THESIS

COMPARISON OF q = 2, 3, 4 AND 5 STATES OF THE POTTS MODEL FOR TWO DIMENSIONAL SQUARE AND TRIANGULAR LATTICES

PONGTHACHAT NEAMSONG

GRADUATE SCHOOL, KASETSART UNIVERSITY
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THESIS

COMPARISON OF q = 2, 3, 4 AND 5 STATES OF THE POTTS MODEL FOR TWO DIMENSIONAL SQUARE AND TRIANGULAR LATTICES

PONGTHACHAT NEAMSONG

A Thesis Submitted in Partial Fulfillment of
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Potts Model is the model for studying the behavior of a magnet which nearest neighbor interaction has q spin direction discontinuously in each site. It is called q state Potts Model. The properties of internal energy per spin, specific heat per spin, magnetization per spin and magnetic susceptibility per spin with q = 2, 3, 4 and 5 for square and triangular lattices with sites 10x10, 15x15, 20x20 and 25x25 varying with temperatures are studied.

In the regions where the temperature is less than critical temperature, when the temperature increases, usually the internal energy, specific heat and magnetic susceptibility also increase but the magnetization decreases. When the temperature tends to the critical temperature, the slope of the internal energy is going to the maximum value and gives the maximum specific heat. The magnetization decreases rapidly and gives the maximum magnetic susceptibility. When the temperature is higher than the critical temperature, the internal energy increases and the magnetization is at minimum.

If the number of spin state increases, the value of the critical temperature will decrease. When the calculation is done at higher number of lattice sites the critical temperature decreases appreciably. Square lattice which has spin interaction less than triangular lattice, gives lower critical temperature comparing to the triangular lattice at the same state.

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Student’s signature Thesis Advisor’s signature

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INTRODUCTION

Magnetization of magnetism is resulted by orbital of electron around nucleus and the electron has the behavior resembles small-sized magnet (electron spin).

Ferromagnetism will show magnetic properties that vary by the temperature. When the temperature is lowers than critical temperature (Curie temperature) and no external field, ferromagnetism has spontaneous magnetic dipole. Spin will behave in same direction causes minimum internal energy and maximum magnetization. When the temperature increases cause internal energy increases too. When temperature reaches critical temperature, the internal energy will increase rapidly. That causes direction of spin will point to any way then magnetization decreases to zero.

The study of magnetic phase transition that is the fundamental analysis makes formula to show relation with thermodynamic quantities. Another way to study is to use model for magnetism.

Ising model is a simplest model. It is assumed that spin of atom has two pointing directions (up pointing or down pointing). In which spins of magnetism have more two states. So Potts model have q states. Which can pointing to q direction equally space and it realizes for magnetism better than Ising model. Two states Potts model is equivalent Ising model.

OBJECTIVES

1. Compare the internal energy, specific heat, magnetization and magnetic susceptibility at state 2, 3, 4 and 5 in the same lattice with site 10x10, 15x15, 20x20 and 25x25 relate with temperature.

2. Compare the internal energy, specific heat, magnetization and magnetic susceptibility at site 10x10, 15x15, 20x20 and 25x25 in the same state relate with temperature.

3. Calculate critical indices α, β, γ and δ.

LITERATURE REVIEW

1. Magnetism in Matter

Magnetism is the power that can exert an attractive on magnetic material. All materials are influenced to present magnetic field but in most case the influence to small to detect. Magnetic field is fundamental field that arise from the movement of electrical charge.

Normally magnetic bar are seen as dipoles having South Pole and North Pole interacting with earth magnetic field. Therefore, when place in a magnetic field, a magnetic dipole will tend to align itself in opposed polarity to that field.

The physical cause of the magnetism of objects, distinct from electrical currents, is the atomic magnetic dipole. Magnetic dipoles, or magnetic moments, result on the atomic scale due to the two kinds of movement of electrons. The first is the orbital motion of the electron around the nucleus; this can be considered as a current loop, resulting in a magnetic moment along the axis of the nucleus. The second, much stronger, source of electronic magnetic moment is due to a quantum mechanical property called spin (although current quantum mechanical theory states that electrons do not actually physically spin, or orbit the nucleus for that matter).

The overall magnetic moment of the atom is the net sum of all of the magnetic moments of the individual electrons. Because of the tendency of magnetic dipoles to oppose each other to reduce the net energy, in an atom the opposing magnetic moments of some pairs of electrons will cancel each other, both in orbital motion and in spin magnetic moments. Thus, in the case of an atom with a completely filled electron shell or sub shell, the magnetic moments normally completely cancel each other and only atoms with partially filled electron shells will have a magnetic moment, whose strength depends on the number of unpaired electrons.

The spin of an electron has a magnetic dipole moment and creates a magnetic field. (The classical analogue of quantum-mechanical spin is a spinning ball of charge, but the quantum version has distinct differences, such as the fact that it has discrete up/down states that are not described by a vector.) In many materials (specifically those with a filled electron shell), however, the electrons come in pairs of opposite spin, which cancel one another's dipole moments. Only atoms with unpaired electrons (partially filled shells) can experience a net magnetic moment from spin. A ferromagnetic material has many such electrons, and if they are aligned they create a measurable macroscopic field.

The spins (dipoles) tend to align in parallel to an external magnetic field, an effect called Para magnetism. Ferromagnetism involves an additional phenomenon, however: the spins tend to align spontaneously, without any applied field. This is a purely quantum-mechanical effect

Ferromagnetism is a phenomenon by which a material can exhibit a spontaneous magnetization, and is one of the strongest forms of magnetism. It is responsible for most of the magnetic behavior encountered in everyday life, and is the basis for all permanent magnets (as well as the metals that are noticeably attracted to them).

Paramagnetic is the tendency of the atomic magnetic dipoles, due to quantum-mechanical spin, in a material that is otherwise non-magnetic to align with an external magnetic field. This alignment of the atomic dipoles with the magnetic field tends to strengthen it, and is described by a relative magnetic permeability greater than unity (or, equivalently, a small positive magnetic susceptibility).

In pure Paramagnetic, the field acts on each atomic dipole independently and there are no interactions between individual atomic dipoles. Such paramagnetic behavior can also be observed in ferromagnetic materials that are above their Curie temperature.

Paramagnetic materials attract and repel like normal magnets when subject to a magnetic field. Under relatively low magnetic field saturation when the majority of the atomic dipoles are not aligned with the field, paramagnetic materials exhibit magnetization according to Curie's Law

In physics, the Curie point, or Curie temperature, is the temperature above which a Ferro magnet loses its ferromagnetic ability to possess a net (spontaneous) magnetization in the absence of an external magnetic field. At temperatures below the Curie point, magnetic moments are partially aligned within magnetic domains in ferromagnetic materials. As the Curie point is approached, thermal fluctuations increasingly destroy this alignment, until the net magnetization becomes zero at and above the Curie point. Above the Curie point, the material is purely paramagnetic.

Below the Curie point, an applied magnetic field has a paramagnetic effect on the magnetization, but the combination of Para magnetism with ferromagnetism leads to the magnetization following a hysteresis curve with the applied field strength. The Curie temperature is a second-order phase transition and a critical point where the magnetic susceptibility is theoretically infinite

2. Magnetic Phase Transitions

Certain materials like iron, cobalt and nickel show ferromagnetic properties below a transition temperature T_c (Curie temperature). In comparison to paramagnetic behavior which is assumed above Curie temperature, ferromagnetic materials are characterized properties. While field strengths of order of 10^9 A/m are necessary to reach the saturation magnetization in a paramagnet, only a few 10^5 A/m are sufficient to achieve the same for a Ferro magnet. The initial susceptibility of ferromagnetic materials is approximately nine orders of magnitude lager than that of paramagnets. After switching off external field, a permanent dipole moment remains in Ferro magnet which depends strongly on the prior mechanical and thermal treatment of the material. Ferromagnetism can be found only in solids with a well-defined crystalline structure (Walter *et. al.*, 1994).

The spontaneous alignment of the atomic dipoles is due to the exchange interaction of the electron, which mutually couples the magnetic moments. The coupling energy of the atomic dipoles is on the order of 0.1 eV. If the temperature rises beyond a value corresponding to the thermal energy kT_c , the bonds are broken and the dipoles become statistically independent, which leads to paramagnetic behavior above T_c (Walter *et. al.*, 1994).

The atomic magnetic moment is proportional to the total angular momentum. Atomic moments contributing to the magnetization are solely due to the spin of electrons. Only between the spins of the electrons is there an interaction which is sufficiently strong to enforce a spontaneous alignment of the moments. The interaction energy of two electrons is quantum mechanically given by two parts due to

$$\begin{aligned} K_{ij} &= \int \psi_i^*(1)\psi_j^*(2)U_{ij}\,\psi_j(2)\psi_i(1)\,d^3\vec{r}_1 d^3\vec{r}_2 \quad \textit{direct} \\ I_{ij} &= \int \psi_j^*(1)\psi_i^*(2)U_{ij}\,\psi_j(2)\psi_i(1)\,d^3\vec{r}_1 d^3\vec{r}_2 \quad \textit{exchange} \end{aligned} \tag{1}$$

The interaction energy is $K_{ij} \pm I_{ij}$, where the + holds for antiparallel spins and - the for parallel spins. The energy difference between the configuration with parallel spins and that with antiparallel spins is $\in_{\uparrow\uparrow} - \in_{\uparrow\downarrow} = -2I_{ij}$. If $I_{ij} > 0$, a parallel alignment of the spins is preferred and $I_{ij} < 0$ an antiparallel. The ferromagnetism can occur only in materials which have sufficiently many electrons with unpaired spins, whose contributions do not cancel, I_{ij} assumed large value and the exchange energy decreases rapidly with increasing distance among the electron (Walter *et. al.*, 1994).

Just as strongly positive exchange integral I_{ij} enforce a parallel alignment of the spins and negative leads to an antiparallel. It is for ferromagnetic and antiferromagnetic

3. Critical indices

Let define a dimensionless parameter t that called reduced temperature which measures how far away from T_C

$$t = \frac{T - T_C}{T_C} \tag{2}$$

when t=0, it is at the critical temperature.

