Phase transitions - Simulating a 2D Ising model with Monte Carlo

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ABSTRACT

The Metropolis is a useful method for simulating the 2*D* Ising model. This Monte Carlo based algorithm managed to calculate the critical temperature to to decimals precision. Simulations with impurities and magnetic fields also showed how the phase transition collapsed and how the system was impacted. The drawback of the Metropolis algorithm is that it easily falls into local minima, requiring colossal number of sweeps to reduce this probability. To avoid enormous computational complexity, the simulated annealing algorithm was implemented. This algorithm proved suitable to find the global minima even for systems with constraints like impurities.

Keywords: 2D Ising model, Metropolis algorithm, Simulated annealing, Phase transitions, critical phenomena

I. INTRODUCTION

A. Theory

1. *Ising Model*

Ising model is a model for studying phase transitions. It consists of a set of spins, s_i which either can point upwards $s_i = +1$ or downwards $s_i = -1$. In this report the square 2*D* Ising model is investigated, meaning that the spins are ordered in a square lattice. In a a square lattice, each spin has four neighboring spins.

The Hamiltonian, E, is a measure of the energy of the system, and for the 2*D* square Ising model is defined as

$$E = -J\sum_{\langle ij\rangle} s_i s_j - H\sum_i s_i, \tag{1}$$

where J is the coupling constant, H the magnetic field, and $\langle ij\rangle$ notated the indices of neighboring particles[1].

In this report, $J = 1$ the coupling constant is ferromagnetic, which means that a system where all the spins point in the same direction will have the lowest possible energy. If $H \neq 0$, all spins should point in the same direction as the magnetic field to have minimal energy.

A central part of this paper concerns phase transitions, the process where a system drastically goes from one state to another. To describe phase transitions order parameters are often used to measure the degree of asymmetry in the phase transition. An order parameter is non-zero in an ordered state, while it is zero in a disordered system[1]. Therefore the order parameters has a discontinuity at the phase transition. Based on how the order parameter is related to the free energy, which order of the derivative, the phase transition is labeled *first* or *second* order. In this paper the spontaneous magnetization is an order parameter.

Order parameters tend to behave as power-law singularities in the critical regime, around a critical variable such as the temperature, T_C[1]. There are multiple such power-laws for magnetic quantities, but in this report only the following will be used:

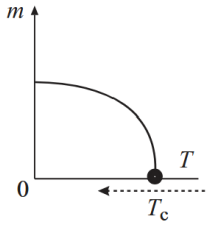


FIG. 1: Second order phase transition. Here the spontaneous magnetization m is used as an example, since it is a second order transition of temperature. Adapted from figure 1.3 in *Elements of Phase Transition and Critical Phenomena*[1]

$$C \propto |\tau|^{-\alpha} \quad (T > T_c), \tag{2a}$$
$$M \propto |\tau|^{\beta} \quad (T < T_c), \tag{2b}$$
$$M \propto |H|^{1/\delta} \quad (T = T_c), \tag{2c}$$
$$\chi \propto |\tau|^{-\gamma} \quad (T > T_c), \tag{2d}$$
$$\xi \propto |\tau|^{-\nu} \quad (T > T_c), \tag{2e}$$

where $\tau = \frac{T-T_c}{T_c}$, H the magnetic field and $\alpha, \beta, \gamma, \delta, \nu$ are the critical exponents for the specific heat C, magnetization M, susceptibility χ and correlation length ξ[1]. The analytical values for these critical exponents are listed in Table I. The analytical value for the critical temperature is $T_C = \frac{2}{\ln(1+\sqrt{(2)})} \approx 2.269$[2].

TABLE I: Critical exponents and their analytical values for 2*D* Ising model, data from Nishimori and Ortiz[1]

Critical exponent	Analytical value
α	0
β	1/8
γ	7/4
δ	15
ν	1

Specific heat C is defined as the temperature derivative of the entropy S, which again is related to the free energy, F by the formula $S = F - T\frac{\partial F}{\partial T}$[3]. Using the fluctuation-dissipation

theorem dissipation one can get the following expression for the specific heat:

$$C = \frac{(\Delta E)^2}{k_B T^2}, \tag{3}$$

where k_B is the Boltzmann constant and $\Delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2}$[2]. Correspondingly, since the magnetic susceptibility is defined as the magnetic field derivative of the magnetization[4], the fluctuation dissipation theorem yields[5]

$$\chi = \frac{(\Delta M)^2}{k_B T} \tag{4}$$

If $H \neq 0$ there is no phase transitions for M as the magnetic field disorder the spins, making sure there never will be a fully non symmetric phase, and therefore no discontinuity in $T = T_C$.

