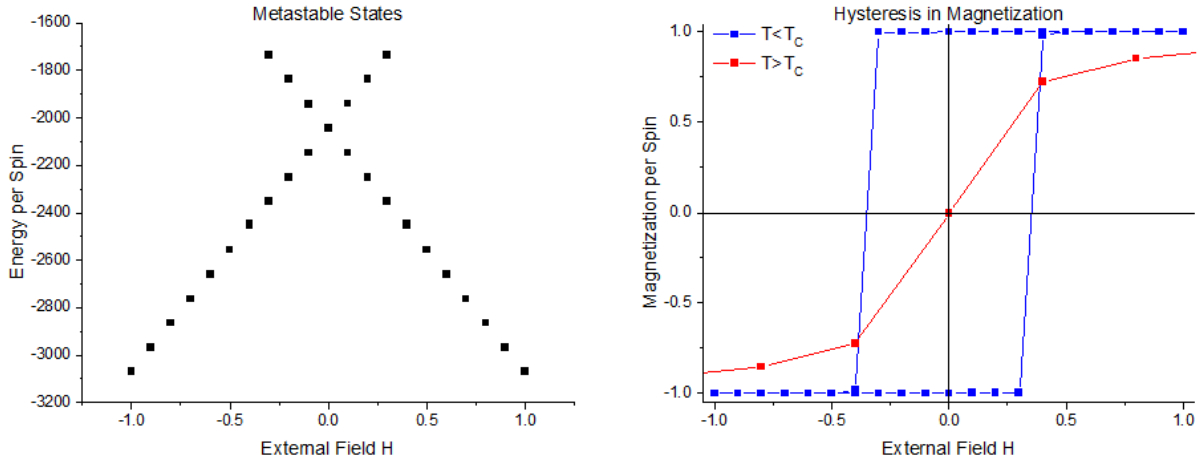


Figure 2: Hysteresis in the magnetization induced by an external field. All curves in both images are generated by ramping the magnetic field from $H = -1$ to 1 and back again. The red curve shows that hysteresis disappears above the critical temperature. Each point is an average over 10^4 independent microstates of a 40×40 spin lattice generated with the Metropolis algorithm.

provided by Kurt Binder [1]. He demonstrated that the fourth order cumulant

$$B(T) = \frac{1}{2}\left(3 - \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}\right) \tag{10}$$

exhibits a fixed point as a function of system size at the critical temperature.[2] We plot this in figure 3, with the result that the critical temperature for our model is $T_c = 2.263$, in good agreement with the theoretical value. Note that the lines in the figure are not fits to the data but merely guide to the eye - because $B(T)$ is concave down at this point, an accurate fit to the data would shift the intersection to the right slightly. We will quantify the nature of the

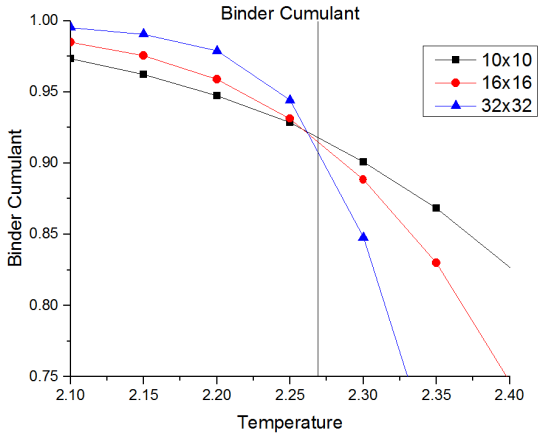
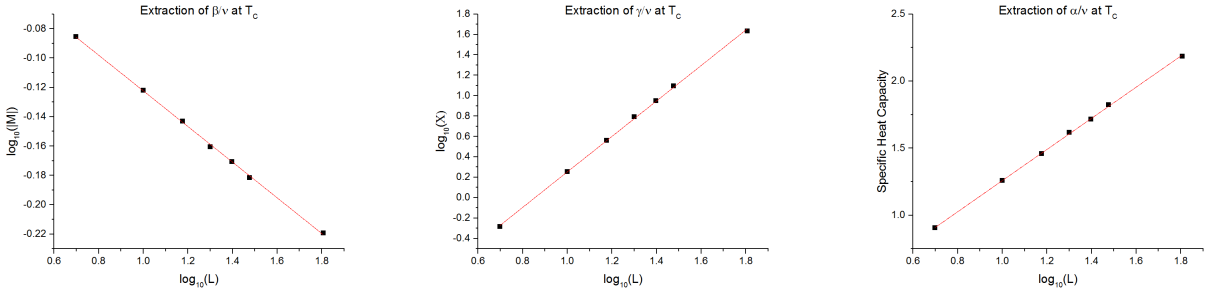