Specific heat with non external field (H = 0) at critical temperature have behavior is infinite value. Critical indices α by

$$C \approx |t|^{-\alpha} \tag{3}$$

The relationship between specific heat at non external field and temperature is show in figure below

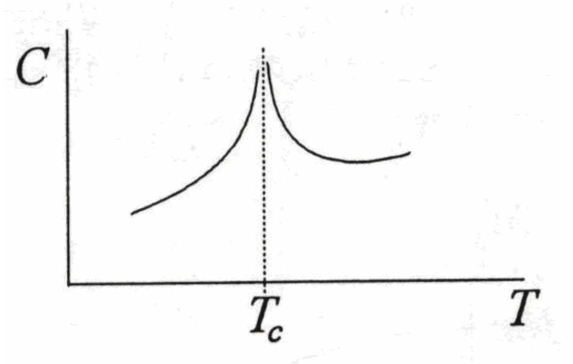


Figure 1 Relation between specific heat and temperature in region critical temperature with non external field

Magnetization is zero at $T > T_C$ and non zero at $T < T_C$. Critical indices β from spontaneous magnetic moment is non zero at temperature below critical temperature

$$m \approx |t|^{\beta} \tag{4}$$

The relationships between magnetization and temperature with non external field is show in figure below

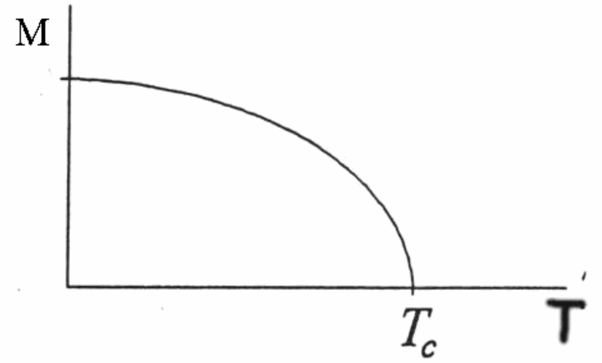


Figure 2 Relation between spontaneous magnetic moment and temperature

The isothermal susceptibility at zero magnetic field (H) is $\chi_0 = \lim_{H\to 0} \chi_T = \lim_{H\to 0}\left(\frac{\partial M}{\partial H}\right)_T$ and the relationships with temperature is show in figure below

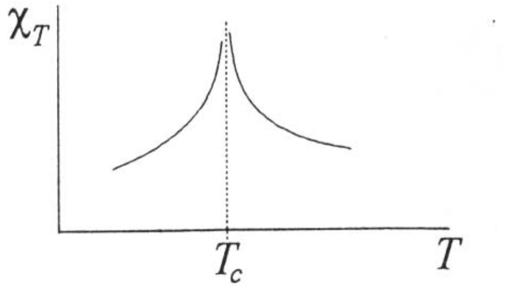


Figure 3 Relation between susceptibility and temperature

Critical indices γ are

$$\chi \approx |t|^{-\gamma} \tag{5}$$

One exponent δ governs the way in which the magnetization of model varies with an applied external field *B* at the critical temperature

$$\text{sgn}(m)|m| \approx H^{1/\delta} \tag{6}$$

where sgn(*m*) = 1 for *m* > 0 or sgn(*m*) =-1 for *m* < 0

4. Spin Model

The science of physics assumes that physical phenomena may be explained and understood as a result of the functioning of physically real systems structured in certain ways and constituted of elements possessing certain properties. The exact nature of the real system in itself is usually unknown, so to gain an understanding if a model is constructed.

The conceptual analogue of the physical phenomenon to be explained is understood as occurring as a result of the properties of the model, and the phenomenon itself is then explained as a result of assumed properties of the real system which are analogous to the properties of the model.

Magnetism (or electromagnetism) is one of the fundamental forces of nature. A field of magnetic force is produced by the motion of an electrically charged particle, and so an electric current (which consists of moving charge) produces a magnetic field.

In 1925 G. E. Uhlenbeck and S. Goudsmit hypothesized that the electron has a "spin", and so behaves like a small bar magnet, and that in an external magnetic field the direction of the electron's magnetic field is either parallel or antiparallel to that of the external field.

Ising model is one of models which spin have one of two values +1 and -1. If the spin more than two states it will be Potts model which spin values have 1 to q. This named after Australian mathematician R. B. Potts who published a study of this model in 1952 just describe later.

Magnetic materials exhibit interesting temperature-dependent behavior. In particular, above a certain temperature any magnetization present disappears. When the temperature is reduced below that temperature regions of stable magnetization spontaneously appear (even in the absence of an external magnetic field). This temperature is called the "critical" or "Curie" temperature. Various discontinuities (called "phase transitions") in measurable properties are found to occur at the critical temperature.

There have been many computational studies of the behavior of magnetic materials at the critical temperature using Ising and Potts spin models. These studies often use so-called "Monte Carlo" techniques (described in Hamersley and Hands comb 1964), which are methods relying on a stream of random numbers to drive a stochastic process, in this case the generation of a succession of many states of the spin model

5. Lattice Geometries

In the magnetic system, spin must have location to relate them with each other and its interaction which usually only nearest neighbor, for simplest case, spin interact. This may have a regular geometric lattice structure which consists of line of joining vertices. Example lattice geometry is below

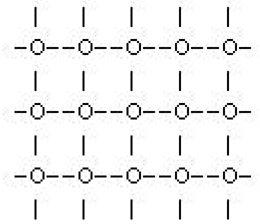


Figure 4 Square Lattice
Source: Yamakuchi (2003)

The similarly lattice in 3 dimensions is called cubic. The 4 and higher dimension is called hyper cubic. The Square and cubic lattice are easiest to represent on a computer. On an infinite square lattice the nearest neighbors of a site with coordination (i,j) will be (i±1,j) and (i,j±1).

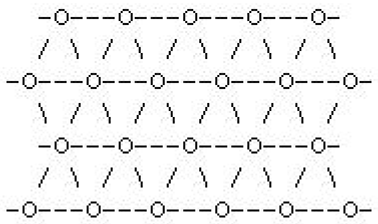


Figure 5 Triangular Lattice
Source: Yamakuchi (2003)

The similarly lattice in 3 dimension called diamond lattice which is structure of carbon atoms in a diamond crystal. A simple trick is set nearest neighbors of spins as easy as square lattice. The nearest neighbors of site (i,j) thus (i±1,j) , (i,j±1) and add (i+1,j-1) and (i-1,j+1)

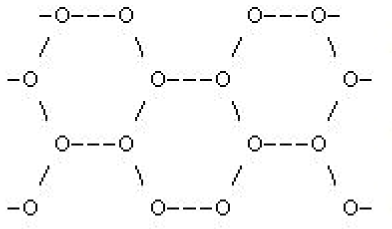


Figure 6 Honeycomb Lattice
Source: Yamakuchi (2003)

Point in the lattice is called lattice point which occupied by spin and it known as site. One of characteristic properties of a lattice geometry is the number of sites directly connected to a site is known as coordination number of the lattice

Example of the coordination numbers of various possible lattice geometries are in table below

Table 1 Coordination number of Lattice

Dimension	Name	Coordination number
2	Square	4
2	Triangular	6
2	Honeycomb	9
3	Diamond	4
3	Cubic	6
3	tetrahedral	12

Source : Yamakuchi (2003)

6. Monte Carlo Method

Statistical mechanics is primarily concerned with the calculation of properties of condensed matter systems which composed of many parts, atoms, or molecule. This system governed by Hamiltonian function which gives the total energy of the system in any particular state. Most of examples have discrete set of states each with its own energy that ranging from lowest energy or ground state E_0 and upwards to E_1 , E_2 ,… possibly with out limit.

Being Hamiltonian system with energy conserve that means the systems stay in the same energy states all the time. It has number of degenerate state with the same energy.

Suppose the system is in state *u*. Let define $R(u \rightarrow v)dt$ to be probability that it is in state *v* at small interval time *dt* later. $R(u \rightarrow v)$ is the transition rate for the transition from state *u* to *v* and assumed time independent.

Define a set of weights $w_u(t)$ which represent the probability of the system will be in state *u* at time *t*.

$$\frac{dw_u}{dt} = \sum_v \left[w_v(t) R(v \rightarrow u) - w_u(t) R(u \rightarrow v) \right] \tag{7}$$

The first term on the right hand side of this equation represent the rate at the system undergoing transition in to state *u* and second term is the rate at which the system undergoing out of state *u* to other states. The probability must obey sum rule $\sum_u w_u(t) = 1$. And this related to the macroscopic properties of the system. If quantity *Q* is interested and it has value Q_u in state *u*. The expectation of any value *Q* at time *t* for the system as

$$\langle Q \rangle = \sum_u Q_u \, w_u(t) \tag{8}$$

If system ever reaches a state in which the two terms on the right hand side exactly cancel one another for all *u*, then the rates dw_u / dt will all vanish and take constant values for the rest of time this is equilibrium state. The equilibrium values call equilibrium occupation probabilities denoted by

$$p_u = \lim_{t \to \infty} w_u(t) \tag{9}$$

In 1902 Gibbs showed that the system in thermal equilibrium with reservoir at temperature *T* has equilibrium occupation probabilities and call Boltzmann distribution

$$p_u = \frac{1}{Z} e^{-E_u / kT} \tag{10}$$

Where Z is partition function which value $Z = \sum_u e^{-E_u / kT}$. k is Boltzmann's constant whose value 1.38 x 10^{-23} J/K

The expectation value of the energy <*E*> is quantity in thermodynamics as the internal energy and it is given by

$$U = \frac{1}{Z} \sum_u E_u e^{-E_u / kT} \tag{11}$$

Numerical method for calculating the partition function of a model is Monte Carlo simulation. This idea is to simulate the random thermal fluctuation of the system from state to state.

The usual goal in the Monte Carlo simulation of the thermal system is the calculation of the expectation value <*Q*>

$$\langle Q \rangle = \frac{\sum_u Q_u e^{-\beta E_u}}{\sum_u e^{-\beta E_u}} \tag{12}$$

That is only tractable in the very smallest system. In larger system, the best we can do is average over some subset of the states, though this necessarily introduces some inaccuracy into the calculation. Monte Carlo techniques work by choosing a subset at random from some probability distribution p_u which we specify. Suppose we choose *M* such states. Best estimate of the quantity *Q* will be given by

$$Q_M = \frac{\sum_{i=1}^{M} Q_{ui} p_{ui}^{-1} e^{-\beta E_{ui}}}{\sum_{i=1}^{M} p_{ui}^{-1} e^{-\beta E_{ui}}} \tag{13}$$

Q_M is called the estimator of *Q*. It has the property that, as the number *M* of states sampled increases, it become a more and more accurate estimate of <*Q*> and when $M \rightarrow \infty$ we have Q_M = <*Q*>

The simplest choice is to pick all state with equal probability and then we get

$$Q_M = \frac{\sum_{i=1}^{M} Q_{ui} e^{-\beta E_{ui}}}{\sum_{i=1}^{M} e^{-\beta E_{ui}}} \tag{14}$$

instead of picking our *M* states in such away that every state of the system is as likely to get chosen as every other, we pick them so that the probability that a particular state *u* get chosen is $p_u = \frac{1}{Z} e^{-E_u/kT}$. Then our estimator for <*Q*> become

$$Q_M = \frac{\sum_{i=1}^{M} Q_{\mu i}}{M} \tag{15}$$

Markov Process is a mechanism which given a system in one state *u* generates a new state of system *v* in random. The probability of generating is called transition probability *P(u → v)* and satisfy two condition: (1) not vary over time and (2) depend only properties current state *u* and *v*. It must satisfy the constraint $\sum_u P(u \to v) = 1$.

