A Study of the 2D Ising Model for 2 Lattices

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Background and Implementation

- Ignoring any external field, the Hamiltonian for a 2D Ising model for a state σ is

$$H(\sigma)/T = -\beta \sum_{<ij>} \sigma_i \sigma_j$$

where $< ij >$ represents the summation over nearest neighbors, σ_i is the spin configuration, which takes the value of $+1$ or -1, and a periodic boundary condition is applied for the lattice grid. If $\beta > 0$, the nearest neighbor coupling is ferromagnetic, where all spins are aligned in the limit $T \to 0$ (i.e., $\beta \to \infty$); conversely, if $\beta < 0$, all spins tend to be anti-aligned in the limit $T \to 0$, which corresponds to the antiferromagnetic state.

- The Monte Carlo method is implemented with the Metropolis algorithm, where a stream of spin configurations is created based on the previous one, and the ensemble of configurations is taken to be equal to the time average. The transition probability of any spin state on the lattice is

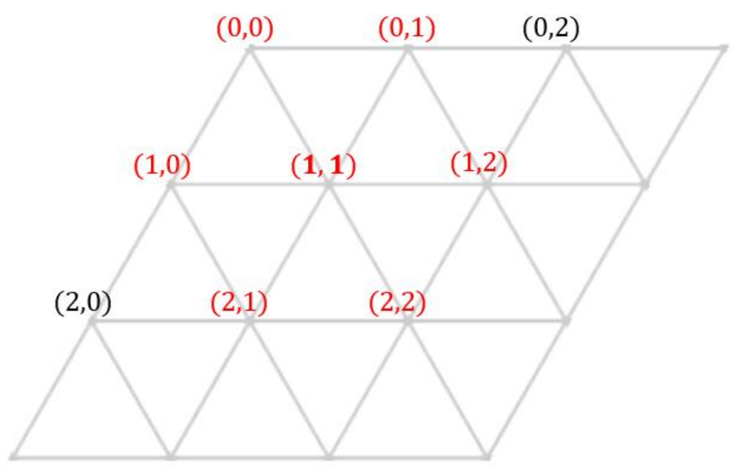
$$w(b \leftarrow a) = min(1, exp(E^a/T - E^b/T)).$$

In the Metropolis algorithm, $r = exp(E^a/T - E^b/T)$ is compared with a random number between 0 and 1. If r is greater than the random number, the spin is changed.

- For the ferromagnetic state, if we plot the average magnetization $m = \sum_i \sigma_i / N_s$ as a function of the simulation temperature, a transition from $m = 1$ to $m = 0$ can be observed as the temperature increases. The critical temperature where the transition happens is the phase transition temperature for the 2D Ising model. Further, the magnetic susceptibility $\chi = \sum_C (m - \bar{m})^2 / N_C$ and heat capacity $C_V = \sum_C (E - \bar{E})^2 / N_C$ are singular at the critical temperature for the second-order phase transition.

- For the antiferromagnetic state, $m = \sum_i \sigma_i / N_s$ is no longer a good measure for the magnetic state, since for both the random and antiferromagnetic spin configurations m takes the value of 0. Instead, $\text{afm} = \sum_{<ij>} \sigma_i \sigma_j / N$, where N accounts for the coordination number, used as a measure of how antiferromagnetic a system is.

