1 Introduction

The Ising model, named after physicist Ernst Ising is a model of discrete random variables representing the magnetic dipole moment of atomic spins, although it has other applications such as modeling pigmentation formation in animals. Classically the two states or "spins" are $+1$ or -1. For the 2D Ising model we consider an $N \times N$ lattice, where at each lattice point $\sigma_i \in \{-1, 1\}$ for $i = 1, ..., N^2$. The system tends to a lower energy state but heat disturbs this tendency allowing for the possibility of different structural phases to arise. We consider such an $N \times N$ square lattice with periodic boundaries. For any given configuration $\sigma \in \mathbb{R}^{N \times N}$, whose entries are σ_i, we can compute the total energy of the system via its Hamiltonian,

$$H(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i, \quad i = 1, 2, ..., N^2.$$

Here J is an interaction between spins, more generally we could write something like J_{ij} to suggest a non constant interaction term between spins for various reasons, however we stick to the simpler consistent interaction coefficient between all spin states J. The second term is representing energy loss in the presence of an external magnetic field h as we would expect more lattice spins to align on average with their neighbors in the presence of some external magnetic field, thus leading to a lower energy configuration.

2 Part A: Plotting Internal Energy & Specific Heat

2.1 Internal Energy

We consider the interacting term $J = 1$, $k_B = 1$ (for simplicity), and $h = 0$, i.e. no external magnetic field being applied to the lattice. We are tasked with plotting internal energy of the system as a function of temperature. We are given the following equations for internal energy,

$$u = \frac{U}{N^2}, \qquad U = \langle H \rangle = \frac{1}{N^2} \frac{1}{Z} \sum_\sigma H(\sigma) e^{-\beta H(\sigma)},$$

where $\beta = (k_B T)^{-1}$ and $Z = \sum_\sigma e^{-\beta H(\sigma)}$ is the partition function which is really a normalizing constant. You may immediately notice that computing $\langle H \rangle$ exactly becomes computationally impossible for even small lattice size considerations. For any lattice size N since every lattice spin can be either spin up or down there are 2^{N^2} possible configurations σ. If we take even a small lattice say, $N = 20$ there are 2^{400} possible configurations, σ for which we need to compute $H(\sigma)$. Clearly we need a better approach so we consider the Markov Chain Monte Carlo (MCMC) simulation to estimate $\langle H \rangle$.

2.2 Procedure: Metropolis Algorithm

Since computing the expected internal energy exactly is out of the picture we instead sample from the Boltzmann distribution of energy states for a given temperature to instead estimate the average internal energy. We first need an initial configuration of spins, naively we could initialize with roughly half spins up and half spins down in a lattice by sampling from the set $\{-1, 1\}$ with uniform probability. However, this is not a likely configuration as the energy is actually too large. Our fix is to apply the **Metropolis Algorithm** to this naive initial configuration

until our configuration is one that is more typical of a Boltzmann distribution. The Metropolis algorithm (see appendix for R code details) can be summarized as the following steps:

(i) Randomly select a single lattice site, say σ_i.

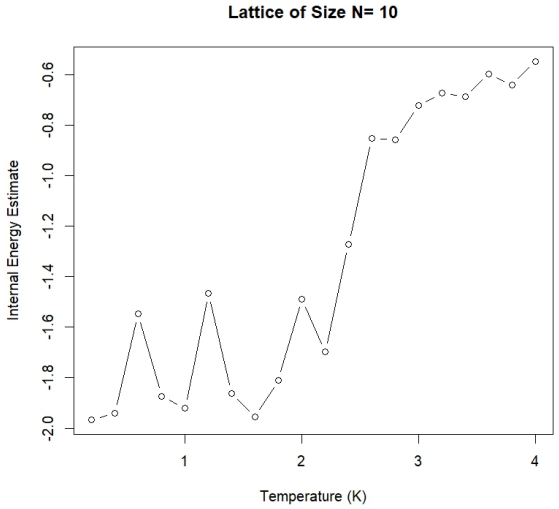
(ii) Propose flipping the spin, i.e. $\sigma_i \to -\sigma_i$.