Markov process is the condition of detailed balance. This condition is that a rate at the system makes transition into and out of any state *u* must be equal.

$$p_u\, P(u \to v) = p_v\, P(v \to u) \tag{16}$$

This is the condition of detailed balance. Insert Boltzmann distribution, The detailed balance equation or transition probability should satisfy

$$\frac{P(u \to v)}{P(v \to u)} = \frac{p_v}{p_u} = \exp(-\beta(E_v - E_u)) \tag{17}$$

Acceptance ratios get transition probability into two parts thus

$$P(u \to v) = g(u \to v) A(u \to v) \tag{18}$$

Where *g(u → v)*is selection probability which is the probability given initial state *u* and *A(u → v)* is the acceptance ratio which say that if we start off in a state *u* and our algorithm generates a new state *v* we should accept that state and change our system to the new state *v*.

7. The Metropolis Algorithm

Metropolis algorithm was introduces by Nicolas Metropolis and his co-workers in a 1953. This is the most famous and widely used algorithm. This chooses selection probabilities for each of the possible states are all equal $g(u \to v) = \frac{1}{N}$. With this selection probability, the condition of detailed balance takes in form

$$\frac{P(u \to v)}{P(v \to u)} = \frac{g(u \to v) A(u \to v)}{g(v \to u) A(v \to u)} = \frac{A(u \to v)}{A(v \to u)} = \exp(-\beta(E_v - E_u)) \tag{19}$$

Now we choose acceptance ratios $A(u \rightarrow v)$ to satisfy this equation, one is to choose

$$A(u \to v) = A_0 \exp\left(-\frac{1}{2}\beta\left(E_v - E_u\right)\right) \tag{20}$$

the constant of probability A_0 cancels out and we can choose any value for it that we like. The largest difference in energy that we can have between two states is $2zJ$, where z is coordination number that means the largest value is e^{-BzJ} , thus in order to make sure $A(u \rightarrow v) \leq 1$ and choose

$$A_0 \le e^{-\beta zJ} \tag{21}$$

Suppose that of the two states *u* and *v*, we are considering here, *u* has the lower energy and *v* has the higher energy. Then the larger of the two acceptance ratio is $A(u \rightarrow v)$, so we set that equal to one. In order to satisfy equation 20 $A(u \rightarrow v)$ must take the value $\exp(-\beta \Delta E)$. Thus the optimal algorithm is one in which

$$A(u \to v) = \begin{cases} e^{-\beta\Delta E} \\ 1 \end{cases} \tag{22}$$

8. Ising Model

The Ising Model is a model of magnet which material is made up from combined magnetic dipole moment of many atomic spin with in the material. The model postulate a lattice with a magnetic dipole of spin on each site

Spins for Ising model assumed is simplest form possible. Each site on lattice have one of two value are 1 or -1 represent up pointing or down pointing of unit magnitude

The Ising model mimics magnetic material by including term in the Hamiltonian proportional to products S_i and S_j of the spins value. For simplest case the interactions are all the same strength denoted by *J* which has dimension of energy. The interactions are only between nearest neighbors spin on the lattice.

To introduce and extend magnetic fields *H* coupling the spin and the Hamiltonian is

$$\mathrm{H} = -J\sum_{<i,j>} S_i S_j + H\sum S_i \tag{23}$$

For $J > 0$ make spin wants to line up in the same direction. A ferromagnetic model is opposed and $J < 0$ for ant ferromagnetic

For $H > 0$ the spin want to line up in the same direction. The states of Ising model are the different set of values that the spins can take.

Easy form of partition function is

$$Z = e^{\left(\frac{-\mathrm{H}}{kT}\right)} \tag{24}$$

Another expectation value can find from this model

Internal energy U is average of H

Specific heat, For $U = \frac{1}{Z}\sum_u E_u e^{-\beta E_u}$ can be written in terms of a derivative of the partition function $U = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{\partial \log Z}{\partial \beta}$. The specific heat can give by the derivative of the internal energy $C = \frac{\partial U}{\partial T} = -k\beta^2 \frac{\partial U}{\partial \beta} = -k\beta^2 \frac{\partial^2 \log Z}{\partial \beta^2}$

Consider $\left\langle E^2 \right\rangle = \frac{1}{Z}\sum_u E_u^2 e^{-\beta E_u} = \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2}$

So $\left\langle E^2 \right\rangle - \left\langle E \right\rangle^2 = \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} - \left[\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right]^2 = \frac{\partial^2 \log Z}{\partial \beta^2} = \frac{C}{k\beta^2}$

then

$$C = \frac{\partial U}{\partial T} = k\beta^2\left(\left\langle E^2 \right\rangle - \left\langle E \right\rangle^2\right) \tag{25}$$

Magnetization

$$\left\langle M \right\rangle = \left\langle \sum S_i \right\rangle \tag{26}$$

Magnetic susceptibility

$$\chi = \frac{\partial \left\langle M \right\rangle}{\partial H} = \beta\left(\left\langle M^2 \right\rangle - \left\langle M \right\rangle^2\right) \tag{27}$$

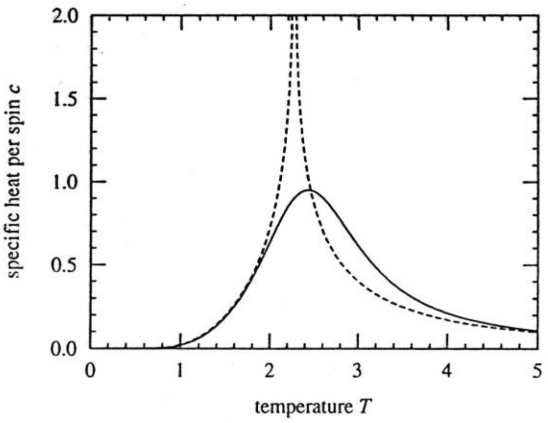


Figure 7 The specific heat per spin for square lattice site 5x5 (solid line) and infinitely big square lattice (dash line)
Source: Walter *et. al*., (1994)

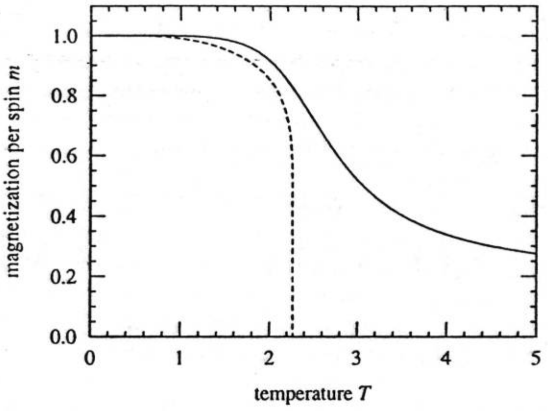


Figure 8 The magnetization per spin for square lattice site 5x5 (solid line) and infinitely big square lattice (dash line)
Source: Walter *et. al*., (1994)

9. The Potts Model

The Potts Model is a model of magnetic spin as same as Ising Model but this model is generalized and it content more than two components of direction of spin. This idea proposed by Domb (Potts 1952) is referred Ising Model which direction of spin is parallel or anti parallel for explore critical properties of magnetism and behavior can show more content for studying critical point theory.

Then an appropriate generalization would be to consider spin system confine in a plane which each spin pointing to one of q equally spaces directions specified by angle

$$\theta_n = \frac{2\pi n}{q} \quad , n = 0,1,\ldots,q-1 \tag{28}$$

In the most general form the nearest neighbor interaction depends only on the relative angle between the two vectors. This is quite generally known Hamiltonian reads

$$H = -\sum_{<ij>} K(\theta_{ij}) \tag{29}$$

Where the function $J(\theta)$ is 2π periodic and $\theta_{ij} = \theta_{n_i} - \theta_{n_j}$ is the angle between the two spins at neighboring site *i* and *j* . The model suggested by Domb (Potts, 1952) is to choose

$$K(\theta) = -J\cos\theta_{ij} \tag{30}$$

that called planar potts model

Potts was able to determine the critical point of this model on the square lattice for *q=2,3,4*. While unable to extend this finding to *q>4*, Potts reported as a remark at the end of his paper the critical point for all *q* of the following model that called standard potts model.

$$K(\theta) = -J\delta_{kr}(n_i, n_j) \tag{31}$$

Each lattice site has spin value S_i which represents Spin direction. These spin values of Potts 'Model is discrete and positive. It starts from 1 to *q* and called *q* state Potts 'Model. Each spin can get one values of *q*.

Any two neighboring spin then contribute amount $-J$ to the Hamiltonian for the same value and zero for otherwise. Most thus Hamiltonian with out external magnetic field is

$$H = -J\sum_{<i\,j>} \delta_{Si,Sj} \tag{32}$$

For $J > 0$ this is Ferromagnetic case which has *q* ground state and $J<0$ for anti ferromagnetic

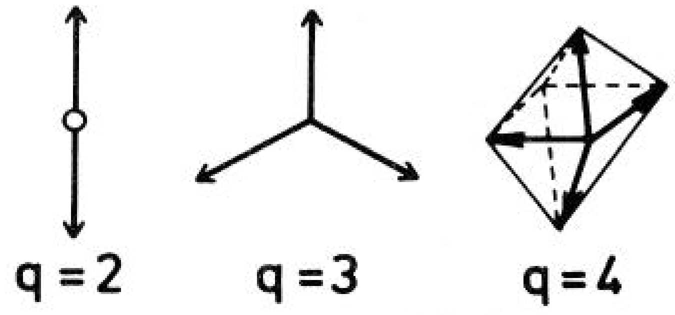


Figure 9 The q unit vectors pointing in the q symmetric directions of a hyper tetrahedron in q-1 dimensions
Source: Wu (1982)

The simulation of Potts 'Model is the same of Ising Model and simplest simulation is single spin flip method. In this thesis use Metropolis Algorithm for Potts 'Model

First choose spin i from lattice by random which each spin have value S_i then random new spin value, not same value, and calculate change of energy for consider acceptance ratio thus

$$\begin{aligned} A &= e^{-\beta\Delta E} && \text{for} \quad \Delta E > 0 \\ &= 1 && \text{for} \quad \text{otherwise} \end{aligned} \tag{33}$$

10. Finite Size Scaling

The finite size scaling method is the way of extracting values for critical exponents by observing how measured quantities vary as the size L of the system study change. This technique not requires us to know T_c, but in fact returns a value of T_c itself. We illustrate for the case of the exponent γ from equation (5).

