Determining the Critical Temperature in a Two-Thirds Filled Blume-Capel Model on a Triangular Lattice

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To better understand the onset of charge ordering in high-temperature superconductors, we perform Monte Carlo simulations using the Blume-Capel model on a 2D triangular lattice. By working in the canonical and grand canonical ensemble, we identify transitions in both charge and spin ordering on the lattice. To aid in this process we introduce several new measurements focused on identifying loops of spin or charge. We also make modifications to the Binder cumulant to make it applicable to the model.

I. Introduction

Superconductivity was first demonstrated experimentally in 1911 by Kamerlingh Onnes who, using liquid helium, reduced the temperature of mercury to 4.2 K and noticed a sudden drop in resistance[1]. However, it wasn't until 1957 that Bardeen, Cooper, and Schrieffer developed a microscopic theory capable of explaining the phenomenon[2]. Although this theory sufficed to explain low-temperature "conventional" superconductors, the emergence of new high-temperature superconductors required new mechanisms[3, 4].

It was discovered in 1986 that $La_{2-x}(Ba,Sr)_xCuO$ had a critical temperature of $T_c \approx 30$ K[5]. This result has spawned a new class of superconductors known as cuprate superconductors which, while superconducting at high temperatures, also have a unique phase diagram. This diagram is shown in Fig. 1. We see that depending on the doping, there are different phases in the material ranging from anti-ferromagnetism to strange metal to superconductivity. So, the question may be raised as to whether some of these unique phases are related to its high-temperature superconducting properties. In this paper, we will address the question of charge ordering and use a classical model to demonstrate how doping can play a role in the creation of charge ordering. In the process, we determine which measurements are suitable for identifying the critical temperature at which charge and spin ordering occur.

II. Order by Disorder

In most scenarios we are accustomed to, increasing the temperature leads to more disorder. But what if, the system was naturally disordered at low temperatures? Now, to understand how that is possible, let us introduce the concept of free energy $F = E - TS$. This expression tells us that the free energy at some absolute temperature T is equal to the difference between the total internal energy of the system and and product of the entropy and absolute temperature T. Now, at a given temperature T, what state will we find the system in? We know that for the system to be in equilibrium this function must be minimized. Thus, by considering how the free energy can be minimized we can understand how the system will behave at a given temperature.

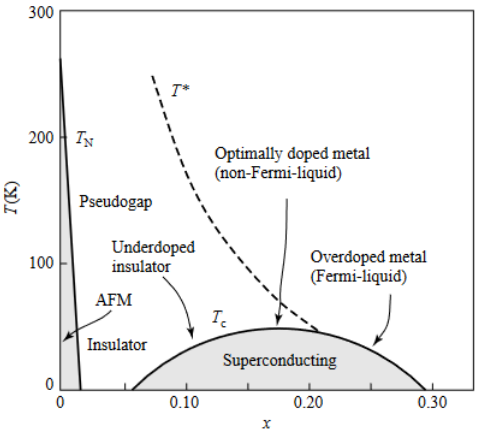

Figure 1: Figure from *Superconductivity: Physics and Applications* by Kristian Fossheim and Alse Sudbø. "Typical overall phase diagram with doping in high-Tc cuprate superconductors (AFM = antiferromagnetic phase)." To the left of the dotted line is a 'strange' metal phase.

From the preceding discussion, we know that the system wants to minimize free energy which at low temperatures just amounts to reducing the internal energy as much as possible, and at high temperatures, to increasing the entropy as much as possible. Thus, if a system has a high number of lowest energy states, at low temperatures, the system can cycle between many low energy states and will be disordered due to the high frequency of fluctuations. It then seems plausible that by increasing the temperature, with less necessity to lower the energy, the system can find a more stable state.

In this paper, we consider a scenario where instead of introducing thermal fluctuations to initiate order by

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disorder we instead allow for fluctuations in the number of particles in the system. This effect can be seen as introducing a new degree of freedom to better model systems in which doping allows for holes. We hope that through the introduction of this degree of freedom, we will see collective behavior even though we are using a classical rather than a quantum model.

III. Frustration in the Triangular Lattice

The goal of this paper is to study the triangular lattice. The main motivation for this approach is the existence of frustration in this geometry. As mentioned before, the most likely set of configurations that we will find the system in at low temperatures is the set of configurations with the least amount of energy. So, our goal is to determine which set of configurations minimize the energy in the triangular lattice to determine if it is a candidate for the mechanism of order by disorder.

First, to determine the energy of the system, we need to start by making some assumptions. In this paper, we will assume that the material can be represented as a lattice of particles that can exist in two states either spin up or spin down. Then, we will assume that the interactions between the spins only occur with spins that are nearest neighbors. Thus, we can determine the total energy of the system by looking at each pair of nearest neighbors and determining the energy associated with each pair. So, in the absence of an external magnetic field, we find that the energy is given by:

$$E = J \sum_{\langle ij \rangle} s_i s_j$$

where J is the energy associated with the interactions between the spins. This equation defines the energy for what is known as the Ising model and can demonstrate a transition between ferromagnetism and paramagnetism. Considering the situations that give the lowest energy, we see that a negative J requires spins to be aligned with their neighbors and a positive J requires spins to be anti-aligned with their neighbors at low temperatures.

In a square lattice, there are only two lowest energy states regardless of the sign of J either all spins being up or all spins being down if J is negative or one of the two alternating patterns of spins if J is positive as shown in Figure 2. Thus we expect the system to be incredibly stable at low temperatures.