(iii) Compute the difference in energy of the two configurations, $\Delta H = H(\sigma_{flip}) - H(\sigma_{original})$,

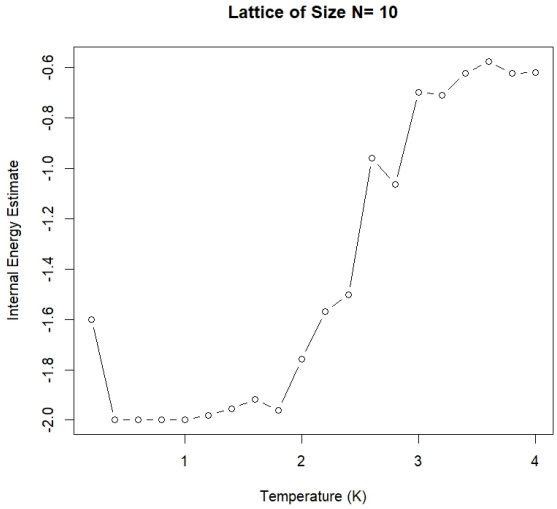
(iv) If the energy configuration post flip is lower ($\Delta H \leq 0$), we accept this new configuration.

(v) If the energy configuration post flip is higher we do not automatically reject the new configuration, instead we accept it with probability $e^{-\beta \Delta H}$.

One slight computation improvement to this algorithm, as it is currently stated, is not computing the total energy of each configuration but only the local energy change at the lattice site, as the rest of the configuration remains the same. The idea now is to take the initial configuration of uniformly distributed spin up and spin down lattices and apply the Metropolis algorithm many times until we approach a typical configuration of the Boltmann distribution. The problem is how many metropolis algorithms do we apply until we can begin to sample? A common unit used is called a **sweep**[1], which is defined as N^2 MC steps, in this case N^2 Metropolis algorithm steps. The rationale being that in 1 sweep on average each site is visited once.



((a)) 10 Sweeps Burn-in, 20 Sweeps Recording



((b)) 100 Sweeps Burn-in, 20 Sweeps Recording

Figure 1: Noise Levels Depending on Number of Burn in Sweeps

The number of sweeps turns out to be a parameter we can vary and notice varying levels of noise in our output, see fig. 1. The more sweeps applied the more the configuration becomes a typical configuration of the Boltzmann distribution. However we do not want to sample the total energy of the configurations during these initial sweeps as they do not yet resemble the distribution we wish to sample from. These initial sweeps are typically called **burn-in** where we do not sample total energy. Once a sufficient burn-in period has been simulated we then begin to sample once every sweep. We can also visualize this evolution into the appropriate distribution by plotting the system's configuration after a given number of sweeps. You can see some initial pattern formation in fig. 2.