The lattice has correlation length ξ. The divergence of the correlation length near the phase transition then goes like

$$\xi = |t|^{-\nu} \tag{34}$$

magnetic susceptibility from equation (5) and (34) we get

$$\chi \approx \xi^{\gamma/\nu} \tag{35}$$

The value of χ in the infinite system can express by writing

$$\chi = \xi^{\gamma/\nu} \chi_0\left(L/\xi \right) \tag{36}$$

Equation (36) is not a useful form since it still contains the variable ξ. Defining a new dimensionless function $\tilde{\chi}$

$$\tilde{\chi}(x) = x^{-\gamma} \chi_0\left(x^{\nu}\right) \tag{37}$$

Use equation (34), we get

$$\chi = L^{\gamma/\nu}\, \tilde{\chi}\left(L^{1/\nu} |t| \right) \tag{38}$$

Since the behavior of χ is not symmetric on the two sides, we can combine these by extending the definition of $\tilde{\chi}(x)$ to negative values of x .

$$\chi = L^{\gamma/\nu}\, \tilde{\chi}\left(L^{1/\nu}\, t \right) \tag{39}$$

Suppose we perform a set of Monte Carlo calculations fo the system of interest for a variety of different system size L over a range of temperature close to where we believe the critical temperature to be.

For each system size we measure the magnetic susceptibility $\chi_L(t)$ at a set of temperature *t*. we can now rearrange equation (39) thus

$$\tilde{\chi}\left(L^{1/\nu} t \right) = L^{-\gamma/\nu} \chi_L(t) \tag{40}$$

Since the scaling function is supposed to be the same for all system sizes, this will only happen if we use the correct values of the exponents γ and ν. We must use the correct values of the critical T_c.

The idea behind finite size scaling therefore is to calculate $\tilde{\chi}(x)$ for each of our different system sizes, and then vary the exponents γ and ν and the critical temperature until the resulting curves all fall of collapse on top of one another.

This method can extended to quantities other than the susceptibility thus

$$\begin{aligned} c &= L^{\alpha/\nu} \tilde{c}\left(L^{1/\nu} t \right) \\ m &= L^{-\beta/\nu}\, \tilde{m}\left(L^{1/\nu} t \right) \end{aligned} \tag{41}$$

11. The Idea of Metropolis Algorithm for Potts' Model

This choose selection probability for each of the possible states are all equal $g(u \to v) = \frac{1}{N}$ and acceptance ratio in previous.

A. Main Idea
  1. define value of size of lattice , k , temperature and J
  2. process to equilibrium
  3. process to data collection
  4. calculate mean of data and save data

B. Process to Equilibrium
  1. define Monte Carlo step
  2. begin loop
  3. metropolis algorithm
  4. repeat step 3 until full Monte Carlo step

C. Process to data Collection
  1. define Monte Carlo step
  2. begin loop
  3. metropolis algorithm
  4. get data
  5. repeat step 3 until full Monte Carlo step
  6. find average data

D. Metropolis Algorithm
  1. begin loop first spin to last spin
  2. random value a and b
  3. if $a>b$ go to next step and if not go to step 11
  4. calculate energy
  5. random new spin value (not same value)
  6. calculate new energy
  7. calculate different of energy (ΔE)
  8. if different of energy less than zero go to step 11 else next step
  9. random value r
  10. if $r < exp(-\Delta E/kT)$ then this spin has new value else this spin get old value
  11. go to next spin and back to step 2

MATERIALS AND METHODS

Materials

Personal Computer
- Intel Pentium 4 1.6 GHz
- RAM DDR 256 MB PC 2100

Methods

1. Study of Potts Model and Algorithm

Collect article, journal about Ising Model and study about this idea for explaining magnetism phase transition and Monte Carlo method use for model.

Study about Monte Carlo Method and the simplest method is Metropolis Algorithm. Then create program with visual basic and test run in one dimension Ising Model. Observe the change of spin direction related with temperature. After that, use this algorithm for two dimension square lattice site 10x10 to check form of graph internal energy related temperature.

Collect article about Potts Model and study this idea for explaining magnetism. Study about methods that can use for this model. One of methods is metropolis algorithm just simplest method.

Create program follow idea of Potts model. Then test program by using small Monte Carlo step and roughly observe graph about internal energy, specific heat, magnetization and magnetic susceptibility all relating with time.

2. Run Program to Collect Data

For square lattice site 10x10, 15x15, 20x20 and 25x25 set value k_b and J to be equal is 1 and vary state of spin that q = 2, 3, 4 and 5 in each lattice site. Run program at range of temperature are 0.4 to 1.5. Amount of Monte Carlo step each temperature is 1,000,000 Monte Carlo steps. For critical region, run program near critical temperature for more detail of decimal system of temperature at least 2 position and more Monte Carlo step.

For Triangular lattice site 10x10, 15x15, 20x20 and 25x25 set value k_b and J to be equal is 1 and vary state of spin that q = 2, 3, 4 and 5 in each lattice site. Run program at range of temperature are 0.9 to 2.0. Amount of Monte Carlo step each temperature is 1,000,000 Monte Carlo steps. For critical region, run program near critical temperature for more detail of decimal system of temperature at least 2 position and more Monte Carlo step.

3. Plot Graph

Use data from previous method (method 2) to plot graph

A. Internal Energy and Temperature, Specific Heat and Temperature, Magnetization and Temperature and last Magnetic Susceptibility and Temperature for same lattice site 10x10, 15x15, 20x20 and 25x25 with state 2, 3, 4 and 5.

B. Internal Energy and Temperature, Specific Heat and Temperature, Magnetization and Temperature and last Magnetic Susceptibility and Temperature for lattice site 10x10, 15x15, 20x20 and 25x25 with same state.

4. Calculate Critical Indices

Use data of 10x10, 15x15, 20x20 and 25x25 lattice site find critical indices α, β, γ and δ.