With L^2 spins that can have two distinct values, there are 2^{L^2} possible configurations of the system. Of these only two have minimal energy, given that $H = 0$, namely that all spins have the same direction, either up or down. If $H \neq 0$, the state with the lowest energy is the state where all spins are pointed in the same direction of the magnetic field.

II. MODELS AND METHODS

A. Metropolis algorithm

To simulate the 2D Ising model, the Metropololis Monte Carlo algorithms was used to flip spins. The code was written in Julia. The implementation was inspired by the python implementation in *Example: Metropolis algorithm for the 2D Ising model* in the MC-notebook from Tor Nordam[6]. The project also included adding impurities in the grid, which were modelled as spin which could not be flipped. This was done by drawing a random sample of size pL^2, where p was the proportion parameter, and skipping energy calculation and flipping on these spins. The full logic behind the implemented Metropolis algorithm is described as pseudo-code in algorithm 1.

B. Simulated annealing (SA)

As the Metropolis algorithm might converge on a local minimum, the Simulated annealing algorithm was implemented to avoid falling into a global minimum. This algorithm starts at a high temperature to open up the possibility of a jump out of a local minimum because of high kinetic energy. The hope is that the system will have jumped until it is in or close to the global minimum before the temperature gets so cold that the system stabilizes. Algorithm 2 shows the pseudo-code for the SA-algorithm. The implementation was is inspired by the flowchart in this article by Baeldung[7].

Algorithm 1 Metropolis algorithm (MC)

Require: N : number of sweeps, T : temperature, L : system length, p : proportion of impurities.
Ensure: Find spin configuration that minimizes energy
  $grid \leftarrow$ random($[0,1]$, size$= L^2$)
  $M_0 \leftarrow \sum_i s_i$ ▷ Initial magnetization
  $E_0 \leftarrow J\sum_{\langle ij \rangle} s_i s_j - H\sum_i s_i$ ▷ Initial magnetization
  $impcoords \leftarrow$ random($([1:L],[1:L])$), size $= (L^2, 2)$
  for n in $1:N$ **do** ▷ Sweep
    for k in $1:L^2$ **do** ▷ Flips
      if (i,j) not in $impuritycoords$ **then**
        $i, j \leftarrow random(1:L)$
        $s'_{i,j} \leftarrow s_{i,j}$ ▷ Flip spin
        $\Delta E = -2Js'_{i,j}\sum_{j \in \langle ij \rangle} s_{i,j} - 2\mu H s_{i,j}$ ▷ Energy change
        $r \leftarrow$ random($[0,1)$)
        if $\Delta E < 0$ or $r \leq e^{(-\Delta E/T)}$ **then** ▷ Minimize energy or random kinetic jump
          $E \leftarrow E + \Delta E$
          $s_{i,j} \leftarrow s'_{i,j}$
          $M \leftarrow M + 2s_{i,j}$
        end if
      end if
    end for
  end for
  return $grid, E, M$

Algorithm 2 Simulated Annealing (SA)

Require: p : proportion of impurities, N : number of sweeps, T_{max}, T_{min} : start and end temperature, α : cooling rate, L : system length
Ensure: Spin configuration that minimizes energy (optimized)
  $T \leftarrow T_{max}$
  $x \leftarrow$ random($[0,1]$, size$= L^2$) with impurities ▷ Initial Grid
  $M \leftarrow \sum_i s_i$ ▷ Initial magnetization
  $E \leftarrow J\sum_{\langle ij \rangle} s_i s_j - H\sum_i s_i$ ▷ Initial magnetization
  while $T > T_{min}$ **do**
    $x_{new}, E(x_{new}), M(x_{new}) \leftarrow MC'(N, T, p, x)$
    $\Delta E \leftarrow E(x_{new}) - E(x)$
    $r \leftarrow$ random($[0,1)$)
    if $\Delta E < 0$ or $r \leq e^{(-\Delta E/T)}$ **then** ▷ Minimize energy or random kinetic jump
      $x = x_{new}$ ▷ Update parameters
      $E = E(x_{new})$
      $M = M(x_{new})$
    end if
    $T \leftarrow \alpha T$ ▷ Reduce temperature
  end while
  return x, E, M