Now, as the point of the Ising model is to represent magnetism, let us consider what physical states these configurations correspond to. When the spins are aligned in the lowest energy state, we are representing a ferromagnet as the alignment of the spins creates a net magnetic moment. In the case where neighboring spins are anti-aligned in the lowest energy state, we are representing an anti-ferromagnet as the spins are aligning

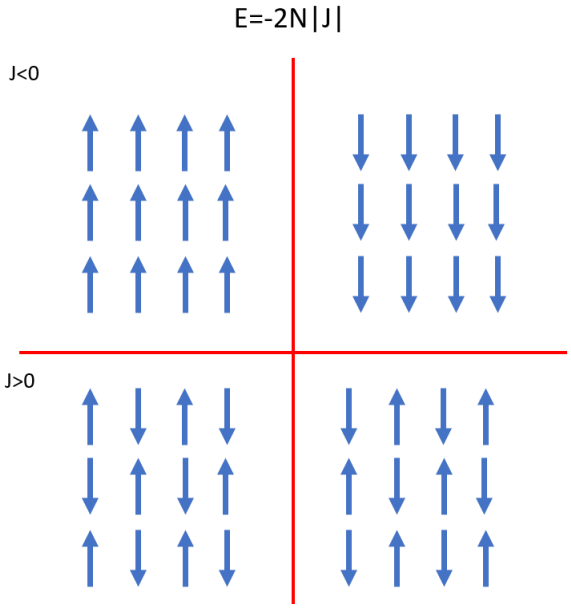


Figure 2: Lowest energy states for the Ising model on a square lattice

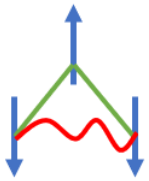


Figure 3: In the anti-ferromagnetic phase, we can't arrange the spins in such a way to eliminate frustration in the triangular lattice.

themselves to ensure the net magnetic moment is zero. In this case, the limited number of lowest energy states leads to order at low temperatures and disorder at high temperatures. However, different geometries will have different lowest energy configurations. So, to explore order by disorder, we likely want to use a geometry in which the number of lowest energy states is large to allow for disorder at low temperatures.

To accomplish this, let us consider the triangular lattice. In this case, if J is positive, all spins can't be anti-aligned with their neighbors (see Fig. 3). This property is known as frustration and leads to there being no stable configuration of spins in the triangular lattice.

Unfortunately, without a stable configuration, the system cannot undergo long-range spin or charge order. To get around this, we allow for the existence of holes in the lattice leading to the possibility of the system finding a stable state when 2/3 of the sites are filled as seen in Fig. 4.

Our goal is to study this system using two different

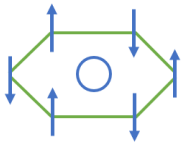


Figure 4: By allowing for vacancies, a stable configuration exists on the triangular lattice in the anti-ferromagnetic case

approaches which we will call the canonical and grand canonical ensembles. We want to see how the filling fraction and temperature affect the onset of both spin and charge order in the material. To clarify, when we refer to spin order we are referring to the alternating pattern of up and down spins whereas charge order just refers to the existence of a honeycomb pattern (or some other stable structure) regardless of the pattern of spins.

IV. Research Question

The goal of our research is to make use of the degrees of freedom granted to us by geometric frustration while also introducing a new degree of freedom. As the Ising model on a triangular lattice has already been studied and shown to have no phase transition in the anti-ferromagnetic case[6], we consider the situation where rather than every site of the lattice being occupied by a particle we can now have vacancies. Thus our possible spin values of $\pm 1, 0$. In studying this system we took two separate approaches, in one approach we allowed fluctuations in the number of spins on the lattice (Grand Canonical Ensemble), and in the other, we fixed the number of spins and only allowed them to swap places or fill holes (Canonical Ensemble). In studying this system we aim to better understand the onset of charge and magnetic ordering on a frustrated lattice to improve our understanding of quantum systems that display these features.

V. Methods

A. Defining Thermodynamic Quantities

Our main goal is to determine the partition function $Z = \sum_s e^{-\beta E_s}$ from this we can calculate all the thermodynamic properties we need. For example:

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z$$

$$C = \frac{\partial \langle E \rangle}{\partial T}$$

$$\langle M \rangle = \frac{\partial}{\partial H} kT \ln Z$$

$$\chi = \frac{\partial \langle M \rangle}{\partial H}$$

where $\langle E \rangle$ is the average energy at a given temperature, C is the heat capacity, $\langle M \rangle$ is the average magnetization and χ is the magnetic susceptibility. Thus our goal is to obtain the partition function Z. So, how should we go about doing this? For a system with a small number of energy levels, we can simply calculate it directly. However, as the number of energy states gets larger this process becomes untenable and we need a new method to obtain these quantities. As an illustrative example, consider the two-dimensional Ising model on a square lattice. In this case, when we have a lattice of N spins, we must pick each spin to either be up or down. Thus, we will have 2^N different configurations of the system and will have 2^N different terms in our calculation of the partition function. So, if we want to study large systems, we will need to find a different way to calculate this quantity. The answer comes in the form of Monte Carlo.

B. Monte Carlo

Before we dive into the how let us answer the what. What is Monte Carlo? In general, a Monte Carlo simulation approximates the answer to some problem by randomly sampling points. For example, you can estimate the area of a circle by randomly throwing darts in a square that contains the circle and comparing the proportion of darts that landed inside the circle to the area of the square. In our work however, we are trying to estimate the thermodynamic quantities by sampling states according to the Boltzmann distribution $p_s = \frac{e^{-\beta E_s}}{Z}$. In the case of the Ising model, the main quantity of interest is the magnetization along with any other quantities that can signal a phase transition such as the specific heat. However, these quantities require us to calculate the partition function which requires a very large sum. So, instead, we create an algorithm that will produce the correct probability distribution without needing to calculate the partition function. This is done by using a Monte Carlo algorithm that goes through the lattice and flips a spin with an acceptance probability that satisfies the detailed balance equation. We do this by using the Metropolis-Hastings rate given by $e^{-\beta \Delta E}$ where ΔE represents the difference in energy between the state we are attempting to change to and the state that we are in[7, 8].

C. Blume-Capel Model

To study charge and spin order on the triangular lattice, we use the Blume-Capel Model. The Blume-Capel model is a variation of the Ising model that allows for vacancies. To control the vacancies, we add a new term

Δ, the chemical potential, to the total energy of the system:

$$E = J \sum_{\langle i,j \rangle} s_i s_j - \Delta \sum_i s_i^2 \tag{1}$$

In this paper, we will be considering the $J > 0$ case. Thus, our goal is to determine the temperature at which the system experiences a transition in both spin and charge order (each occupied site represents a charge) at certain values of Δ or to vary Δ so that the average density is constant and obtain a critical temperature for a particular filling fraction.

1. *Canonical Ensemble*

The first approach we tried was to keep the number of spins in the lattice constant. We began by setting $n_\uparrow = n_\downarrow = N/3$ where N is the number of lattice sites. In this scenario, each proposed change in the Monte Carlo code is a proposed swap between neighboring sites rather than a proposed spin flip. Thus, it will take the system quite some time to reach equilibrium as the particles have to move to their proper location. However, this approach did have the advantage of being able to control the total number of spins without having to determine the proper value of Δ to get a particular average density at a particular temperature.