RESULTS AND DISCUSSION

Results

1. Square Lattice

1.1 Lattice Site Comparison

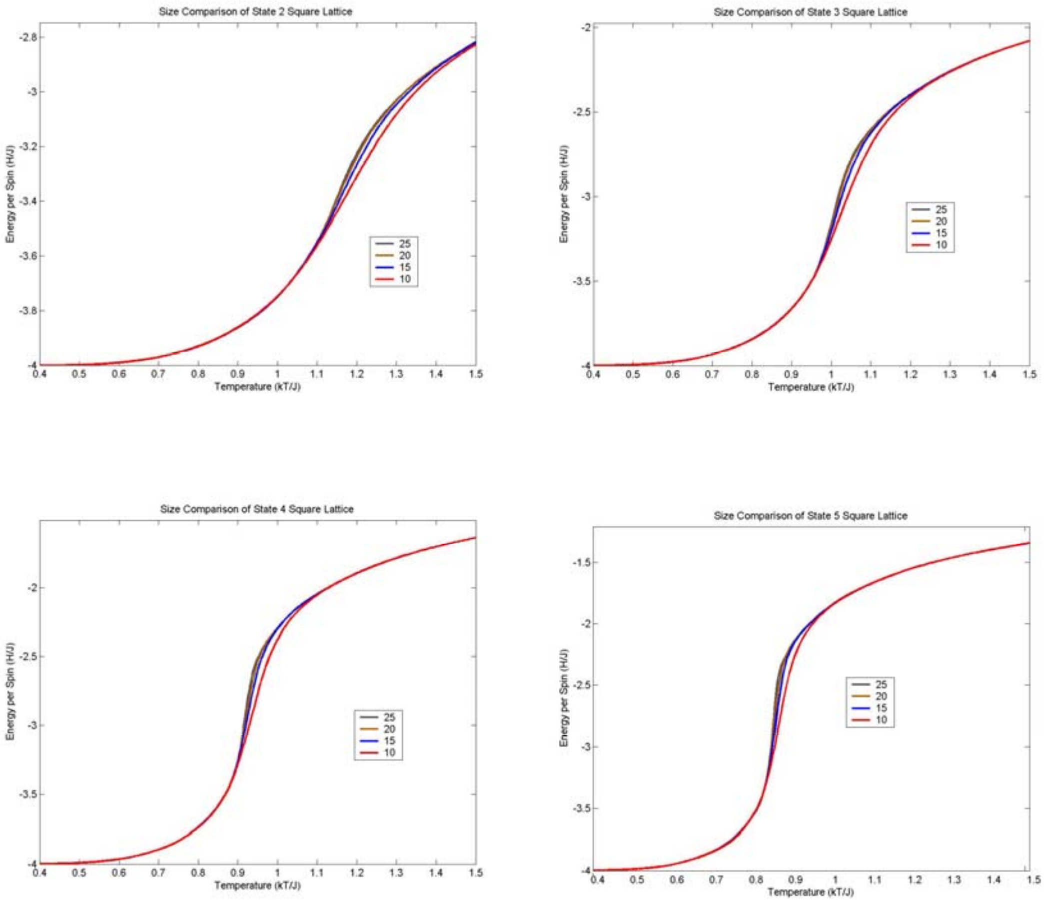


Figure 10 Lattice site comparison of energy per spin for square lattice

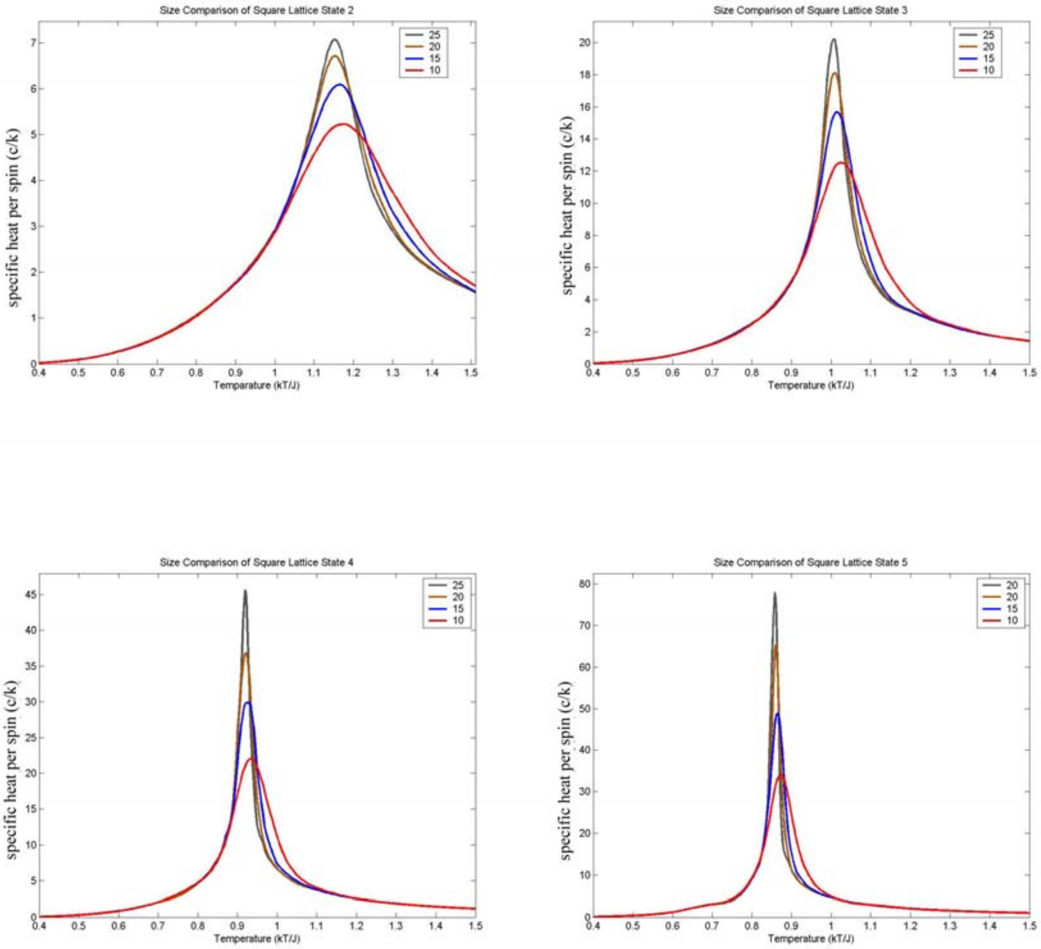


Figure 11 Lattice site comparison of specific heat per spin for square lattice

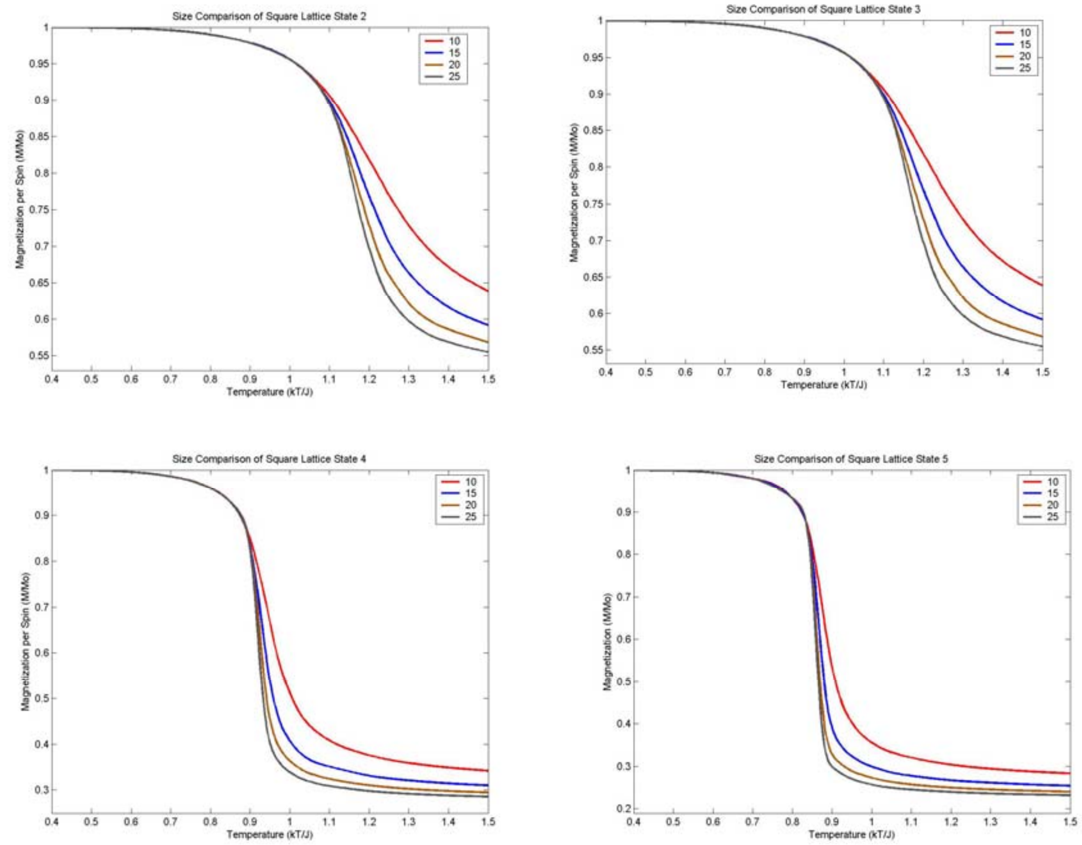


Figure 12 Lattice site comparison of magnetization per spin for square lattice

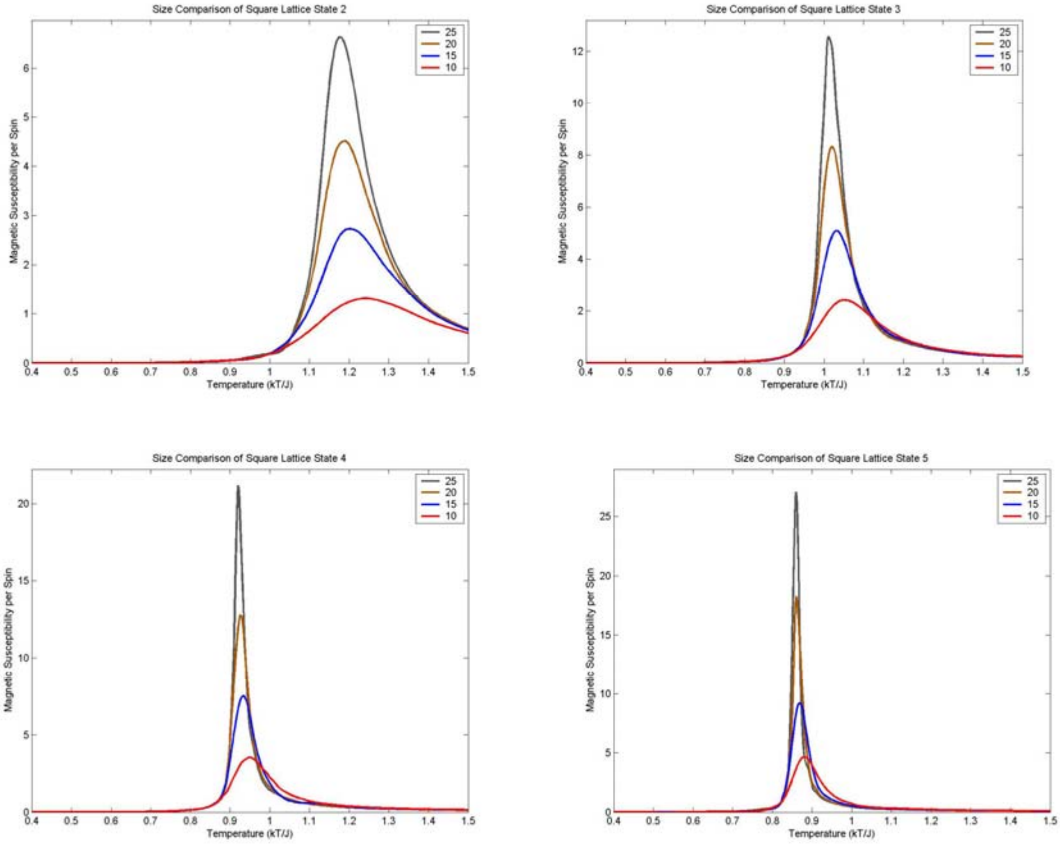


Figure 13 Lattice site comparison of magnetic susceptibility per spin for square lattice