Figure 3: The Binder cumulant B(T), showing a fixed point at the critical temperature as a function of system size. The vertical line shows the theoretical critical temperature. Each point is an average over 10^5 independent microstates generated with the Metropolis algorithm.



(a) (b) (c)

Figure 4: Linear fits of logplots of physical paramters yield ratios of critical exponents in the slope. Data was generated using the Metropolis algorithm with 10^5 independent microstates per point.

divergence of a few physical quantities of relevance at the critical point by calculating several of the critical exponents for the 2D square lattice Ising model. In particular, if we define reduced temperature as $\tau = \left|\frac{T-T_C}{T_C}\right|$, then the asymptotic scaling of the physical parameters considered far at the critical point is such that

$$C_V \sim \tau^{-\alpha} \tag{11}$$

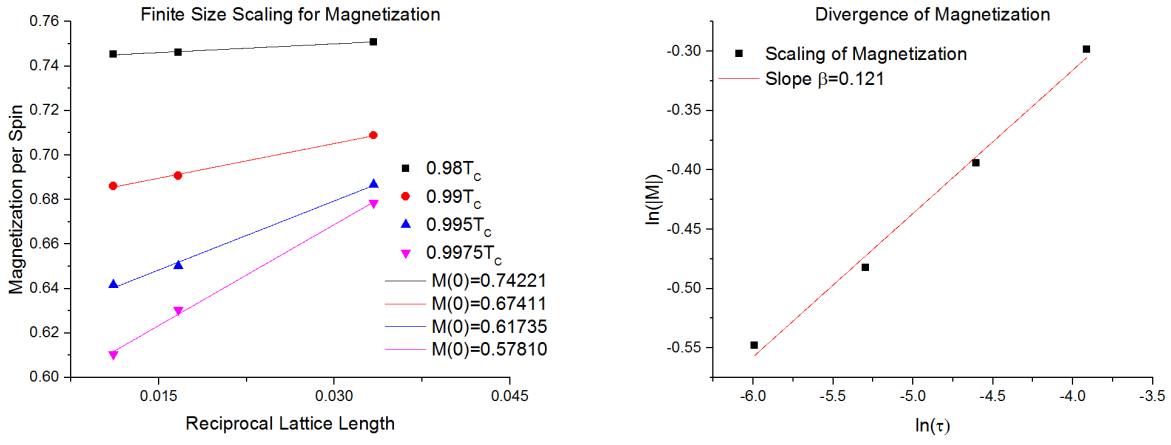
$$\chi_{|M|} \sim \tau^{-\gamma} \tag{12}$$

$$|M| \sim \tau^{\beta} \tag{13}$$

$$\xi \sim \tau^{-\nu} \tag{14}$$

$$|M| \sim H^{\delta} \tag{15}$$

where ξ denotes the correlation length which gives a measure of the size of magnetic domains



(a) (b)

Figure 5: Finite size scaling analysis for the megnetization just below the critical point using 30×30, 60×60, and 90×90 spin lattices. Each point is an average over 10^4 independent microstates generated using the Wolff algorithm.

of the system. These values have been calculated theoretically [6] to be $\alpha = 0$ (we will see that

in fact $C_V \sim \ln \tau$), $\beta = \frac{1}{8}$, $\gamma = \frac{7}{4}$, $\nu = 1$, and $\delta = 15$. These parameters are very sensitive to finite size effects, and as such we must use finite size scaling to extract them. Near the critical point, fluctuation in the correlation length become comparable to the size of the system[2][7], but are obviously limited by it, that is $\xi \sim L$. Therefore, $\tau \sim L^{-\frac{1}{\nu}}$, and so scaling of C_V, $|M|$ and $\chi_{|M|}$ with L will allow us to determine ratios of critical exponents. This method of extracting critical exponents is outlined in [7]. The results of this simulation can be seen in figure 4.