[1] reference

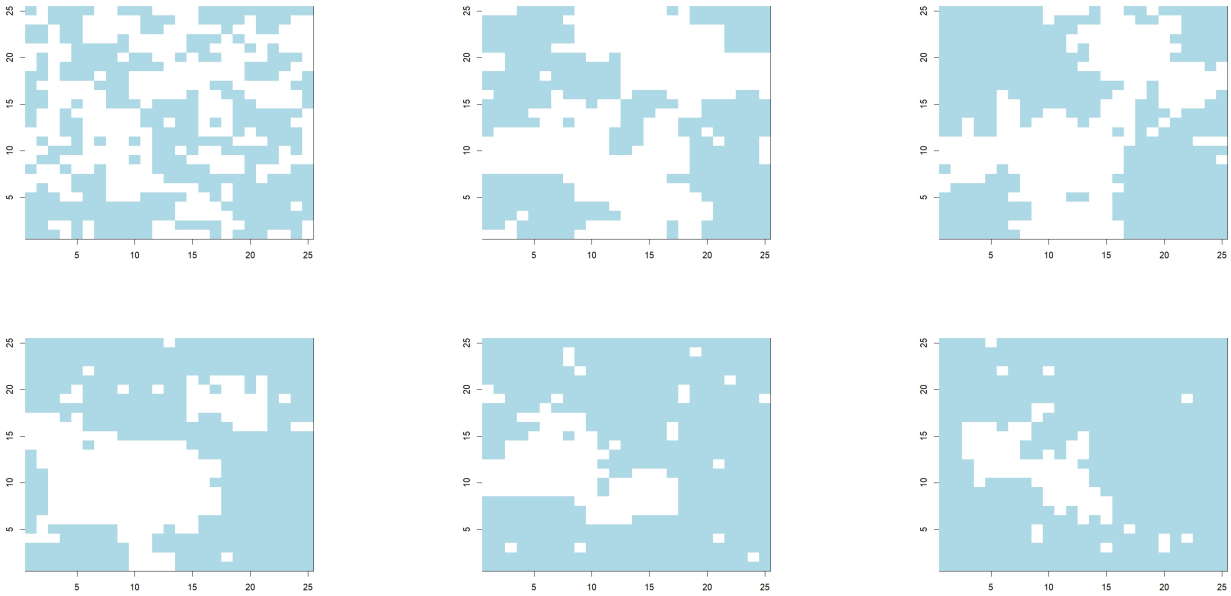
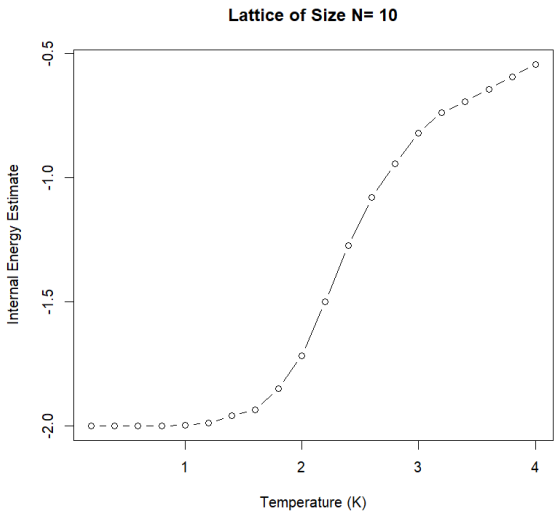


Figure 2: Six snapshots of the 2D Ising model during Metropolis evolution at $T = 2$.

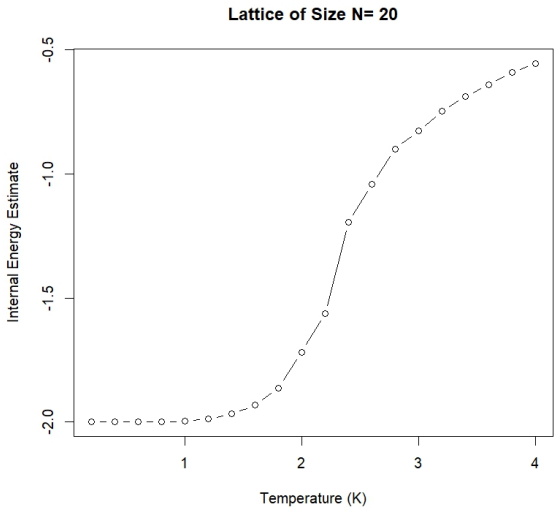
2.3 Internal Energy Results

We begin by selecting a lattice size, I picked $N = 10, 20, 30$, and 40 so as to keep computation time reasonable. Then we look at a range of temperatures for which I picked $(0.2, 0.4, ..., 3.8, 4.0)$. The MCMC is then the following steps:

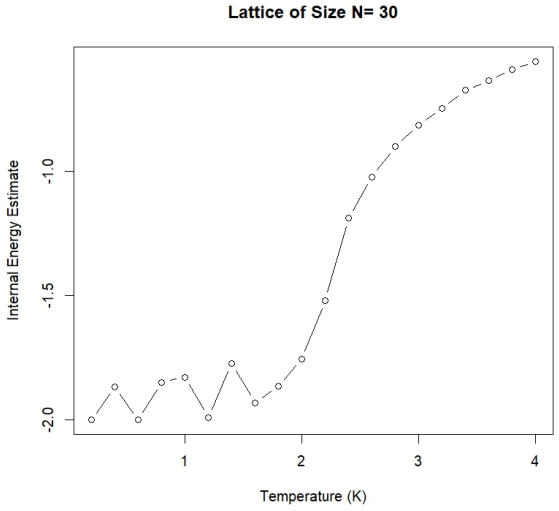
1. Set $T = 0.2$, and consequently $\beta = \frac{1}{0.2}$.
2. Initialize a uniformly distributed $N \times N$ lattice, and run the Metropolis algorithm for a certain number of sweeps (burn-in). *I stuck to around 100 to 200 sweeps, but obviously a longer burn-in period yields less noise.*
3. Once the burn-in period is over we begin sampling total energy by computing $H(\sigma)$ every sweep. *This is yet another parameter, obviously the more we sample the better estimate we will have of* $\langle H \rangle$.
4. Compute and save the sampled average energy at this temperature.
5. Set $T \to T + 0.2$ and repeat the process until $T = 4.0$.
6. Plot T versus our estimates for the internal energy, say $\overline{u}$.



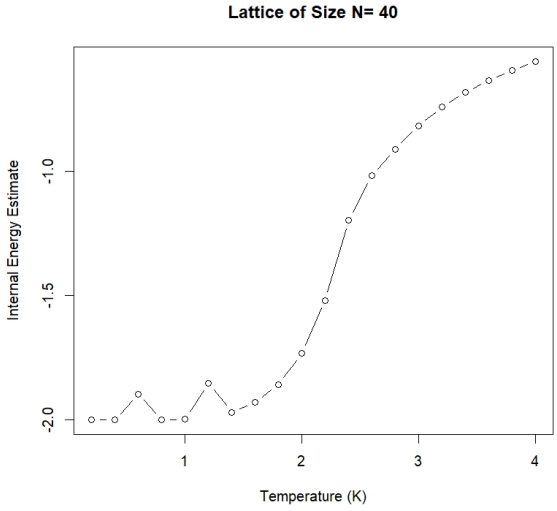
((a)) $\overline{u}$ versus T ($N = 10$)



((b)) $\overline{u}$ versus T ($N = 20$)



((c)) $\overline{u}$ versus T ($N = 30$)



((d)) $\overline{u}$ versus T ($N = 40$)

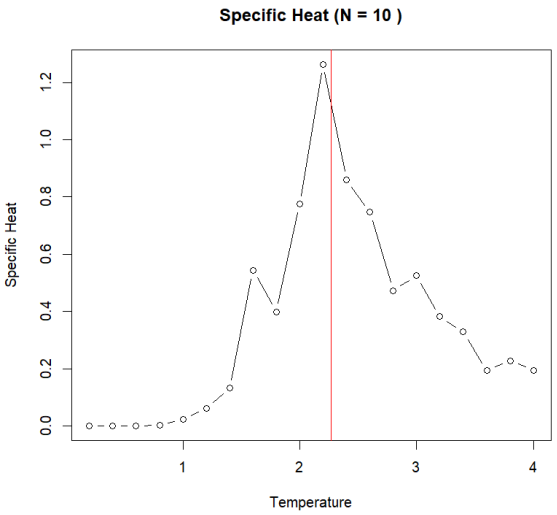
Figure 3: Results: Plotting $\overline{u}$ as a Function of T For Varyiing Lattice Sizes

The results for internal energy as a function of temperature can really be best summarized by fig. 3. Due to computation time restraints the burn in periods were kept constant for all four lattice sizes, namely 250 burn in sweeps and 1000 recording sweeps. We note in all four plots a trend towards -2 internal energy for lower temperatures and a trend towards 0 internal energy for higher temperatures. This is consistent with the idea that for lower temperatures spins spontaneously align (the ferromagnetic state) and for higher temperature (above the critical temperature) spins are randomly oriented, the so called paramagnetic state[2].