1.2 State Comparison

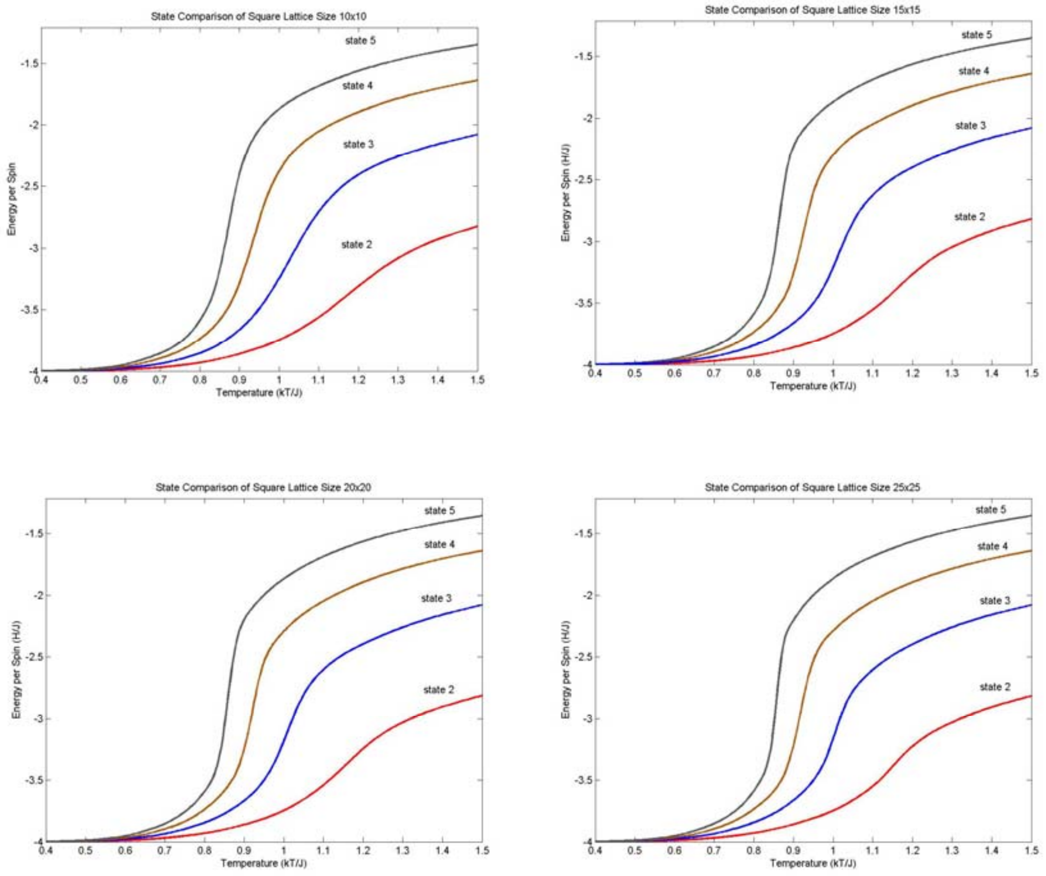


Figure 14 State comparison of energy per spin for square lattice

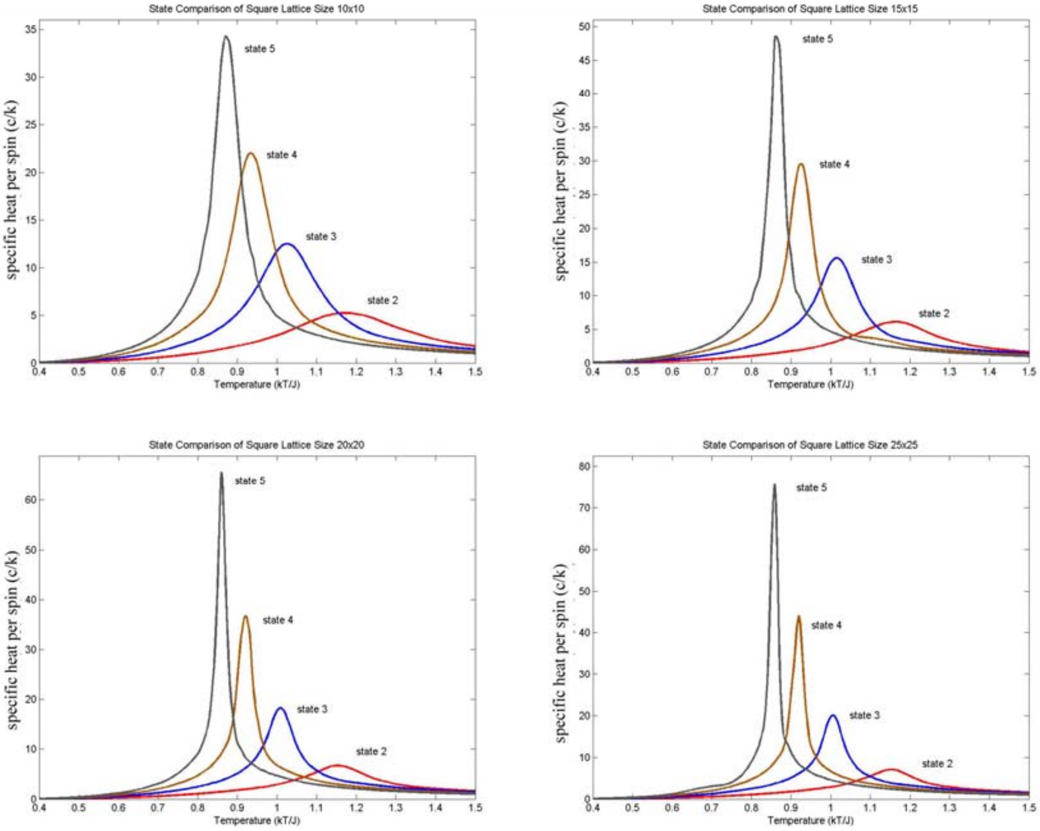


Figure 15 State comparison of heat capacity per spin for square lattice

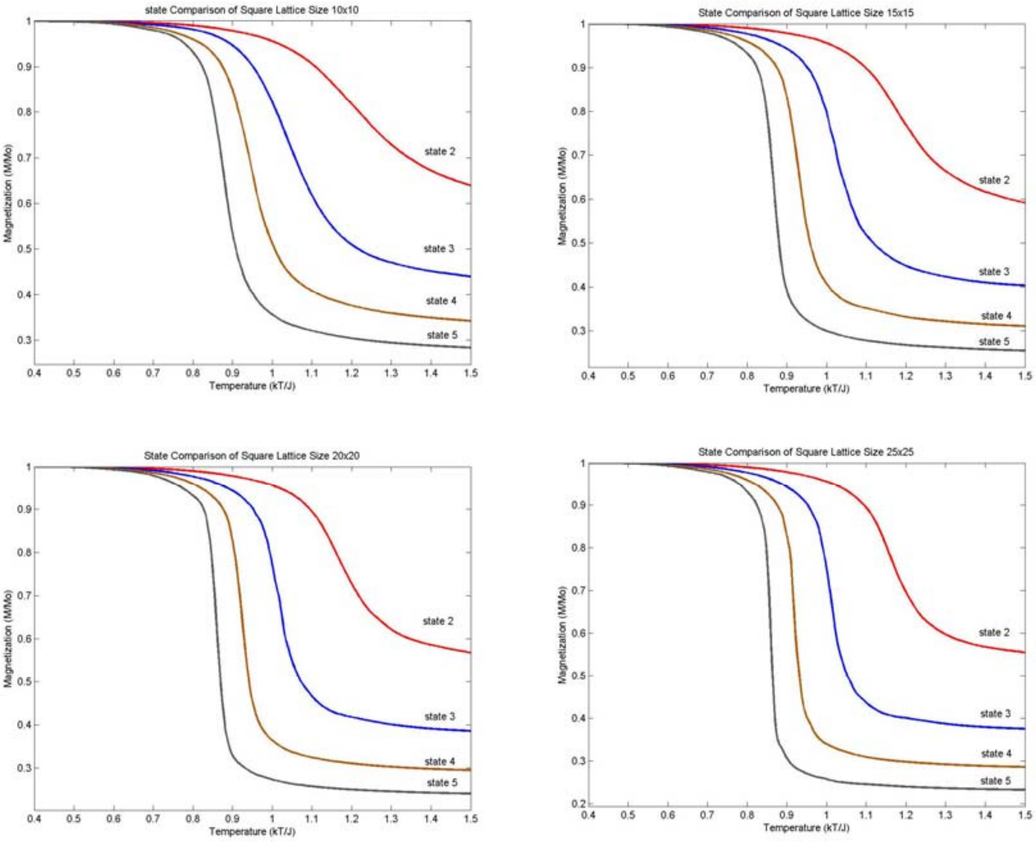


Figure 16 State comparison of magnetization per spin for square lattice

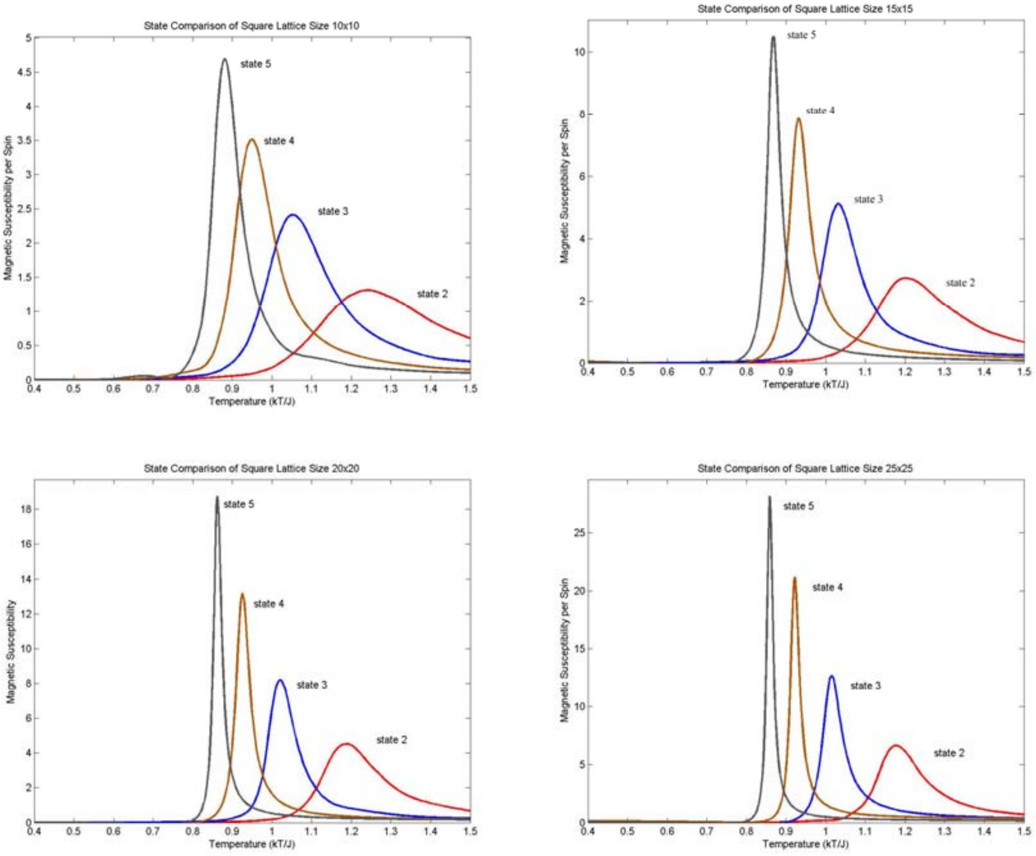
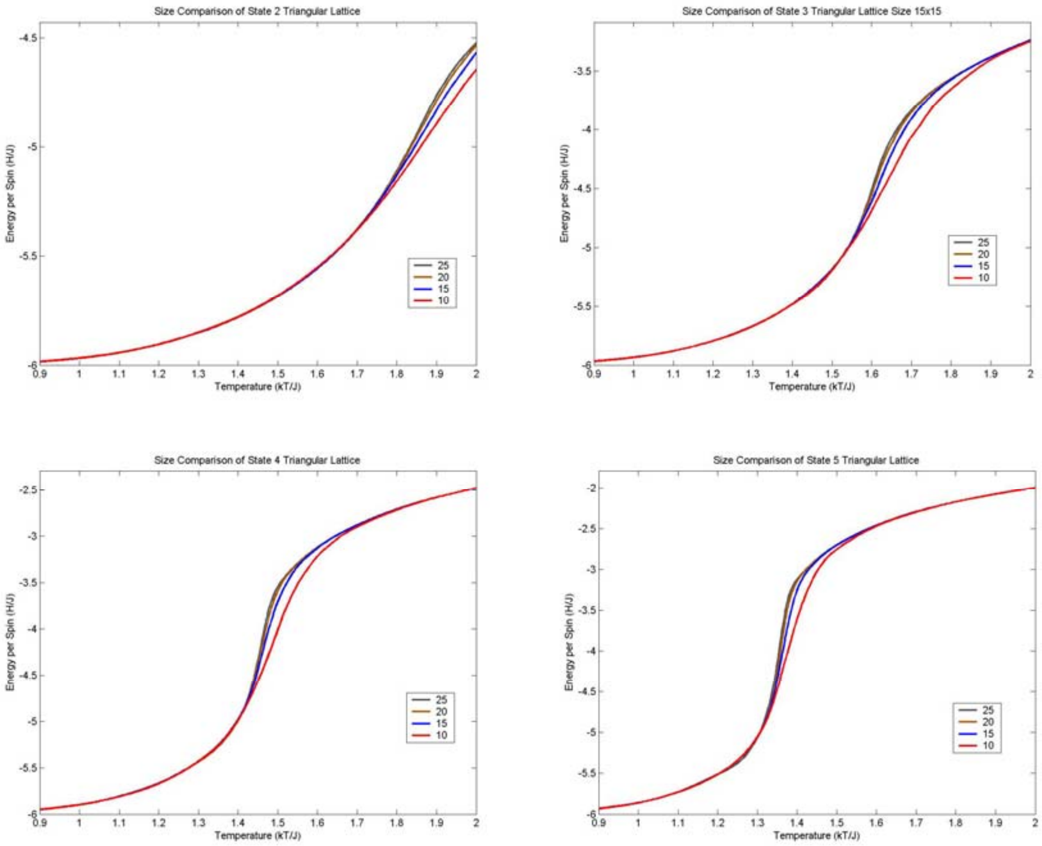