2. *Grand Canonical Ensemble*

The other approach used was the Grand Canonical Ensemble. Although we obtained many preliminary results through the Canonical Ensemble, once we started working in the Grand Canonical Ensemble, we tended to use it to produce the rest of our results. This is because by varying the value of Δ we can realize a much richer phase diagram. Also, since we change the system through spin flips the system can reach equilibrium much quicker. Additionally, if necessary, we can tune the value of Δ to obtain constant average filling. However, in practice we were only successful in obtaining constant average filling for 2/3 filling as the dependence on Δ is incredibly sensitive as seen in Fig. 5.

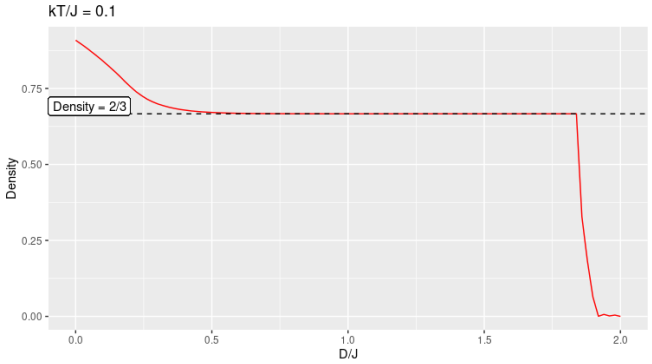


Figure 5: At $kT/J = 0.1$ the density as a function of D (Δ) is very stable for 2/3 filling but is unstable if we go below 2/3 filling.

VI. Results

A. Quantities of Interest

Our work is a variation on the Ising model. The difference between the Blume-Capel and Ising models is the ability for sites to be unoccupied and a new term in the energy (a chemical potential) that relates to the number of occupied sites.

As our work builds off the traditional Ising model, let us look to the Ising model to determine what measurements to make. Important measurements in the Ising model include the Binder cumulant which is defined as $1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}$ where the M refers to the magnetization $M = \sum_i s_i$ in the ferromagnetic case and the staggered magnetization $M_{AF} = \sum_i (-1)^i s_i$ in the anti-ferromagnetic case. Thus, in the low-temperature limit, the absolute magnetization $|M|$ will just be the number of spins as all spins will point in the same direction in the ferromagnetic case or they will be anti-aligned so the absolute value of the alternating sum will give the number of spins. Thus the Binder cumulant will be $1 - N^4/3(N^2)^2 = 1 - 1/3 = 2/3$. In the high-temperature limit, the spins are random. In this case, we see that the fourth moment of the magnetization $\langle M^4 \rangle = \langle \sum_i s_i \sum_j s_j \sum_k s_k \sum_l s_l \rangle$ where all the sums are independent. Because the spins are random, the expectation value will vanish unless we have two pairs of matching indices i.e. $i = j, k = l$ or $i = k, j = l$, or $i = l, j = k$ thus the expectation value of the numerator is $3N^2$ as there are three ways to pair the indices and N values associated with each pair of matching indices. The denominator in the high-temperature limit will be $3\langle M^2 \rangle^2 = 3\langle \sum_i s_i \sum_j s_j \rangle^2$ where again, the expectation value will vanish unless the indices match which will happen N times making the denominator $3N^2$. Thus, in the high-temperature limit, the Binder cumulant becomes $1 - \frac{3N^2}{3N^2} = 0$. This is the case no matter the lattice size. However, at the critical temperature, the value of the Binder cumulant will be the same regardless of the lattice size. This means that the critical temperature can be determined by noticing where the Binder cumulants of different lattice sizes cross.

Another quantity of interest is the magnetic susceptibility. The magnetic susceptibility χ is the response of the magnetization to a change in the applied magnetic field $\chi = \frac{dM}{dB}$. In the Ising model, the energy in the pres-

ence of an external magnetic field is given by:

$$E = J\sum_{\langle i,j\rangle} s_i s_j - B\sum_i s_i \tag{2}$$

where the probability of the system being in a given configuration s is given by the Boltzmann distribution

$$p_s = \frac{e^{-\beta E_s}}{\sum_s e^{-\beta E_s}}$$

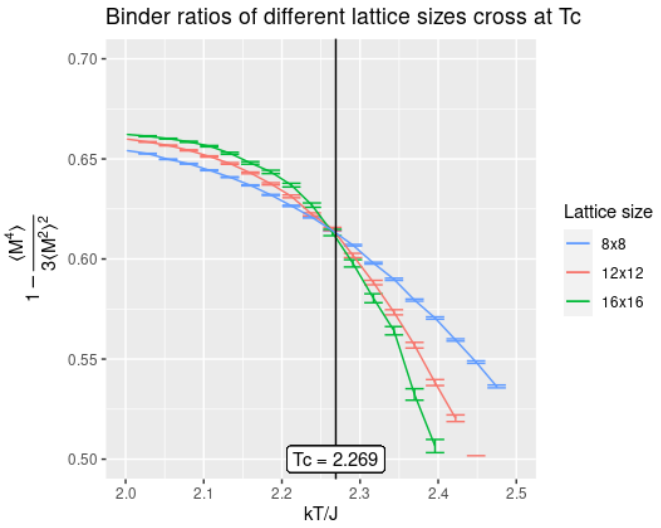
so the average magnetic susceptibility χ is given by:

$$\begin{aligned}\frac{d\langle M\rangle}{dB} &= \frac{d}{dB}\sum_s M_s p_s \\ &= \frac{d}{dB}\frac{\sum_s M_s e^{-\beta(J\sum_{\langle i,j\rangle} s_i s_j - BM_s)}}{\sum_s e^{-\beta(J\sum_{\langle i,j\rangle} s_i s_j - BM_s)}} \\ &= \beta\left[\frac{\sum_s M_s^2 e^{-\beta E_s}}{\sum_s e^{-\beta E_s}} - \left(\frac{\sum_s M_s e^{-\beta E_S}}{\sum_s e^{-\beta E_s}}\right)^2\right] \\ &= \beta\left(\langle M^2\rangle - \langle M\rangle^2\right)\end{aligned}$$

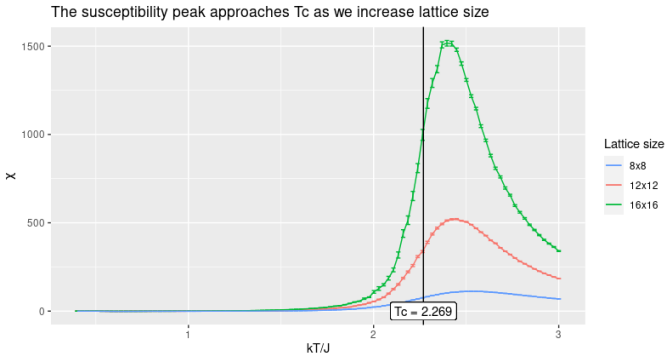
This quantity will diverge at the critical temperature as the magnetization will suddenly change at the critical temperature.

