An Investigation of the Use of Various Lattice Shapes in the 2D Ising Model

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Abstract

In this investigation, the 2D Ising model was constructed using three different lattice shapes, the square, the triangle, and the hexagon (honeycomb). Properties of these Ising models were then investigated as they reached equilibrium using a Monte-Carlo Metropolis algorithm. It was also attempted to utilise a convolutional neural network to predict the ground state given the initial state, but this was dropped due to technical issues with 4D input tensors.

The Ising Model

The Ising model is a very useful model in the fields of solid state physics and computer science alike. The model consists of some array of units, each of which has a binary state. In the realm of solid state physics, this can be interpreted as a lattice with a binary state of electron spins, either ± 1. For two adjacent atoms, i.e. nearest neighbours, their energy is lower if their spins are aligned. Additionally, an external magnetic field can be applied, such that an electron's energy is lower if it is aligned with the magnetic field. The Hamiltonian is therefore defined as

$$H = -J \sum_{<ij>} S_i \cdot S_j - h \sum_i S_i$$

where

$$< ij > = \text{nearest neighbours}, S_i = \text{ spin of electron } i,\ J = \text{interaction value},\ h = \text{magnetic field value}$$

In the choosing of nearest neighbours, periodic boundary conditions are applied for electrons on the extremity of the lattice.

Generally, the application of an external magnetic field makes the model behave more predictably and less interestingly; thus, for this investigation, the value of h was set to zero. Non-collinear values of the spin can also be chosen.

System Evolution and the Metropolis Algorithm

To investigate how the system evolves with time, we can assign a probability that the spin of one electron will flip, depending on the change in the system energy. From statistical mechanics[1], the probability of a state k is given by

$$P_k = \exp \frac{-\beta E_k}{Z}$$

where

$$\beta = \frac{1}{K_B, T},\ K_B = \text{Boltzmann's constant},\ T = \text{temperature, and}$$

$$Z = \sum_N \exp\left(-\beta E_N\right) \text{ (the sum over all possible states)}$$

For the model, a lower energy is desirable, so if flipping an electron's spin results in an overall decrease in energy, the electron will flip. However, if this is not the case, it is still possible for an electron to flip. From Bayes' theorem, it can be derived that the probability of an electron flipping is given by

$$P_{\text{flip}} = \exp\left(-\beta \delta E\right)$$

Thus, if $\delta E \leq 0$, the electron flips, but if $\delta E > 0$, it flips with probability P_{flip}.

To evolve the system with time, we simply choose a random electron, and see if it will flip. This is repeated thousands of times until the system reaches a stable equilibrium, and is known as the Monte Carlo Metropolis algorithm.

The Square Lattice

The Ising model is known for undergoing a famous phase transition upon reaching a critical temperature T_C. In 1944, Lars Onsager derived an analytical solution for the square lattice with the magnetic field value h equal to zero. For an infinite square lattice the transition temperature was derived[2] to be ≈ 2.27, with units of J/K_B. These units will be used in this investigation for simplicity. This phase transition can be interpreted as the transition from paramagnetism to diamagnetism in the case of a ferrous material.

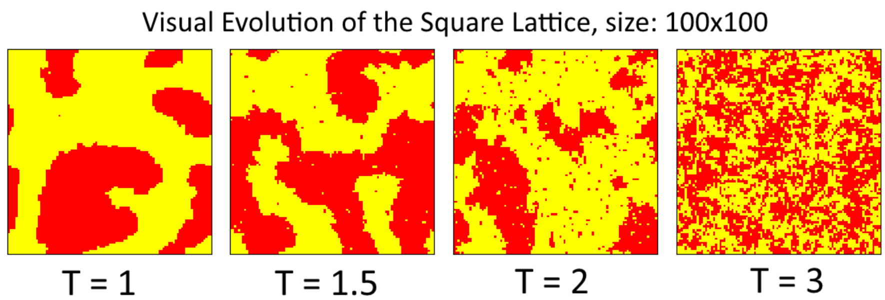

Fig. 1: Evolution of a 100x100 square lattice over 1 million iterations. The phase transition is seen occurring at a temperature of approx. 2 to 3. This happens due to the probability of an energy-increasing electron flip increases, and results in the system never reaching a stable equilibrium.