Figure 17 State comparison of magnetic susceptibility per spin for square lattice

2. Triangular Lattice

2.1 Lattice Site Comparison


Size Comparison of State 2 Triangular Lattice

Size Comparison of State 3 Triangular Lattice Size 15x15

Size Comparison of State 4 Triangular Lattice

Size Comparison of State 5 Triangular Lattice

Figure 18 Lattice site comparison of energy per spin for triangular lattice

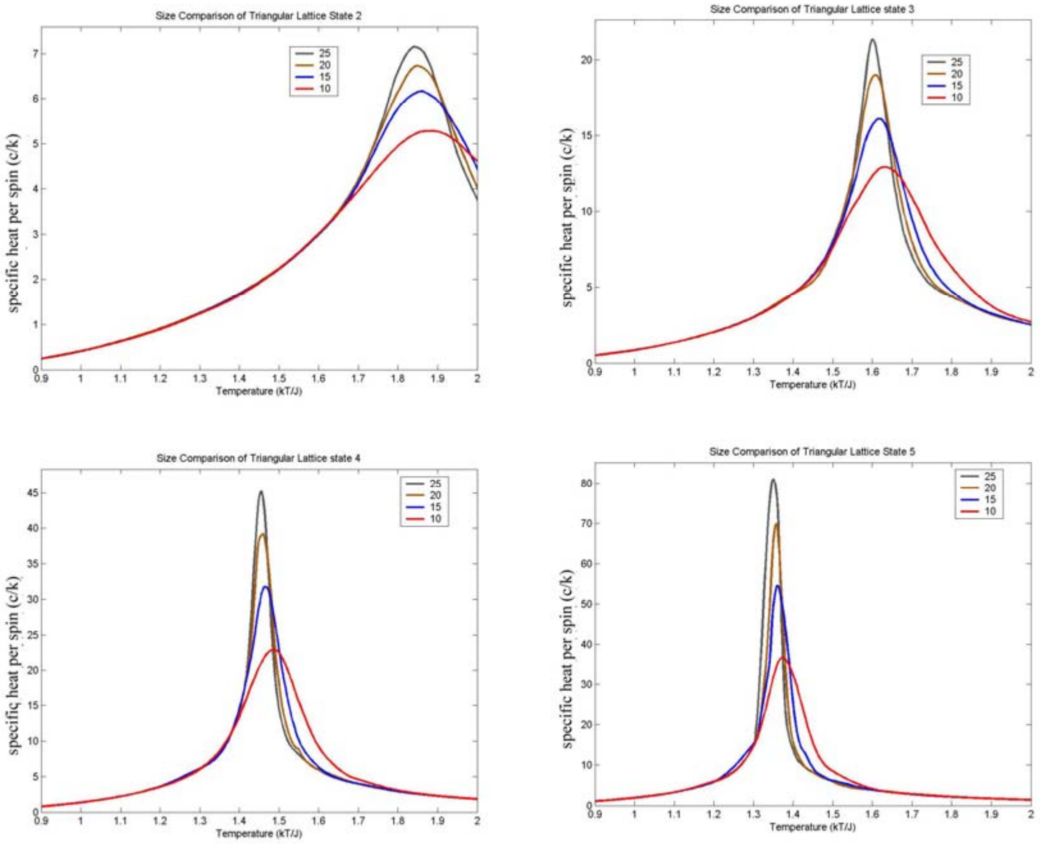


Figure 19 Lattice site comparison of specific heat per spin for triangular lattice

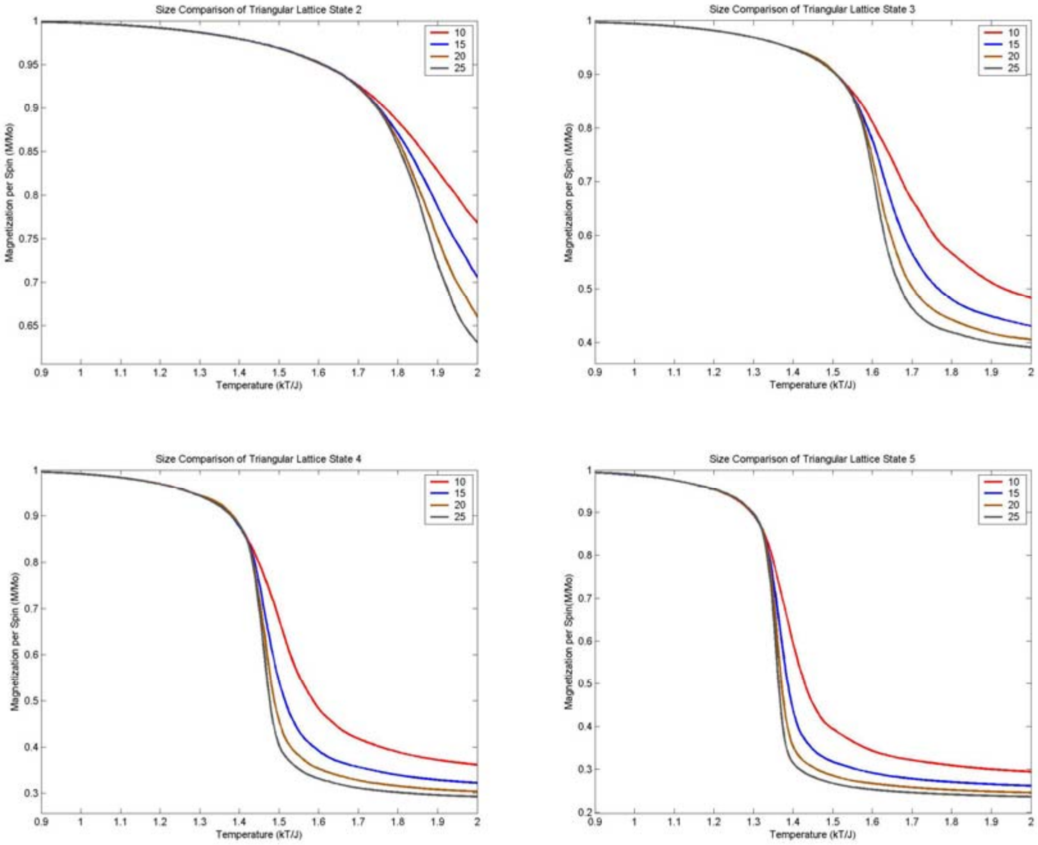


Figure 20 Lattice site comparison of magnetization per spin for triangular lattice

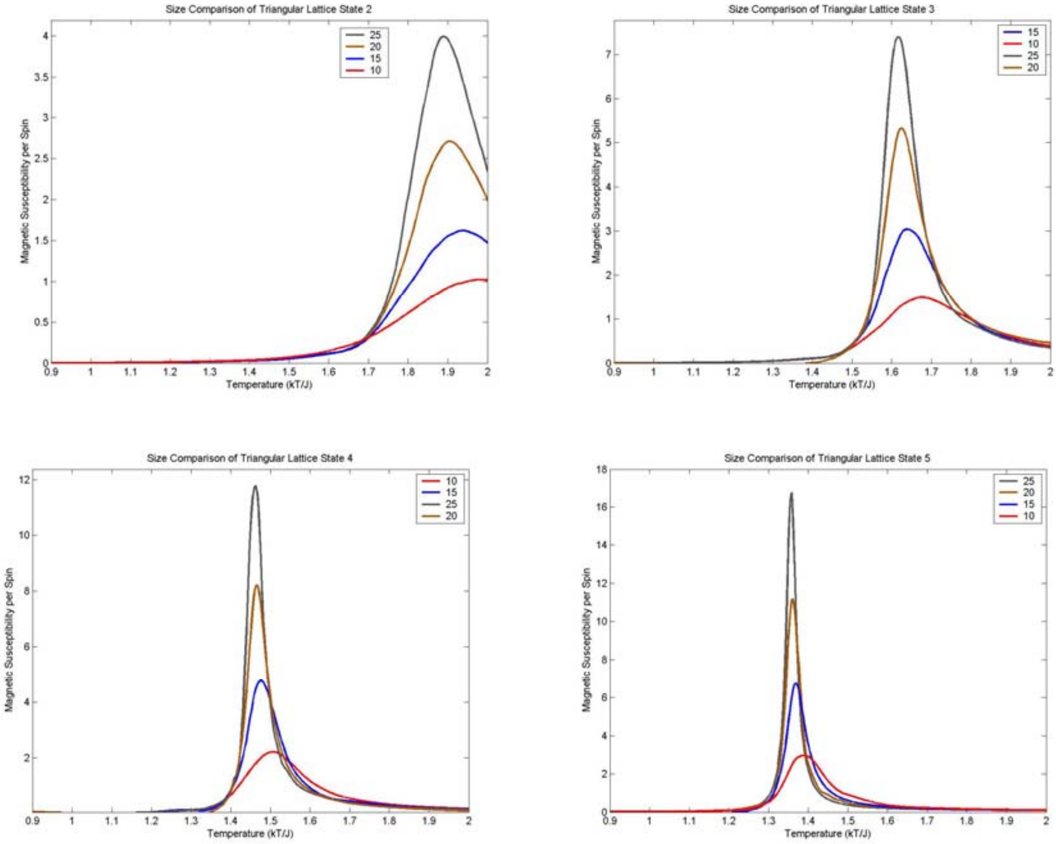


Figure 21 Lattice site comparison of magnetic susceptibility per spin for triangular lattice