Finally, we consider the specific heat which is given by $C = \frac{d\langle E\rangle}{dT}$ which similarly to the susceptibility can be shown to be equal to $\frac{1}{kT^2}\left(\langle E^2\rangle - \langle E\rangle^2\right)$. This quantity will also diverge at the critical temperature as it takes a lot of energy to change the temperature of a system while it is undergoing a phase transition. This can be seen by examining the results of simulations performed on the Ising model on a square lattice as seen in Fig. 6.

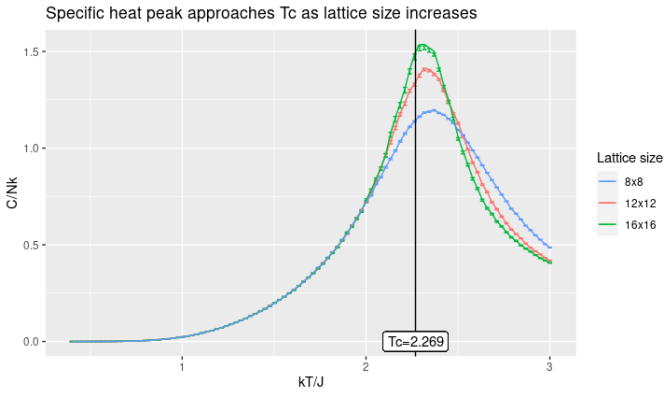
However, since we want to determine where spin and charge order appear, we will also introduce new measurements. Before getting into these measurements, however, it makes sense to redefine our lattice in terms of sublattices. If we are at 2/3 filling, we expect to obtain a honeycomb structure with alternating spins along the perimeter of the honeycomb. So, let us define the set of all nodes containing an up spin to be one sublattice, the set of all nodes containing a down spin to be another, and the set of all empty sites to be the final sublattice (see Fig. 7). Now, we will define the measurements in terms of these sublattices. We introduce two new measurements to help us see changes in both spin and charge order. For both of these measurements, we will consider a small loop on the lattice that is the perimeter of the honeycomb structure we expect to see. One measurement involves taking the product around this loop while the other involves taking the sum of the square of the elements of the loop (see Fig. 8). The first measurement will return the value of -1 if the loop only contains elements of the two sublattices that contain spins. This is because we are taking a product over six spins with half up and half down. This measurement is sensitive



(a) Binder cumulant in the Ising model on a square lattice. The crossing of Binder cumulants of different lattice sizes indicates a phase transition.



(b) Susceptibility in the Ising model on a square lattice. The peak in the susceptibility indicates a phase transition.



(c) Specific heat in the Ising model on a square lattice. The peak indicates a phase transition.

Figure 6

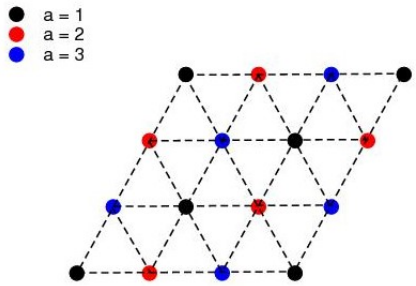
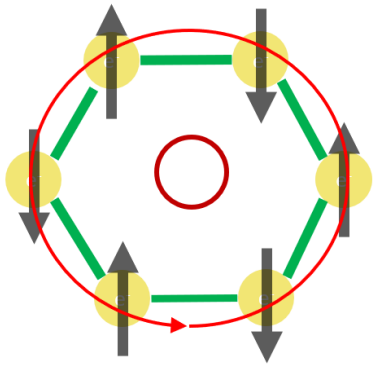


Figure 7: The three different sublattices on a triangular lattice. Each sublattice a is given an index $a = 1, 2, 3$ and is represented by a different color. In a perfectly ordered phase, one sublattice will only contain up spins, one sublattice will only contain down spins and the other will be empty.



Loop operator:

$$Z_C = \prod_{i \in S \subseteq A \cup B} s_i$$

Proportion of neighbors occupied:

$$\text{If } s_i = 0 \rightarrow \sum_{neighbors} \left(s_{neighbor}\right)^2$$

Figure 8: Diagram showing the new measurements involving loops that we are using to detect spin and charge order. The loop operator takes the product of spins in a loop and the proportion of neighbors occupied counts the number of occupied neighbors surrounding an empty site.

to a change in spin order as a single spin flip will cause the value to drastically change. The second measurement, involving the sum of the squares of the elements of this loop, will only tell us about charge order as both up and down spins will return the same value.

B. Simulation Results

Now that we know what we want to measure, let us see how the system behaves. Our first step was to confirm the simulation worked by comparing our results to

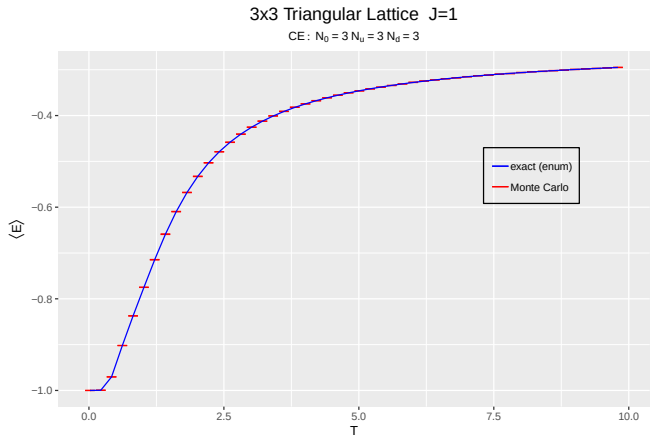


Figure 9: Comparison of Monte Carlo results (red bars) with exact enumeration (blue line) for a 3×3 lattice in the canonical ensemble with $N_\uparrow = N_\downarrow = N_0 = 3$. The high temperature limit is $\langle E(T = \infty) \rangle = -1/4$. See Eq. 3.