C. Finding critical exponent α

A method based on finite size scaling was used to approximate the critical exponent α. From Equation 2e, one can get that $|\tau| \propto \xi^{-\frac{1}{\nu}}$ for $T > T_C$. Inserting this expression for $|\tau|$ into Equation 2a, one gets that

$$C \propto |\xi|^{\frac{\alpha}{\nu}} \quad (T > T_C). \tag{5}$$

From Equation 2a it is obvious that C diverges as $T \to T_C$, which means that according to Equation 5 $\xi \to \infty$ as $T \to T_C$

too. Further, one can from Equation 2e, find the exponent $-\nu$ as the slope of a line through the points $\frac{\log\xi}{\log|\tau(T)|}$. Similarly one should be able to find the ratio $\frac{\alpha}{\nu}$ as the slope of a line through $\frac{\log C(T)}{\log\xi}$.

First one need an approximation for T_c. The method used here was to find out for which temperature the magnetization behaved as a power law. This was done by fitting a line through the $\log M(t)$ as a function of $\log\xi$ for different temperatures, here $T\in[1.0,3.5]$. The index with the best R^2 value was chosen and the temperature at this index was the approximation to T_c. Then the temperatures maximizing the heat coefficient for each L was found, and these temperatures was put into $\tau'(L)=\left|\frac{\max_T\{C(L)\}-T_c}{T_c}\right|$. Then $\log\xi$ was fitted against $\log\tau(L)'$ to find the the parameters ν. Then the maximum values of the heat coefficient $C_{max}(L)$ was found before a line was fitted through $\log(C_{max}(L))$ as a function of $\log\xi$ to find the factor $\frac{\alpha}{\nu}$. Since both ν and $\frac{\alpha}{\nu}$ now where known, α could be calculated.

III. RESULTS AND DISCUSSION

To be able to analyze the critical behavior of the system, it is important that the system achieve equilibrium. The equilibrium energy is though temperature dependent, as shown in Figure 3a. The higher the temperature, the more thermal fluctuations, preventing the system of reaching the global minimum energy, effectively increasing the equilibrium energy, as seen in Figure 4a. These fluctuation are visible in Figure 3b, where the system is achieves equilibrium as almost all spins point in the same direction, here up. For the higher temperatures, the fluctuations reduce the probability of ending up in the symmetric state. Further the higher the temperature, the lower the magnetization, as spins flip more often due to thermal energy, resulting in a more evenly distributed pattern, as can be seen in Figure 2. The phase transition between this ordered and the discorded state is clearly visible in Figure 4b, which greatly reassembles the plot of a second order phase transition, Figure 1 there exist a phase transition between the ordered state where the spins point mostly in the same direction to a state of disorder, as seen in Figure 1.

From the energy plot Figure 3a, the energies quickly stabilizes, indicating that there is not many sweeps necessary to reach equilibrium. However, as the magnetization in Figure 3b fluctuations significantly, even after $1.6e7$ time steps, the system may converge locally, which therefore demands many steps to be able to escape. Local converging is like the reason for the magnetization has some outliers to the left of the critical temperature. For low temperatures the probability for jumping of of a local minima due to thermal energy is low, and therefore a enormous number of sweeps are necessary to be able to reduce the number of outliers. An alternative is to use the simulated annealing algorithm, algorithm 2.