A simple least squares fit gives the ratios $\frac{\gamma}{\nu} = 1.74 \pm 0.02$, in excellent agreement with the theoretical value, and $\frac{\beta}{\nu} = -0.122 \pm 0.001$, in slightly poorer agreement.Finally, since $C_V \sim \log L$, we have $\alpha = 0$ as required.

Extracting absolute values for the critical exponents requires an absolute estimate of at least one of ν, β or γ. We will extract β from the magnetization near the critical temperature following the example of [3]. By plotting magnetization as a function of reciprocal lattice size L^{-1} for several temperatures near the critical point, the y-intercept of a simple linear fit will give an estimate of the magnetization of an infinite system, which can then be used to extract temperature scaling. The Metropolis algorithm proved inadequate for this purpose, and so the Wolff algorithm was implemented specifically for this simulation. Figure 5a shows the results of extrapolating magnetization to infinite system size for several values of temperature, which is then used in figure 5b to extract β as the slope of $\ln \tau$ versus $\ln |M(\tau)|$, yielding $\beta = 0.121 \pm 0.007$. Standard error propagation then gives our final results for the temperature scaling of the phase transition, outlined in the table below.

Exponent	Value	Theory
α	0	0
β	0.121 ± 0.007	0.125
γ	1.72 ± 0.07	1.75
ν	0.99 ± 0.07	1

In principle an identical analysis could be performed to extract δ by considering the magnetization induced by a small external field H near the critical temperature. However, because of the poor performance of the Wolff algorithm in the presence of external fields, the necessary statistics proved to be beyond a desktop computer.

3 Frustrated Spin Systems

While the basic 2D Ising model is well-understood, there are generalizations of the model which are still the subject of active research. One such extension of the model is the introduction of anti-ferromagnetic impurities in the system. These impurities have the effect of frustrating the system: spins with both ferromagnetic and antiferromagnetic neighbours cannot adopt a configuration which gives minimal interaction energy with all of its neighbours. We will loosely follow the recipe provided by [5], and attempt to answer some of the questions they raise in their work. The system considered in [5] involves vertical ferromagnetic nearest neighbour

interactions, while horizontal nearest neighbour interaction strengths in odd numbered rows are assigned an antiferromagnetic character of strength γ with probability p. Defining the interaction strength between spin (i, j) and spin $(i, j + 1)$ as B_{ij}, we have

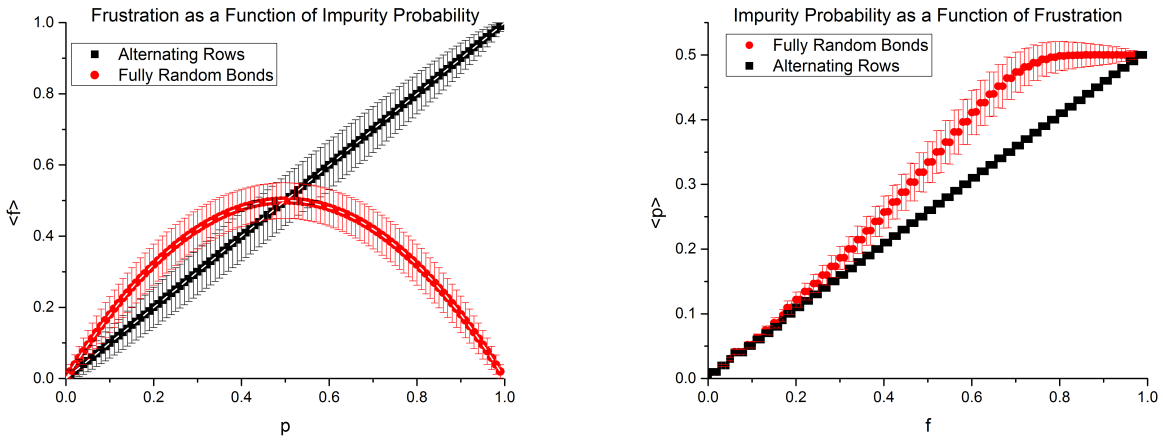
$$B_{ij} = \begin{cases} 1 & \text{i even} \\ -\gamma & \text{i odd, with probability } p \end{cases} \tag{16}$$