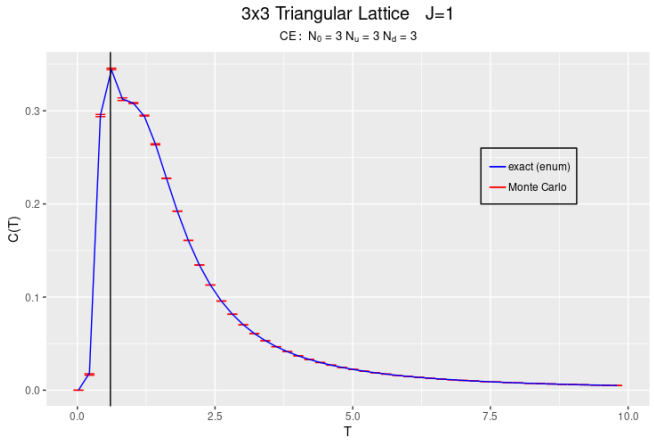


Figure 10: Comparison of Monte Carlo results (red bars) with exact enumeration (blue line) for a 3×3 lattice in the grand canonical ensemble with $D/J = 2$.

results obtained via exact enumeration over all of the states (see Figs. 9 and 10).

We see that our code does agree with enumeration and thus are confident enough to go forward and try larger lattice sizes. Also, it should be noted that in the canonical ensemble, the energy of the system does not vanish at high temperatures. This is due to our restriction on the amount of spins of a certain type. To make this clearer, at high temperatures we expect the system to want to maximize entropy so all states should be equally likely thus, we would expect there to be an equal likelihood of the neighboring spin to be up, down, or empty meaning on average the product of a spin with its neighboring spin should be zero. Thus, when we sum over all nearest-neighbor pairs of spins, we should get zero on average and the energy should vanish at high tempera-

tures. However, this is not what happens in the canonical ensemble. The reason for this is that by limiting the number of spins, we are not equally likely to have each type of spin as a neighbor. To see this, without loss of generality, consider sitting at a site with an up spin, then there are $N/3$ down spins, $N/3$ empty sites, and $N/3-1$ up spins left to choose a neighbor from, thus the likelihood of having a neighbor with a down spin is $\frac{N/3}{N-1}$, the likelihood for a neighbor being empty is $\frac{N/3}{N-1}$ and the likelihood of the neighbor being an up spin is $\frac{N/3-1}{N-1}$ assuming we have no bias towards a particular spin type. Thus, if we consider the energy per particle we get:

$$\begin{aligned}\lim_{T\to\infty}\left\langle\frac{E(T)}{N}\right\rangle &= \frac{1}{N}\frac{zJ}{2}\left(\frac{N}{3}\left((1)(1)\frac{N/3-1}{N-1}+(1)(-1)\frac{N/3}{N-1}\right.\right.\\ &\qquad\left.\left.+(-1)(1)\frac{N/3}{N-1}+(-1)(-1)\frac{N/3-1}{N-1}\right)\right)\\ &= \frac{zJ}{6}\left(\frac{-2}{N-1}\right)\\ &= \frac{zJ}{3(N-1)}\\ &= \frac{2J}{N-1} \quad \text{For a triangular lattice} \qquad (3)\end{aligned}$$

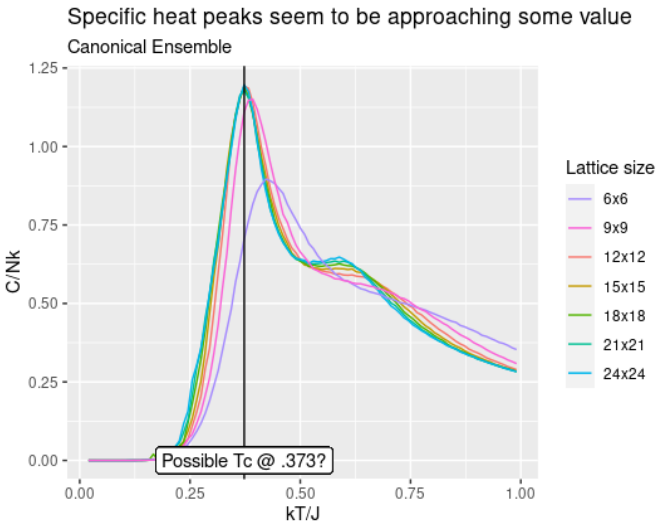
Thus, we see that the energy will vanish at high temperatures in the thermodynamic limit ($N\to\infty$) but only converge to that result at a slow $1/N$ rate.

Now that we have a working code, we want to compare our results from both the canonical and grand canonical ensembles. First, let us consider the constant Δ case. In this case, the density can change in the grand canonical ensemble so we don't expect it to agree with the canonical ensemble. However, let us see what results we get in both cases. The results are given in Fig. 11.

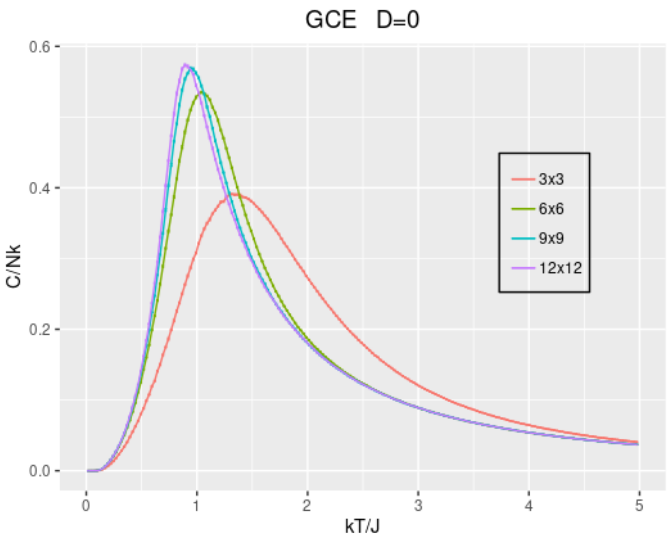
We find that despite the density being able to change with temperature in the constant Δ case, the specific heat curve is smooth. And with our data in the canonical ensemble, we see that we have a shoulder in the specific heat. The mechanism responsible for this shoulder is still unknown but it is an interesting feature that we don't see in the Ising model on a square lattice.