2D triangular lattice

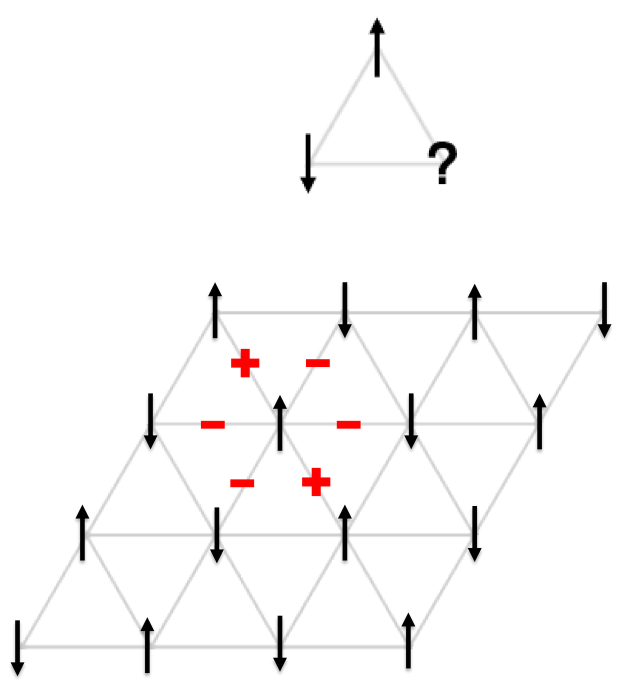


For the triangular lattice, each spin site has 6 nearest neighbors, as shown in red for the site $(1, 1)$. The simulation for the triangular lattice is the same as in the square case, except for the addition of two more nearest neighbors.

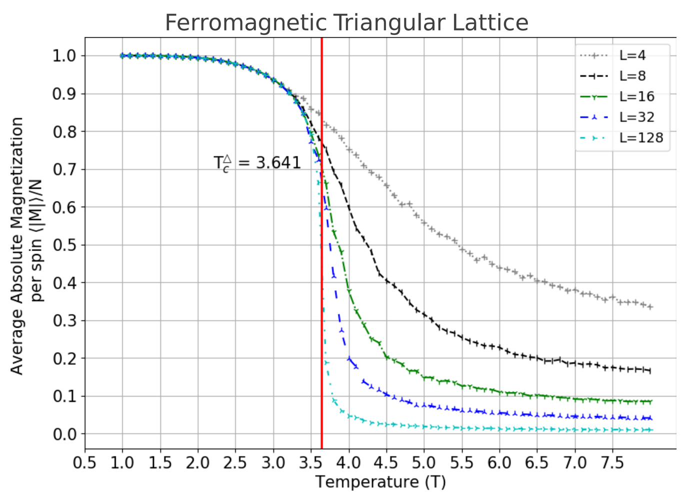
Ferromagnetic

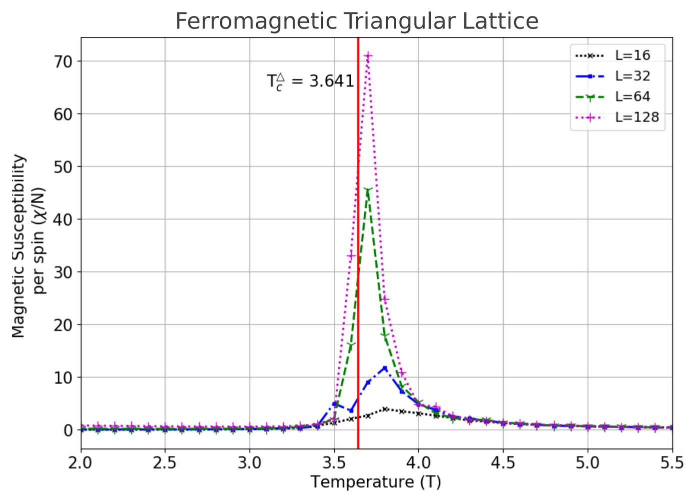
For the ferromagnetic state of the triangular lattice, the simulated transition happens at around $\beta = 0.28$ $(T \approx 3.6)$, which corresponds to a higher transition temperature than in the square lattice case. Physically, this means that for a system with more nearest neighbors, the stronger inter-site coupling makes the ferromagnetic state more stable, even at higher temperature.