A. Without magnetic field

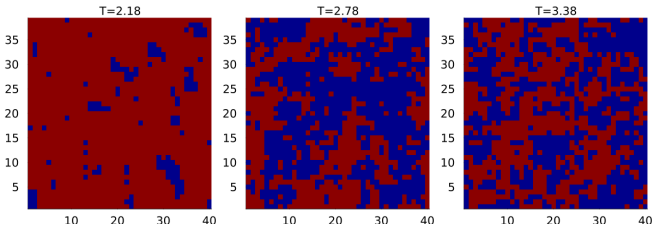
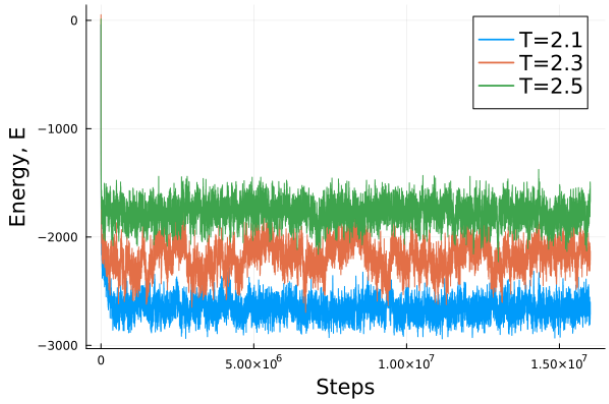
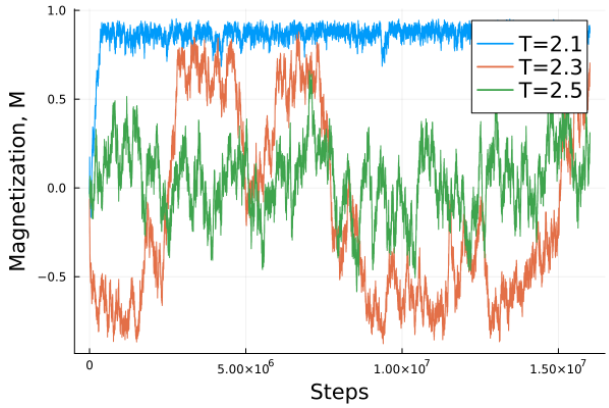


FIG. 2: Final spin configuration for the three temperatures $T\in[2.18,2.78,3.38]$. Red spins point upward $(s_i=+1)$, while blue points downwards $(s_i=-1)$.



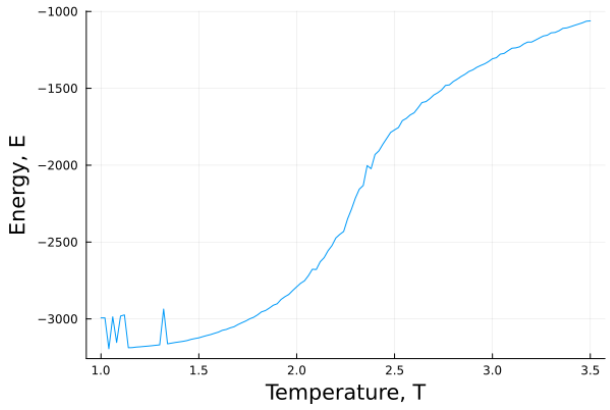
(a) E



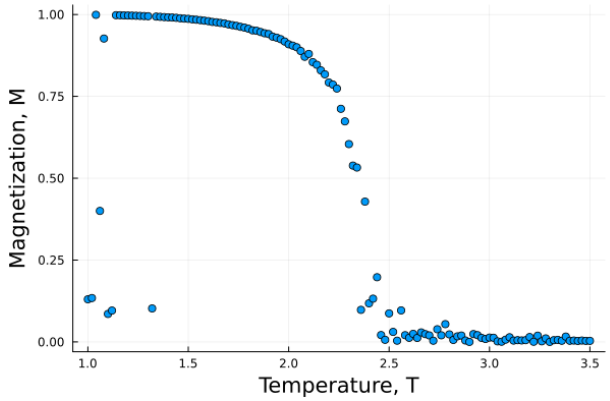
(b) M

FIG. 3: Energy (a) and magnetization plot (b) for a lattice of lengths $L=40$, there are $L^2=1600$ steps per sweep. The simulation was run for 10000 sweeps to ensure system converged. Both plots was run for the temperatures $T\in[2.1,2.3,2.5]$.

The temperatures giving the highest peaks in Figure 5b are in the interval $T\in[2.2,2.32]$, with a mean of 2.27. This results is in great agreement with the analytical result for the critical temperature as presented in section I A. To investigate how the estimated critical temperatures giving the the highest