Now, let us see how our specific heat data from the GCE with constant average density compares with that obtained from the canonical ensemble. The results, shown in Fig. 12 show that any results we get for 2/3 filling in the canonical ensemble can easily be reproduced in the grand canonical ensemble by tuning the value of Δ to ensure an average of 2/3 filling at a given temperature.

From our specific heat results, we see that we have a critical temperature near $kT = 0.373J$. We now look to other measurements to confirm these results. Let us consider the new measurements involving loops. We will start with a measurement of the number of neighbors an unoccupied site has. In the canonical ensemble, we looked at the number of neighbors surrounding an occupied site. The reason we chose this measurement



(a) Specific Heat in the Canonical Ensemble. We can use the peak to determine a phase transition. An interesting feature is the shoulder on the graph. It is not yet understood where this shoulder comes from.

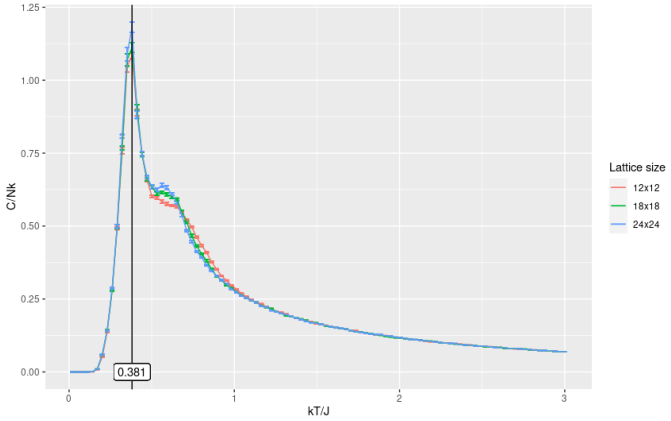


(b) Specific Heat in the grand canonical ensemble where $\Delta = 0$. Although the density isn't being held constant, the curve is smooth. We can also see that the shoulder has disappeared and the peak is at a different place. Thus, to compare the canonical and grand canonical ensembles, we need a way to hold the density constant.

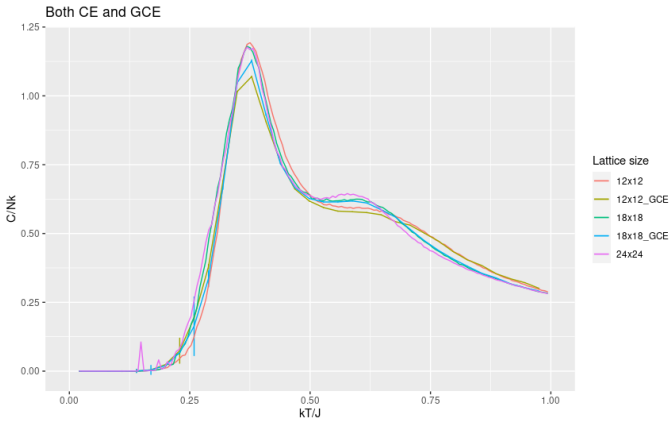
Figure 11

was because in the ordered phase we expect it to have a value of one and at high temperatures it should be 2/3, so we hope to see a large drop at the critical temperature indicating a phase transition.

The results, shown in Fig. 13 show that we have the sharpest change in the proportion of occupied neighbors near $kT = 0.375J$ which agrees with our previous approximate critical temperature of $kT = 0.373J$.



(a) Specific Heat GCE with $\langle\rho\rangle = 2/3$. We see that in holding the density constant, we can reproduce the results of the canonical ensemble.



(b) Specific Heat CE and GCE with $\rho = 2/3$. Comparing the canonical and grand canonical ensemble with the Δ tuned to give constant density shows agreement between the two.

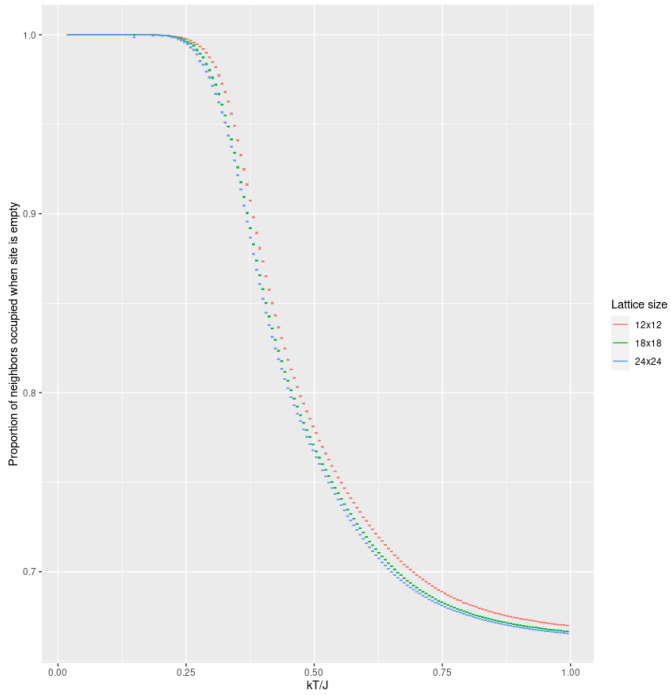
Figure 12

This seems to suggest the specific heat peak is telling us where charge order occurs in the 2/3 filled lattice case.