The case $-\gamma = 1$ recovers the basic model considered already. Following the example in [5], we define a plaquette to be the square formed by four nearest neighbour bonds. It's easy to see that a plaquette is frustrated if and only if the product of the bonds surrounding it is negative. The particular form of the frustration chosen by the group is done simply for the sake of an analytic solution, since fully random distribution of antiferromagnetic bonds is a much more challenging problem analytically. The results in [5] show the presence of additional phase transitions at low temperature (up to three transitions between 4 phases in the case of $\gamma = 1.2$ and $p = 0.82$).

Attempts to reproduce these effects failed, for reasons which will be discussed shortly. However, it is possible to answer one of the open questions that they pose at the end of their work, namely, whether or not the artificial order imposed by having antiferromagnetic bonds only in alternating rows has any impact on their results. The answer seems to be yes, but the reason does not require very complex simulations to elucidate.

Because antiferromagnetic bonds occur only in alternating rows, every such bond introduces two frustrated plaquettes into the system. If we define f to be the fraction of frustrated plaquettes, then is is easy to see that $\langle f \rangle = p$, where $\langle \cdot \rangle$ denotes an average over realizations of equation 16. On the other hand, for antiferromagnetic impuruties which are randomly distrbuted throughout the horizontal bonds in the system, a plaquette will be frustrated with probability $\langle f \rangle = 2p(1-p) < 0.5$. Thus, some degree of ordering is required to achieve $f > 0.5$ as is required for the appearance of additional phase transitions in [5]. The only way to achieve a fixed $f > 0.5$ while maintaining maximal disorder is to choose a bond at random, and reverse its character only if doing so will increase frustration in the sytstem. Figure 6 shows both approaches. In particular, we see that in order to fix $f > 0.5$ the scheme outlined here does not introduce more random bonds into the system (p levels off around 0.5 in figure 6b) but instead simply rearranges existing bonds until the level of frustration is achieved, moving the sytem closer to the partially ordered state used in [5]. Since the additional phase transitions appear only for $f > 0.5$ and seem to become more pronounced as f increases, the ordered state, or one which comes close, is necessary for its appearance.

Since we are unable to reproduce the results in [5] with the resources at our disposal, we will instead turn to a qualitive look at the effects of frustration on the physics observed in the simple Ising model. The parameter space is enormous, since we may now consider the effects of frustration level, antiferromagnetic interaction strength, temperature, and external field, so we will focus our efforts on the maximally frustrated system with antiferromagntic interaction



(a) (b)

Figure 6: Four different approaches to frustrating the system. In a), we use equation 16 and alternating limit antiferromagnetic bonds to alternating rows (black points) and calculate average frustration, and relax the constraint of alteranting rows with the same value of p (black points). In b), we randomly choose bonds and reverse their character only if it increases total frustration, until a fixed chosen level of frustration is achieved in the case of alternating rows (black points) and fully random bonds (red points) . Each measurements represents an average over 10^4 realization of each particular scheme, and error bards show standard deviations.

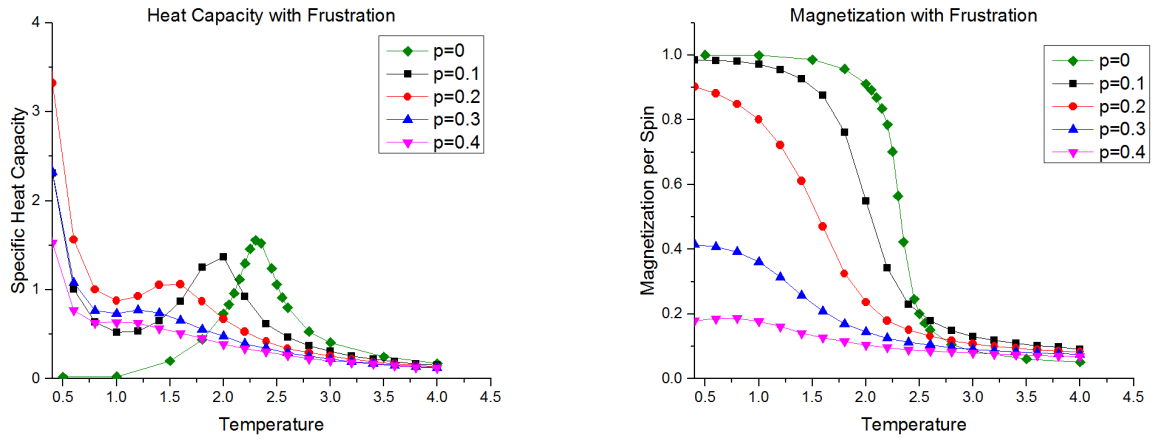
strength equal to the ferromagnetic bond strength, that is