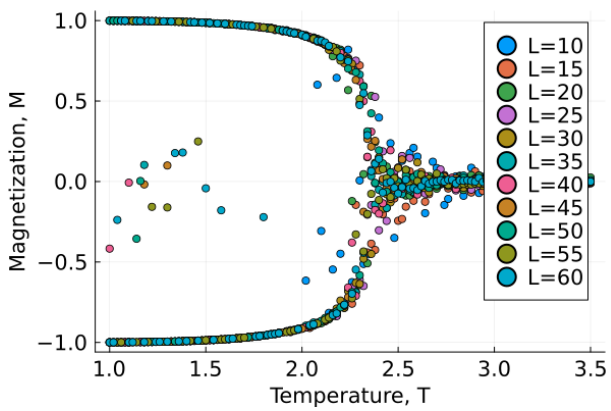


(a) E

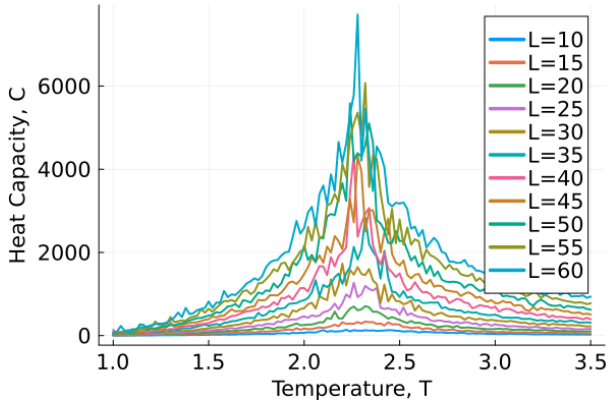


(b) $|M|$

FIG. 4: Energy (a) and absolute value of magnetization (b) as functions of temperature. 10000 sweeps used.



(a) M



(b) C

FIG. 5: Energy (a), magnetization (b) and specific heat (c) as functions of temperature for different system lengths L.

peaks in C, one can do a linear regression through the data points $C(L)$. Figure 11 shows a such linear regression. The graph has slope of almost zero, and the R^2 is so low, that a linear dependency between L and T_max is not not likely. The data points are also so spread, that there is no foundation to conclude whether the system size has a influence on the value at which the specific heat C diverges. As T_c is constant for the system, one should not expect the system size to be influence the point at where the critical phenomena takes place.

1. *Finding* α

The temperature that maximizes the R^2 value for M as a function of $|\tau|$ is 2.64, which is far from the analytical value of 2.269. This deviation is most likely due to the limitations of the finite size scaling and that the data of Figure 5a is messy around T_C. Also the R^2 values fluctuated randomly, having large peaks throughout the temperature interval, as seen in Figure 12. Still the approximated critical temperature value was used to calculate the critical exponent ν, which got a number of 0.53, which is far from the analytical value in Table I. This deviation might also be due to the low values for L, as $\xi \to \infty$ at T_c, therefore giving a R^2-value of 0.012 and a $p-$value of 0.75, indicating that there is no linear dependency between L and $|\tau|$. The log-log plot of C_{max} as a function of L got a almost linear fit with $R^2 = 0.993$ and $p < 1e-10$, resulting in $\frac{\alpha}{\nu} = 2.27$, giving $\alpha = 1.2$, which is not close to the analytical value of zero. The large deviations between the obtained results and the analytical values, indicates that this method based on finite size scaling is not suited for a $2D$ Ising model of such small scales. If ξ should diverge, $L \to \infty$.

The average magnetization do not seems to be effected by the system size L, as the data points in Figure 5a mostly fit on the line of theoretical data as plotted in Figure 4b, but here with both positive and negative values. The explanation of this independence is that the plotted magnetization is averaged over the number of spins in the system, L^2, which means that only the relation between the number of positive and negative spins that is important. According to Figure 5b, the temperature where the specific heat diverges is not affected by the system size L. However, the magnitude of the peaks increases with L, as there are more spins in the system, and therefore possible larger energy fluctuations in the critical regime.