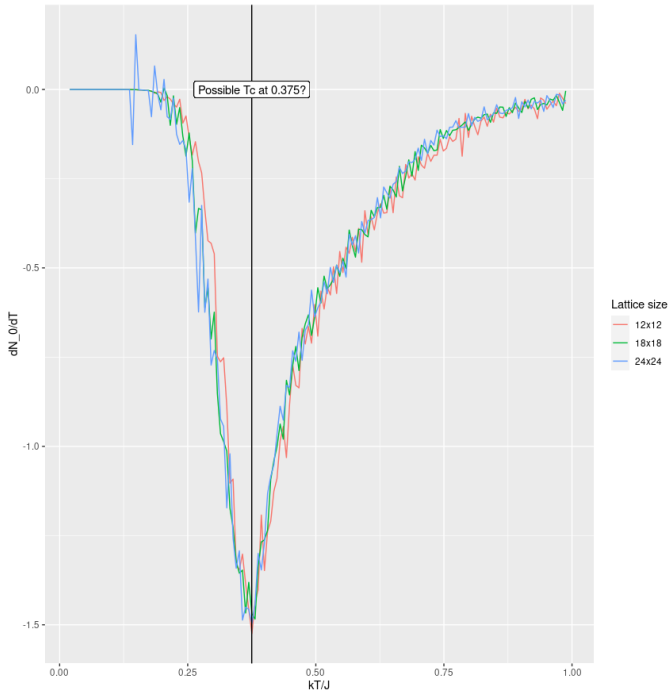
Next, we look at the loop operators which should tell us about both charge and spin order as a single hole in the loop causes the loop operator to return a value of zero, and a single spin flip in the loop causes the sign of the loop operator to change. In the case of the loop operators however, rather than taking the loop around empty sites, I took all the loops around the sites in the sublattice with the largest amount of vacancies (lowest charge density). The three different sublattices on the triangular lattice are shown in Fig. 7.

The results obtained from the loop operator are shown in Fig. 14.

As we can see, the loop operator gives a slightly different critical temperature. So, since this measurement is sensitive to spin order as well as charge order, it may be the case that the spin order disappears at a lower temperature than the charge order leading to the discrepancy in the critical temperature between the loop oper-

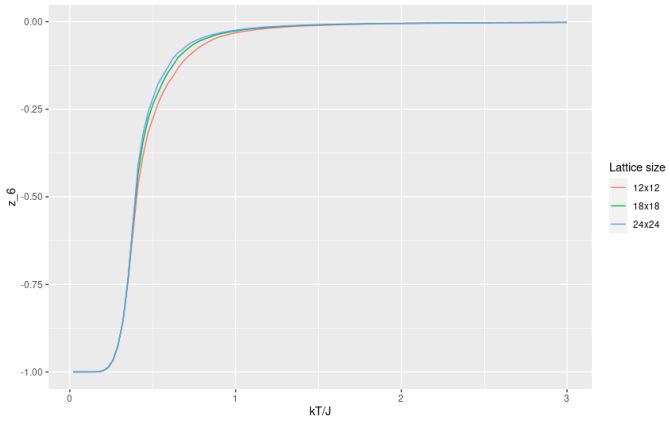


(a) Proportion of occupied sites surrounding an unoccupied site in the canonical ensemble. A phase transition isn't obvious from this graph so we take the derivative to see if we can see where one occurs.

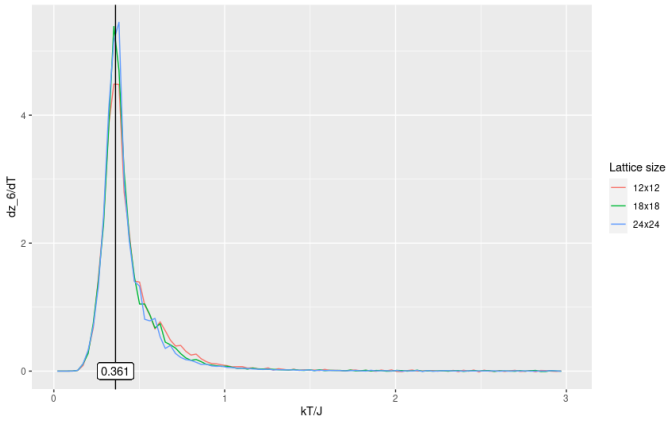


(b) Derivative of the previous graph. We see that there is a spike in the derivative and it occurs near our critical value of $kT = .373J$

Figure 13



(a) Average value of the product of the loop surrounding an element of the sublattice with the smallest number of spins.



(b) Derivative of the previous graph. We see that the spin order may have been lost before the charge order. However, this critical temperature is still close to our critical value of $kT = 0.373J$.

Figure 14

ator and the specific heat.

Finally, we want to see if we could recreate the Binder crossing. However, if we were working in the canonical ensemble, the number of spins is fixed so the magnetization will always be zero. A way to get around this was to take the magnetization of each sublattice separately. The first thing we tried was to define the Binder ratio as the average Binder ratio of each sublattice. However, as one sublattice was empty at low temperatures this caused issues as the Binder ratio is defined as $\frac{\langle M^4\rangle}{\langle M^2\rangle^2}$ so zero magnetization would lead to division by zero. We can get around this by removing the Binder ratio from the average if it involves division by zero. However, this still doesn't fix the problem completely. To see this, consider a sublattice that receives a single spin at one time step of the Monte Carlo simulation and is empty the rest of the time. Then, $\langle M^4\rangle = \frac{(\pm 1)^4}{N} = \frac{1}{N}$ whereas $\langle M^2\rangle^2 = \left(\frac{(\pm 1)^4}{N}\right)^2 = \frac{1}{N^2}$ giving a Binder ratio of $\frac{1/N}{1/N^2} = N$ (the number of Monte Carlo steps). Thus, if we run our simulation for a long time this mostly empty sublattice will bias our average Binder ratio to be huge. To get around this, instead of directly taking the average Binder ratio, we take the ratio of the weighted average of $\langle M^4\rangle$ and the square of the weighted average of $\langle M^2\rangle$ where the weights are determined by the average number of spins in that sublattice:

$$B_{\text{weighted}} = \frac{\sum_\alpha \langle M^4\rangle w_\alpha}{\left(\sum_\alpha \langle M^2\rangle w_\alpha\right)^2}$$

$$\text{Where the weight } w_\alpha = \frac{\langle \sum_{i\in\alpha} s_i^2\rangle}{\sum_\alpha \langle \sum_{i\in\alpha} s_i^2\rangle}$$

In this case, we unfortunately do not have any crossings. However, when taking the derivative, we see a peak near our specific heat peak as shown in Fig. 15 We see that we get a slightly higher critical temperature than we got in the specific heat. This may be a sign that in the canonical ensemble, spin order disappears at a higher temperature than charge order which is the opposite of the case we found in the GCE. However, seeing as we have a fixed number of spins, this may account for that discrepancy.