Evolution of Properties

In this model, four important properties were investigated: the total energy given by the Hamiltonian, the excess magnetic spin given by the sum over all spins, the specific heat capacity, and the susceptibility. The calculation of the latter two are not discussed here but are available in literature. The values of the specific heat capacity and susceptibility should spike noticeably at the location of the phase transition temperature T_C.

Property Evolution

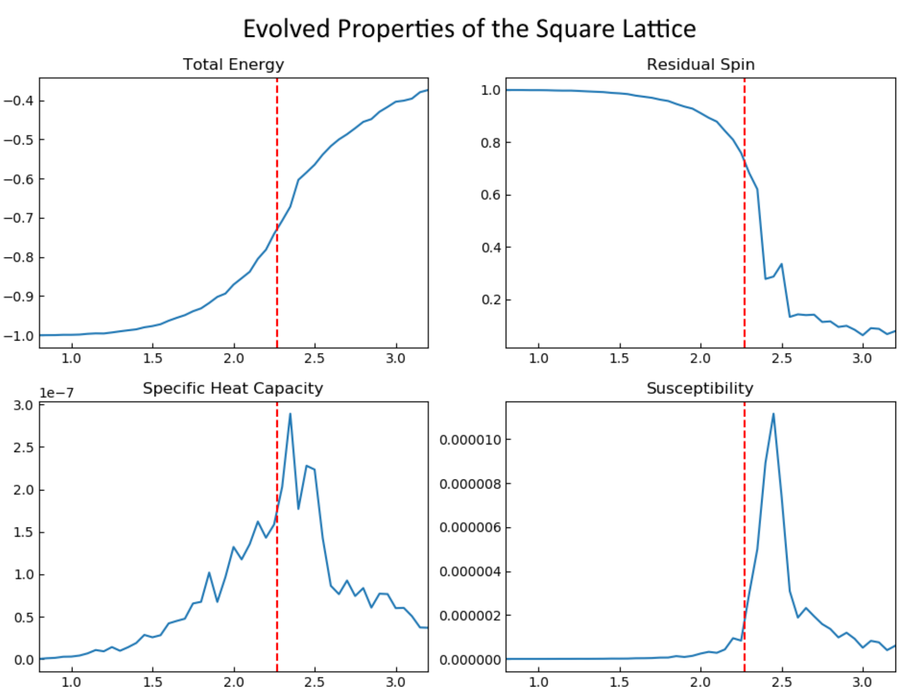

Fig. 2: Evolution of the square lattice. As the temperature increases and the lattice becomes more disordered, the total energy approaches zero, as does the residual spin. The red line gives the location of the theoretical T_C, and corresponds closely to the spikes in the specific heat capacity and susceptibility. Because a lattice of only 30x30 was used, the spikes are shifted slightly to the right.