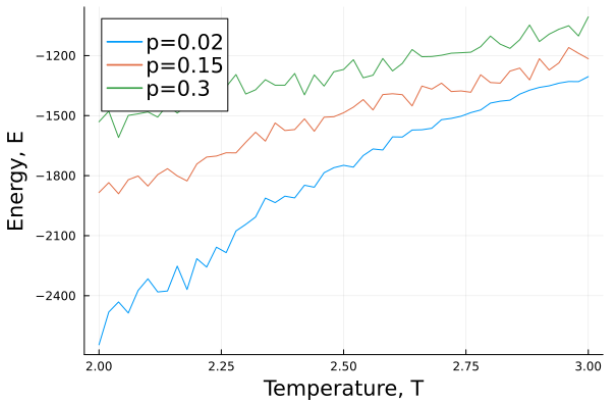
2. *With impurities*

Impurities was added as as described in 1. From Figure 6a, it is evident that the lower the proportion of impurities p, the lower the energy, especially for low temperatures. The effect of impurities gradually weakens as the temperature increases, due higher thermal energies disorders the system, leaving the configurations more random. From Figure 6b, it is clear that the impurities destroys the phase transition between a order spin state and a disordered one, as it collapses the magnetization to fluctuate insignificantly around zero. The reason for this collapse is that impurities induces local clusters, since there are multiple spins of different orientation that cannot change. Such clusters are visible in Figure 7, where larger ps introduce more and smaller cluster. The formation of clusters makes it more difficult for the Metropolis algorithm to find the global minimum, and therefore the simulated annealing algorithm was used. Comparing the values of Table II with the values from, the SA obtained lower energy for all ps and larger magnitudes of M for $p = 0.02$. The SA did though iterate down to $T = 0.1$, further than the normal Metropolis was allowed. The energy of the different systems for the same p did no vary much, but the magnetization did for larger values of p. Since the impurities are drawn at random, one initialization could contain many impurities pointing the same way near each other like in $p = 0.15, i = 2$ in Figure 7, where the most stable system contained large areas of spins point the same direction, resulting in a larger magnetization. In comparison $p = 0.15, i = 2$, contains smaller clusters more distributed, resulting in a low magnetization magnitude. This adaptability makes the SA algorithm suitable for tackling a wide range of systems.

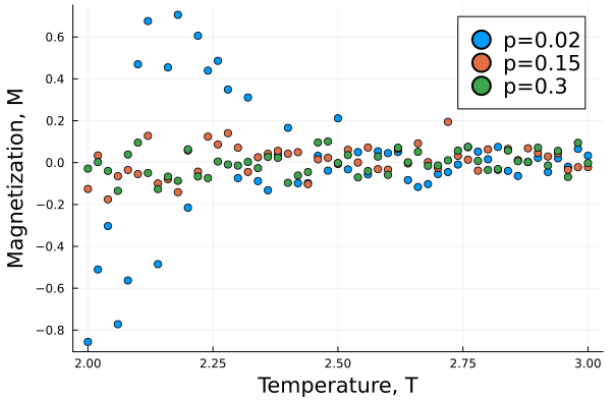
From Figure 6c it is evident that the specific heat reduced with the number of impurities. More impurities, the fewer spins are able to flip, and therefore the maximum energy variance is reduced. Formation of local clusters further reduce the energy difference achievable, as the system is far away from the global energy minima where all spins point in the same direction. Therefore Figure 6c also displays the collapse of the phase transition.

TABLE II: Final energy E and magnetization M for different proportions of impurities p and different initializations i. 500 sweeps were used.

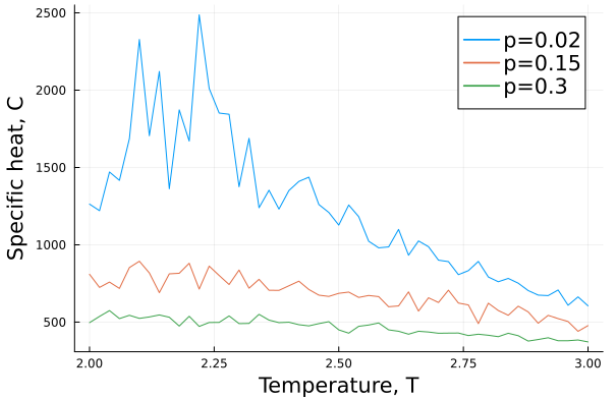
	E			M		
	$p = 0.02$	$p = 0.15$	$p = 0.30$	$p = 0.02$	$p = 0.15$	$p = 0.30$
$i = 1$	-3088.0	-2484.0	-2048.0	0.97875	0.47125	-0.00875
$i = 2$	-3060.0	-2492.0	-1972.0	0.9775	0.0275	0.22875
$i = 3$	-3120.0	-2464.0	-1952.0	-0.9875	-0.03625	-0.03375



(a) E



(b) M



(c) C

FIG. 6: Energy (a), magnetization (b) and specific heat (c) as functions of temperatures with impurities added. A run was used for impurity proportions $p \in [0.02, 0.15, 0.3]$.