$$B_{ij} = \begin{cases} 1 & \text{with probability } 1-p \\ -1 & \text{with probability } p \end{cases} \tag{17}$$

Frustration actually has a drastic effect on the system even at low frustration levels. First and foremost, it has the effect of slowing down the time required to reach equilibrium, especially at low temperatures. For this reason, simulations of frustrated systems are done using $10N^2$ spin-flips between microstate outputs instead of the previous N^2. In order to simulate an average over equation 17, bonds are reinitialized to a new value between every output of a member of the ensemble.

The effect on the ferromagnetic transitions can clearly be seen in the heat capacity in figure 7a. While the peak near the former critical temperature is still visible at low p, it is smoothed over and moves to lower temperature as frustration increases, since the additional energy introduced by frustrated interactions requires lower temperature before thermal energy is sufficiently for a nonzero magnetization to appear.

Most striking, however, is the sudden appearance of increased heat capacity at low T. The divergence of heat capacity is clearly unphysical, since the laws of thermodynamics requires the vanishing of heat capacity at absolute zero. The reason for this numerical artifact is rooted in fluctuation-dissipation theorem through equation 7. Because reinitialization of the bonds results in a new energy minimum each time, energy fluctuations over the ensemble become relatively large even at small T. A similar effect manifests itself in the magnetic susceptibility, becoming



(a) (b)

Figure 7: The effects of increasing levels of frustration on a 16×16 spin lattice is shown on a) heat capacity and b) magnetization. Each point represents an average over 10^4 microstates, except for the $p = 0$ curves which are taken directly from figure 1.

more pronounted in both cases as the level of frustration increases. At high temperatures the fluctuations introduced by randomizing the impurities are small compared to typical thermal fluctuations and the effect becomes less obvious. For an ensemble average over any particular realization of equation 17, this divergence would not be present. In light of this, it is not at all surprising that we failed to reproduce the results of Pasquini et al [5], since all the additional phases they observed were at relatively low tempature. If we fix the level of frustration instead of the probability for an antiferromegnetic bond, the divergence is suppressed slightly, but is still present at very low temperatures.

While low temperature results are suspect, at high temperatures the fluctuations induced by randomizing bonds are small compared to thermal noise, as evidenced by the convergence of all the curves at high temperature in figure 7, and so it is still possible to comment on qualitative trends. Unsurprisingly, the magnetization is no longer complete at any temperature, since random distribution of antiferromagnetic bonds introduces a tendency to seed oppositely magnetized domains. While the ferromagnetic vertical bonds are sufficient to ensure that a nonzero magnetization menifests itself at low temperature regardless of frustration, there is no longer a sharp transition between paramegnetism and ferromagnetism.

4 Conclusion

We have investigated the ferromagnetic phase transitions in 2-dimensional Ising spin systems and successfully quantified the temperature scaling of the transitions through the critical exponents. In particular, we find that the magnetization diverges with exponent $\beta = 0.121 \pm 0.007$, the susceptibility diverges with exponent $\gamma = 1.72 \pm 0.07$, the heat capacity shows a log divergence with exponent $\alpha = 0$, and the correlation length diverges with exponewnt $\nu = 0.99 \pm 0.07$, all in agreement with theoretical predictions. Moreover, we have studied the effect of adding a

proportion of antiferromagnetic impurities to the system, showing that they result in greatly increased fluctuations in energy and magnetization even at low temperatures, though the appearance of a divergence in the heat capacity and magnetic susceptibility is attributed to the method used to simulate the impurities as opposed to a real physical effect.

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