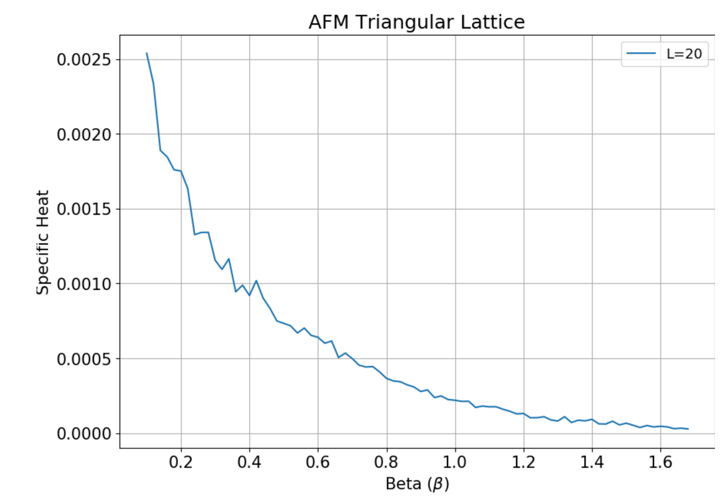
Anti-ferromagnetic

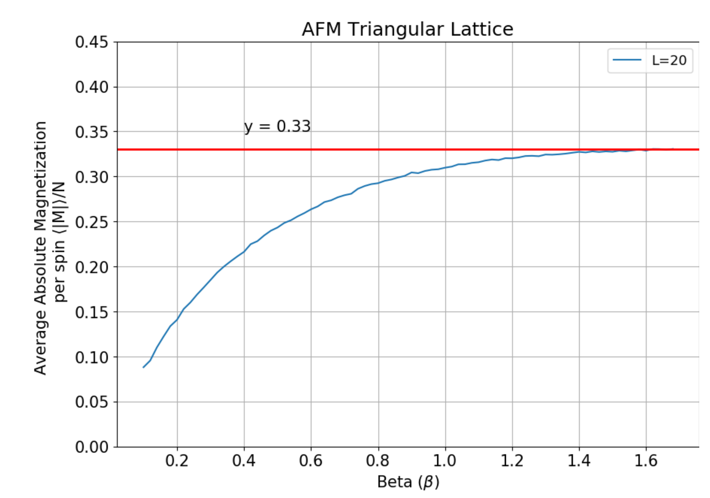


For the antiferromagnetic state, there is the famous magnetic frustration problem, as shown on the left. However, there is a similar spin configuration as for the square lattice, where the nearest neighbors are the most anti-aligned. By our measure for the AFM state, out of the six nearest neighbors, in net there are two anti-aligned neighbors. The largest level of antiferromagnetism is $\text{afm} = 2/6 \approx 0.33$. Indeed, this is the case from our simulation. Also, notice that the temperature required to reach this order is higher than in the ferromagnetic case.