B. With magnetic field

Comparing the magnetization plots in Figure 3b and Figure 8, the importance of the magnetic field becomes clear. Comparing the graph for the same temperature $T = 2.3$, the magnetization is almost stabilized compared to the wildly fluctuating example of Figure 3b. One can even see that when the magnetization is beginning to drop, there is some mechanism that counteracts this change, which is the magnetic force. Looking at Figure 9, one can observe that most of the spins point in the same direction as the magnetic field. It is important to mention that each instance is different and that

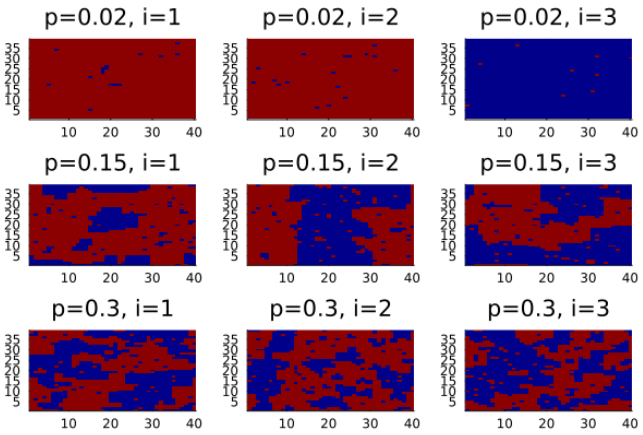


FIG. 7: Final grids from the SA algorithm. These grids are the lowest energy configuration given the initial grid. Here p is the proportion of impurities, while i is the label for the initialization. Here 500 sweeps was used.

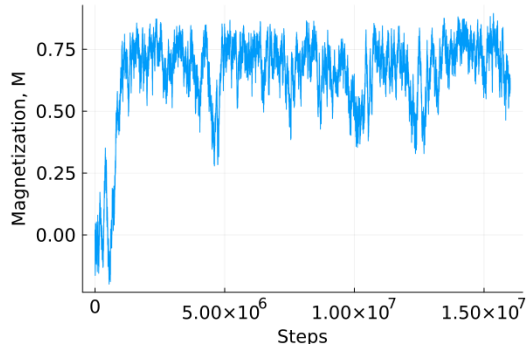


FIG. 8: Magnetization, M as a function of number of steps, with magnetic field $H = 0.01$ and temperature $T = 2.3$. 10000 sweeps used, where each sweep is 1600 steps. The starting temperature was 10 and the end temperature was 0.1. The cooling rate was set to 0.96, and $L = 40$.

the the systems might end up with a total different behavior than presented here, but the magnetic field will help the system stabilize for even higher temperatures. Figure 10a depicts this effect, as the magnetic field smooths out the phase transition, effectively removing the discontinuity and therefore the abrupt change between a ordered state and a disordered state, as predicted in section I A. The larger the H, the higher the temperature before the system reaches state of almost zero net spin, and therefore the less resemblance to a phase transition. Figure 10b also shows this conduct as the higher the H, the lower the peaks and the more continuous the function $\chi(T)$ becomes. In the opposite limit, as $H \to 0$, the peaks becomes higher and the behavior more and more diverging, leading to a phase transition in $H = 0$.