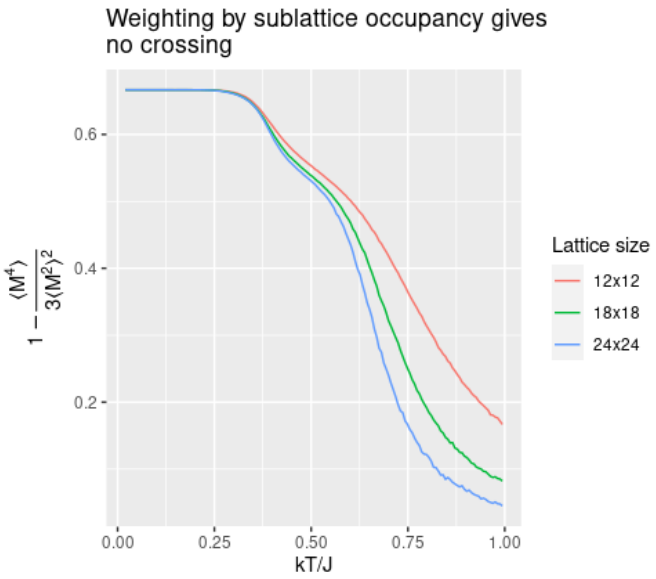
Another attempt at defining a sublattice Binder ratio shown in Fig. 16 was obtained by just throwing out Binder ratios greater than 3 (as that's the high-temperature limit for the Binder ratio) and averaging what's left over. However, in this case, the Binder ratio isn't smooth and has no clear crossing, so it seems like this definition doesn't properly weigh the sublattices either.

VII. Conclusion

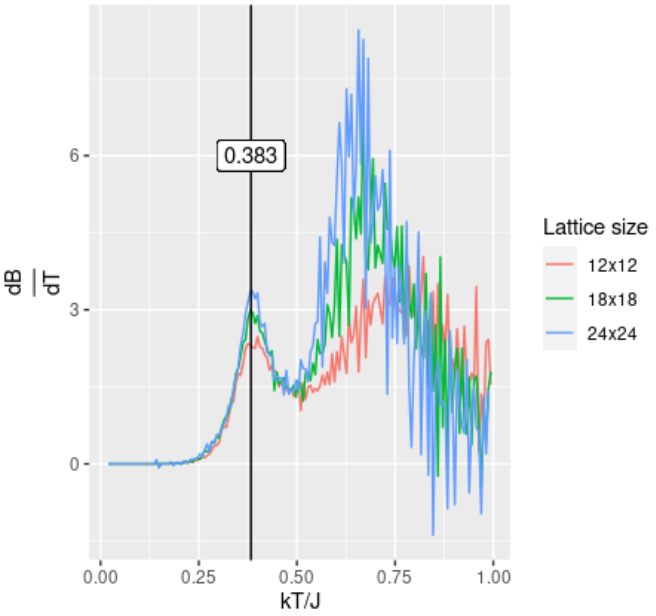
In conclusion, the Blume-Capel model on a triangular lattice allows us to explore spin and charge order in a purely classical model. Our results show that it is likely that the spin order is lost at lower temperatures than the charge order.

The clash between spin order and charge order may be the key to understanding the shoulder in the specific heat. However, based on our data, there is no obvious correlation between the two, and the cause of the shoulder is still unknown. On the other hand, through this model, we obtain an estimated critical temperature of $kT \approx 0.373J$ based on the specific heat plot with the loss of charge order being more closely related to this peak.

Furthermore, our attempt to modify the Binder ratio turned out to be unsuccessful. This is likely because one sublattice will nearly always be empty while the other two are nearly always full at low temperatures thus we need some method of controlling the value of the Binder ratio at low temperatures if we are to consider the fluctuations in magnetization in all three sublattices or ignore a sublattice entirely. Both solutions



(a) Weighted Binder ratio in the Canonical Ensemble. We see that in the way it is currently defined, we have no crossing.



(b) Derivative of the previous graph. The derivative of the weighted Binder ratio gives a small peak near our critical temperature of $kT = 0.373J$ so it seems that this measurement does somehow relate to the critical temperature just not in the usual way we would expect the Binder cumulant to behave.

Figure 15

result in a Binder cumulant that is unable to obtain a crossing and is thus unable to be used to determine a critical temperature. As a result, we must rely on the critical temperature obtained from the specific heat and our loop measurements.

Further work is still needed, however, to create a phase diagram, understand the shoulder in the specific

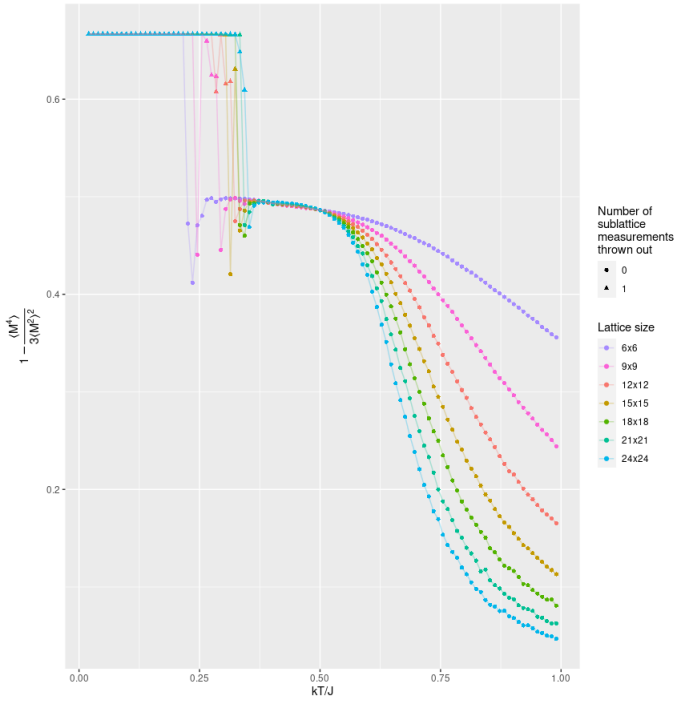


Figure 16: Calculating the Binder cumulant for each sublattice and averaging over them after throwing out Binder cumulants greater than 3. We see that there is no clear crossing.

heat, and obtain critical exponents associated with the phase transitions.

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