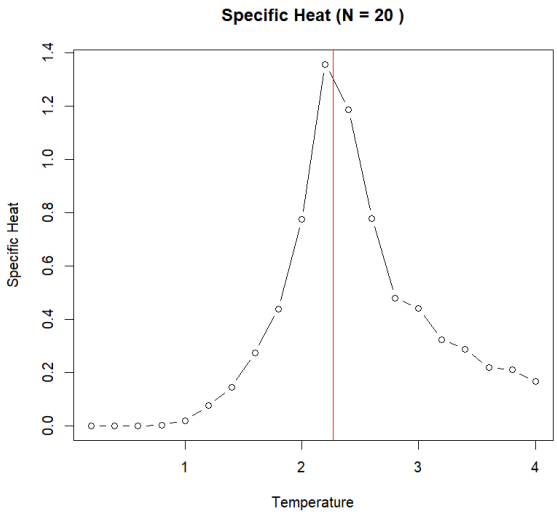
2.4 Specific Heat

The process of recording the specific heat as a function of temperature under no external magnetic field is nearly identical to except we record $\overline{c}$ the estimate of specific heat at some T.

[2]reference



((a)) $\bar{c}$ versus T ($N = 10$)



((b)) $\bar{c}$ versus T ($N = 20$)

Figure 4: Results: Plotting $\bar{c}$ as a Function of T For Varying Lattice Sizes

The only real difference is that the number of sweeps required for lattices increases drastically from the numbers required in the internal temperature plots. They require longer burn in periods as well as longer recording periods in general for smoother graphs and a well defined peak.

2.5 Results: Identifying Phase Transition

From theory we expect a critical temperature of $T_c = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$. This is exactly what is seen in fig. 3 and fig. 4. In fig. 3 we note that the transition becomes sharper for larger N although this sharpness is most visible going from $N = 10$ to $N = 20$ and that that phase transition clearly happens at $T \approx 2.269$. That is also the temperature where we see the peak in the specific heat plots, which clearly indicates the specific-heat singularity associated with the phase transition. Although the amount of data here is sparser we can clearly see a slight sharpness increase going from lattice size $N = 10$ to $N = 20$.

3 Part B: Magnetization

For magnetization we would like to first fix temperature and then record magnetization as a function of h, the external magnetic field strength. Since we will use the same Metropolis algorithm we do not need to modify the scheme described in part A significantly. The changes to the algorithm are the following:

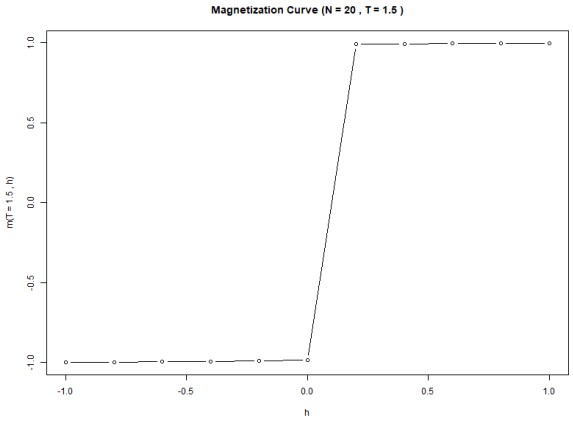
(I) The Hamiltonian has changed so that means that we must update how the local ΔH is computed after a flip is proposed.

(II) Temperature is not varying it is fixed. Instead vary h, I chose $h \in \{-1.0, -0.8, ..., 0.8, 1.0\}$.