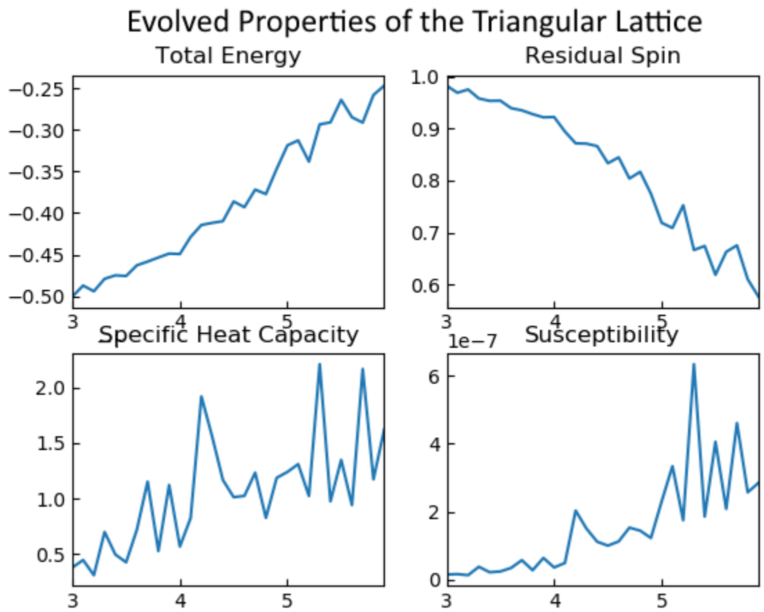

Fig. 3: Evolution of the triangular lattice. There is no analytical solution for the critical temperature for this lattice. Although the data is noisy due to a more complicated lattice, the specific heat capacity and susceptibility spikes are seen to be at $T \approx 5.3$.

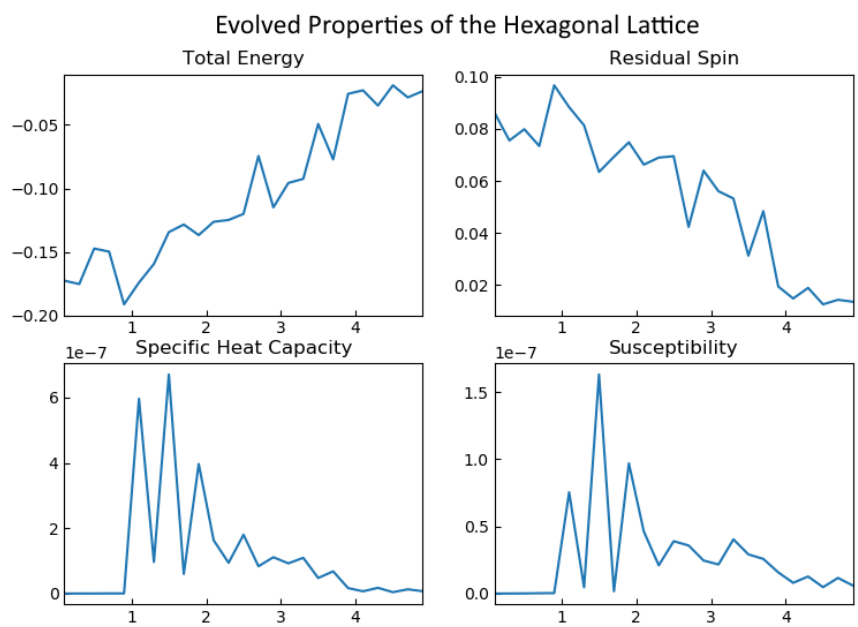

Fig. 4: Evolution of the hexagonal lattice. Again, there is no analytical solution for the critical temperature for this lattice. The specific heat capacity and susceptibility spikes are seen to be at $T \approx 1.5$.

Conclusion

The Ising model is a versatile and fascinating model which has applications reaching far beyond its apparent simplicity. Besides its use to make predictions in solid state physics, the model also has surprising connections to the field of machine learning, being the inspiration for Hopfield networks[3], a form of recurrent neural network that can be used for error correction (content-addressable memory). It also related to Boltzmann machines[4], which are used widely in deep learning.

Although these applications are perhaps more interesting than the evolution of the lattice properties depending upon temperature, this investigation could be extended by constructing the Ising model with various other shapes, as they need not be Bravais lattices. Theoretical derivations of T_C for other lattice shapes may also involve the development of useful methods in other fields.

[1]: McQuarrie, A. (2000) Statistical Mechanics, University Science Books, California
[2]: Baxter, Rodney J. (1982), Exactly solved models in statistical mechanics (PDF), London: Academic Press Inc. [Harcourt Brace Jovanovich Publishers], ISBN 978-0-12-083180-7, MR 0690578
[3]: `http://ecee.colorado.edu/~ecen4831/hoplecs/hoplec1.html`
[4]: `https://www.cs.toronto.edu/~hinton/csc321/readings/boltz321.pdf`