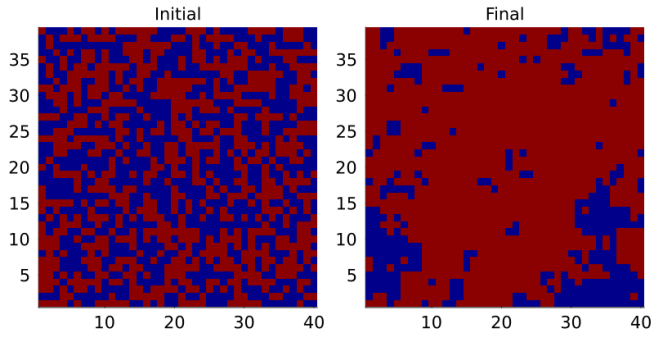
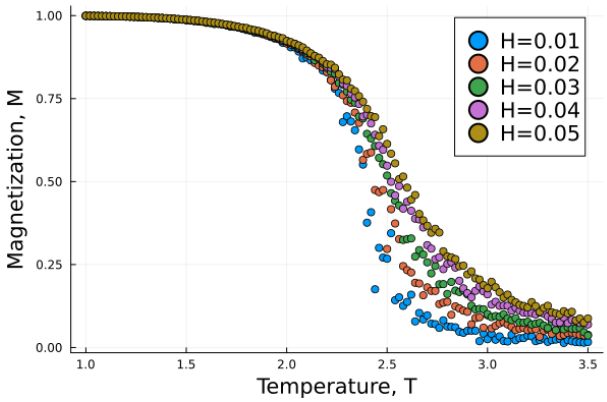
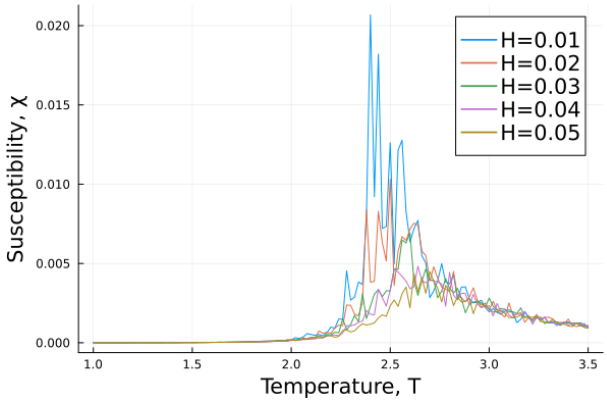


FIG. 9: Initial and final grid, with magnetic field $H = 0.01$ and temperature $T = 2.3$. Red spins point upward $(s_i = +1)$, while blue points downwards $(s_i = -1)$.



(a) $|M|$



(b) χ

FIG. 10: Magnetization magnitude (a) and susceptibility χ (b) as functions of temperatures for different magnitudes of magnetic field $H \in [0.1, 0.5]$.

IV. CONCLUSIONS AND FUTURE WORK

Critical phenomena of the 2D Ising model could effectively be studied using Monte Carlo simulations. Using Monte Carlo simulations the critical temperature was calculated to to decimal precision. Simulated annealing was effective to find

global minima, systems with impurities.

Further work includes a larger simulation for large numbers of L to better find the critical exponent α. Interesting would also a study in data collapsing with scaling laws to better illustrate the different behavior around the critical regime.

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V. APPENDIX A:FIGURES FOR FINDING α

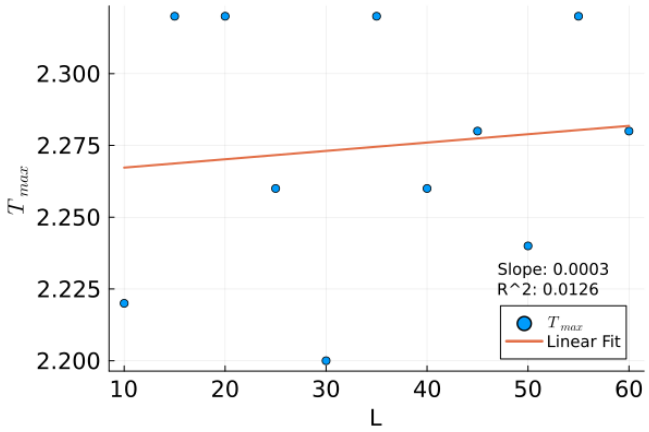

FIG. 11: Linear regression for temperature values that maximize the specific heat, as a function of system length L.

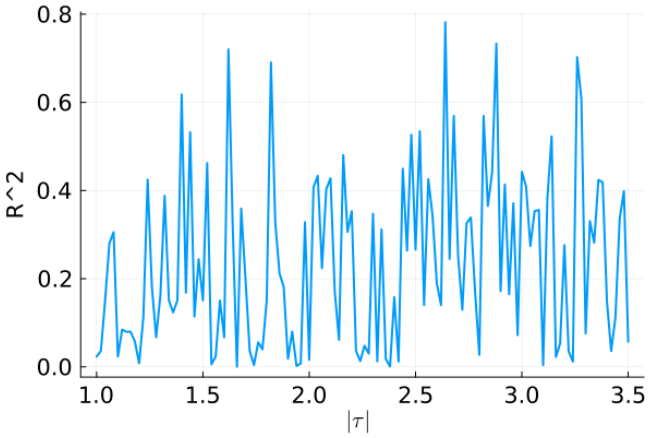

FIG. 12: R^2 values for M as as function of τ.