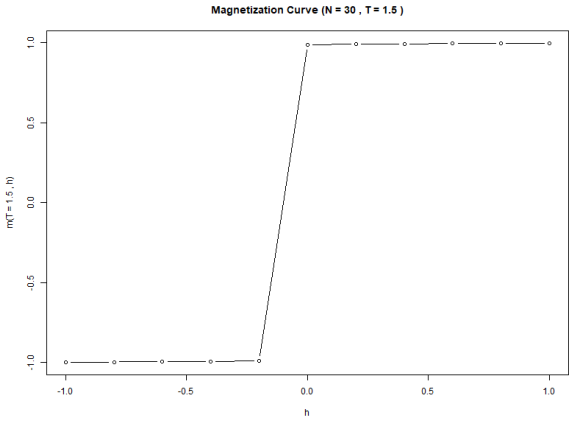
(III) All other steps remain the same, including: measuring in sweeps, run many burn in sweeps before beginning to record.

3.1 Results

Let $\overline{m}$ represent the estimate for magnetization that we found using MCMC. To obtain these results we update the Hamiltonian and estimate $m = \frac{\langle \sum_i \sigma_i \rangle}{N^2}$ by first running 300 burn in sweeps and then recording for 1200 sweeps for temperatures below, near, and above $T_c \approx 2.269$.



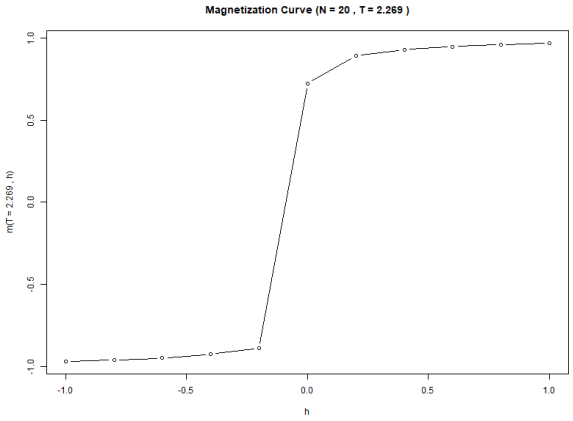
((a)) Lattice Size of 20



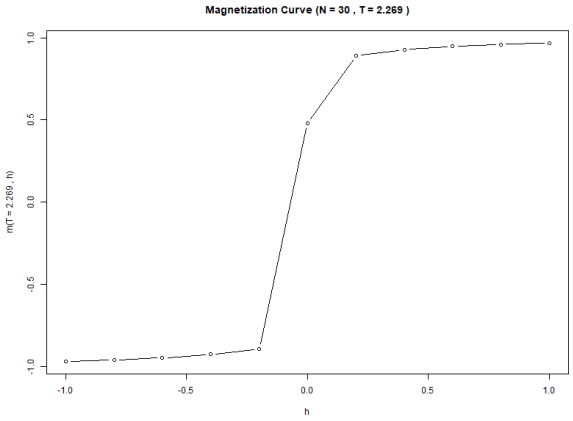
((b)) Lattice Size of 30

Figure 5: Plot of $\overline{m}$ against h for $1.5 = T < T_c$

For temperatures below the critical value we see near steady values at $\pm m$ for the magnetization with a sharp discontinuity at $h = 0$, when the external magnetic field is turned off.