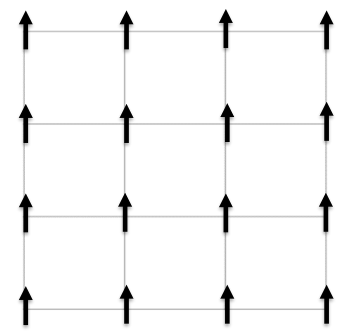




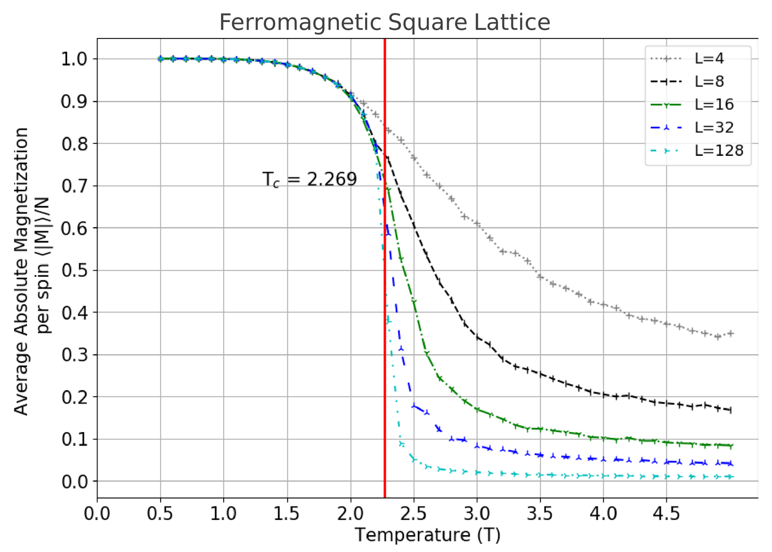
2D square lattice

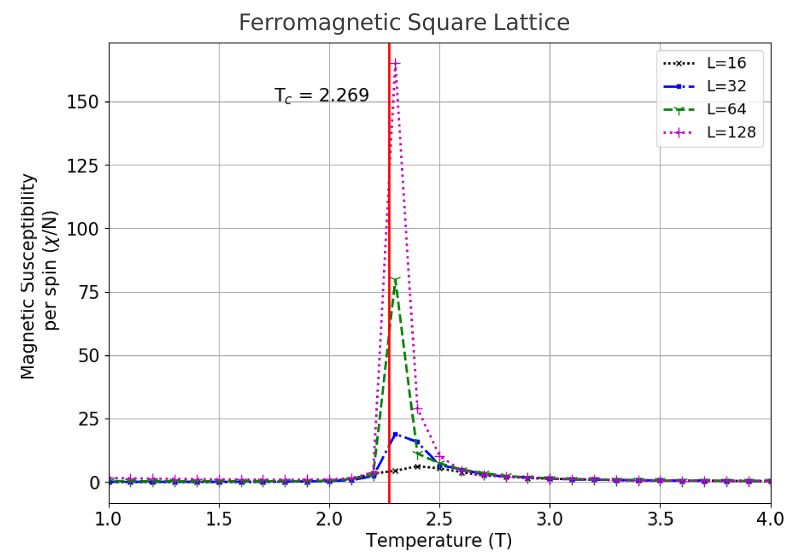
Ferromagnetic

The analytical critical temperature for the 2D square lattice Ising model is $\beta = 1/k_B T = \ln(1+\sqrt{2})/2 \approx 0.44$ (T $\approx$ 2.27). From the simulated average magnetization and susceptibility plot, a similar value of critical β is observed.



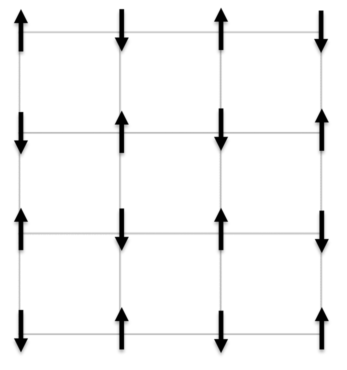
Ferromagnetic square lattice



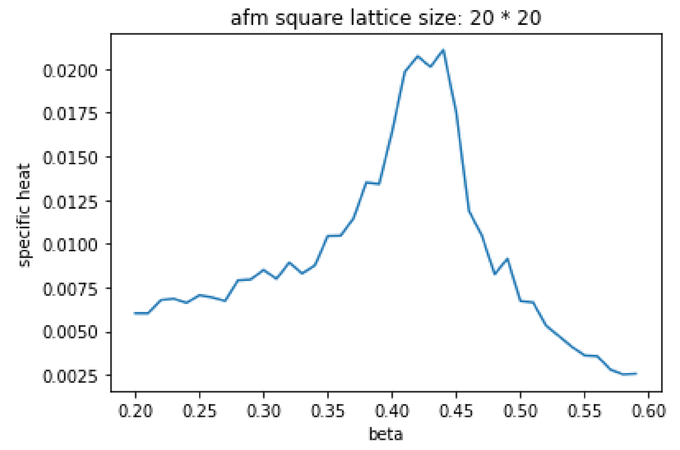


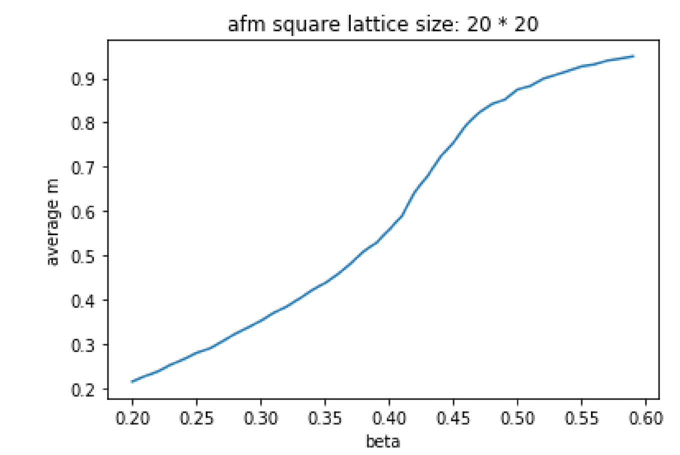
Anti-ferromagnetic

Since the square lattice is bi-partite, the anti-ferromagnetic 2D square lattice has the same transition temperature as in the ferromagnetic case.



Anti-ferromagnetic square lattice





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References

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2. Numerical Ising Model Simulations on Exactly Solvable and Randomized Lattices, Stephen L. Eltinge, 2015.