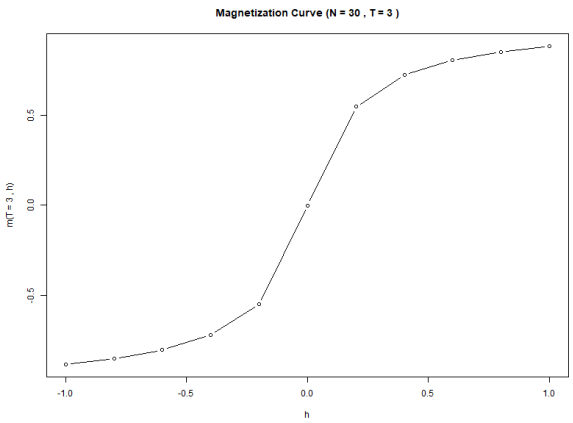
((a)) Lattice Size of 20



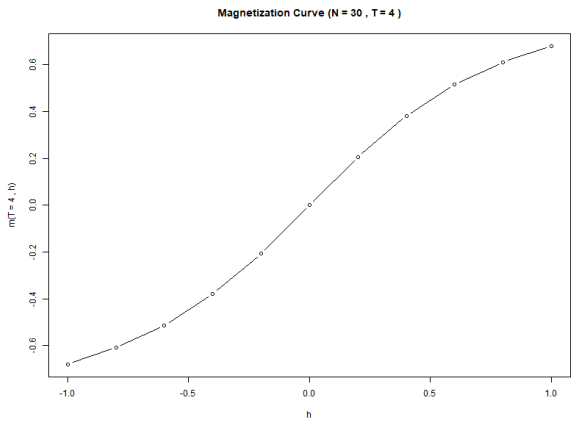
((b)) Lattice Size of 30

Figure 6: Plot of $\overline{m}$ against h for $2.269 = T \approx T_c$

For temperatures near T_c in this case $T = 2.269$ we still have a rapid change in magnetization is still evident but slightly more curved than the low temperature case.



((a)) Lattice Size of 30, $T = 3$



((b)) Lattice Size of 30, $T = 4$

Figure 7: Plot of $\overline{m}$ against h for $T > T_c$

For the higher temperature case we get some interesting behavior where we see the magnetization become roughly linear as T increases. This is exactly the behavior we expect to see in these plots. Below T_c neighboring interactions dominate thermal noise and therefore the system prefers $+m$ or $-m$ see fig. 5. At the critical temperature the system becomes sensitive to even tiny fields hence the slope goes to infinity at $h = 0$ fig. 6. Finally at $T > T_c$ thermal noise dominates and in the paramagnetic system magnetization becomes roughly proportional to h, fig. 7. The simulation certainly supports these ideas. It seems like these plots reveal the transition from an ordered ferromagnetic phase to a disordered paramagnetic phase as temperature increases past the critical temperature.

4 Conclusion

The 2D Ising model is a rich canvas to practice code, simulate fascinating physics, and explore a worthy application of the MCMC. There are many improvements that could be made to this project in terms of plot outputs, the main one of course is the smoothness of the graphs could be improved by increasing both the number of burn-in sweeps and the number of recording sweeps. This would likely get rid of artifacts like those seen in the $N = 30$ and $N = 40$ subplots in fig. 3 for low temperatures. Increasing the number of sweeps would also likely exaggerate the level of steepness in the internal energy graph as we expect the slope to tend to infinity at the critical temperature. Having the patience and the computational power to compute for larger N would also greatly increase the quality of these plots.

5 R Code Appendix

```r
## Metropolis Algorithm
  Metro <- function(A, Beta){
    ## Pick site
    i <- sample(seq(1, nrow(A)),1)
    j <- sample(seq(1, ncol(A)),1)

    ## Random number
    r <- runif(1,0,1)

    ## Propose flip
    Accept <- A
    Accept[i,j] <- -1*Accept[i,j]

    ## Periodic Condition
    nr <- nrow(A)
    nc <- ncol(A)
    ip1 <- if (i == nr) 1 else i + 1
    im1 <- if (i == 1) nr else i - 1
    jp1 <- if (j == nc) 1 else j + 1
    jm1 <- if (j == 1) nc else j - 1

    ## Local Energy Change
    H_pre <- -1* A[i,j] * (A[i, jp1] + A[i, jm1] + A[ip1, j] + A[im1, j])
    H_post <- -1 * Accept[i,j] * (Accept[i, jp1] + Accept[i, jm1] +
                                    Accept[ip1, j] + Accept[im1, j])
    Delta_H <- H_post - H_pre

    prob_accept <- exp(-1*Beta*Delta_H)
    ## Decision
    if(Delta_H <= 0){
      return(Accept)
    }
    else if (r <= prob_accept){
      return(Accept)
    }
    else{
      return(A)
    }
  }
```