2.2 State Comparison

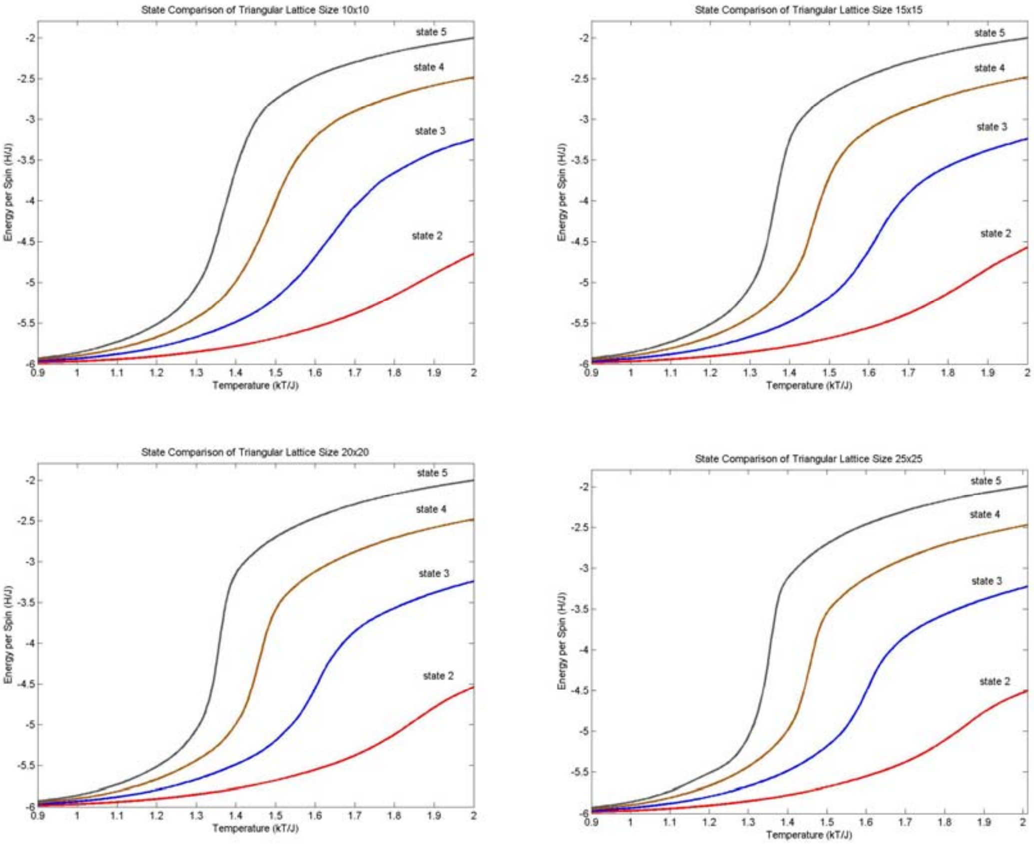


Figure 22 State comparison of energy per spin for triangular lattice

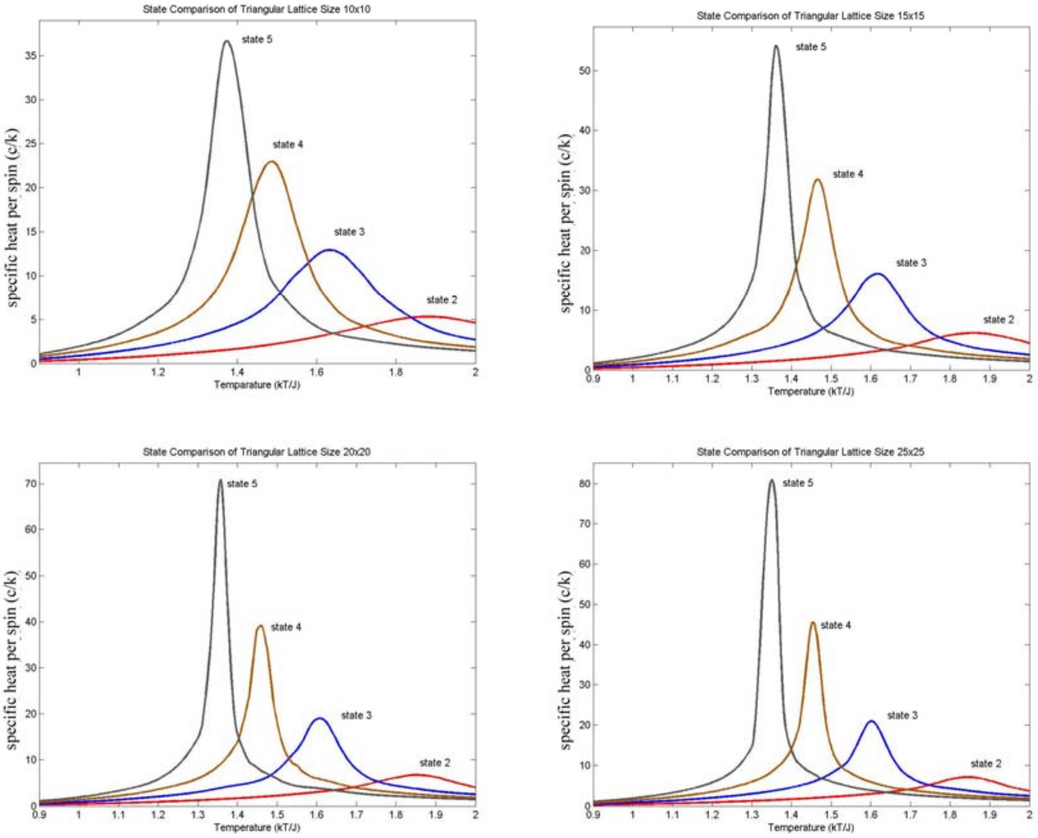


Figure 23 State comparison of specific heat per spin for triangular lattice

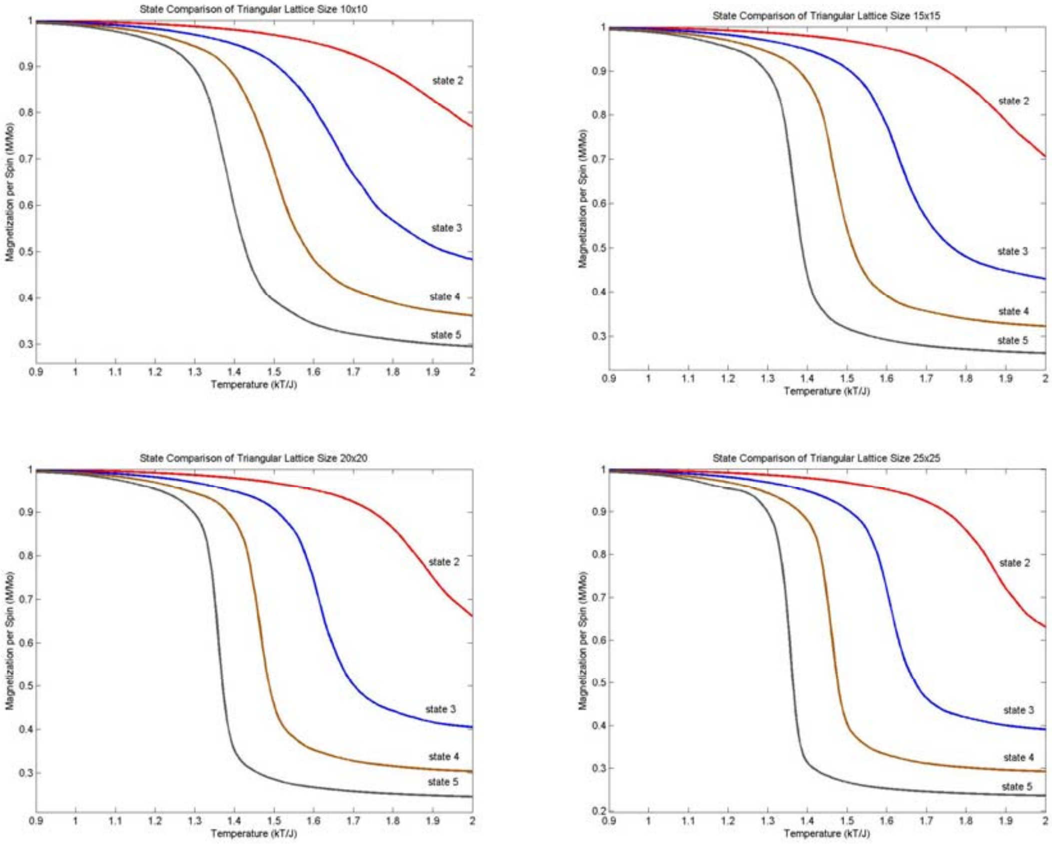
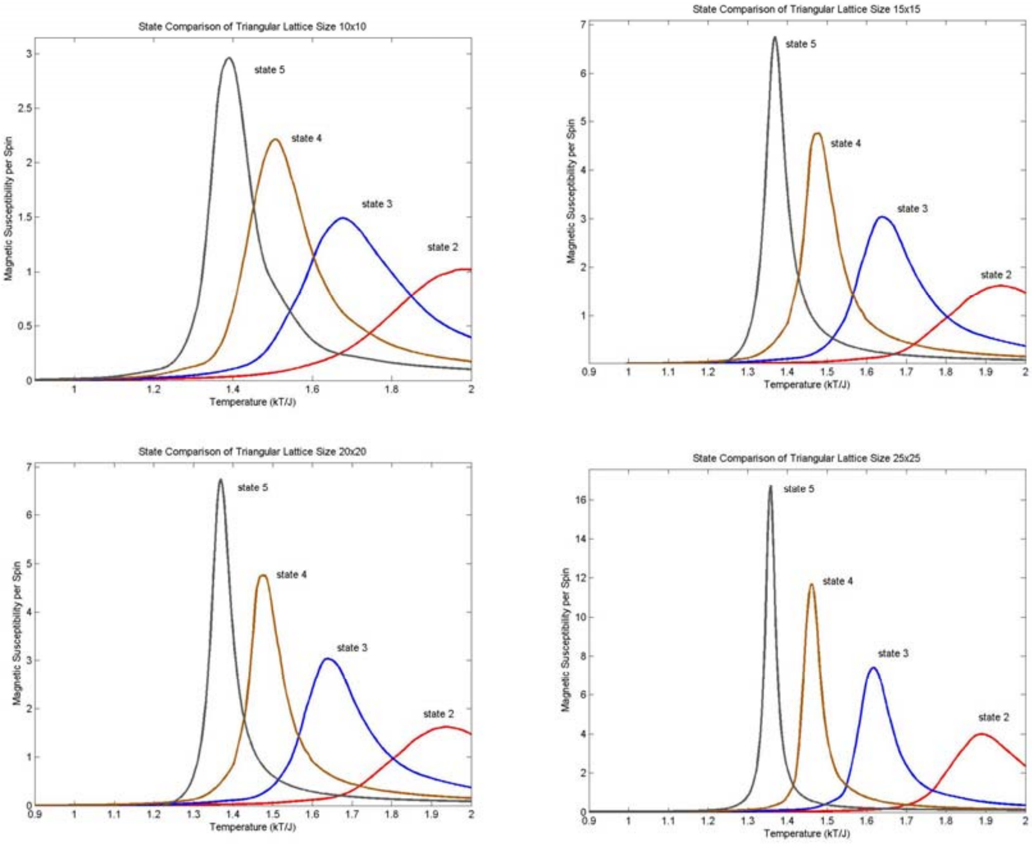


Figure 24 State comparison of magnetization per spin for triangular lattice



State Comparison of Triangular Lattice Size 10x10

State Comparison of Triangular Lattice Size 15x15

State Comparison of Triangular Lattice Size 20x20

State Comparison of Triangular Lattice Size 25x25

Figure 25 State comparison of magnetic susceptibility per spin for triangular lattice

Table 2 Critical Indices of Square Lattice

state	kTc/J	α	β	γ	δ
q = 2	1.15	0.299	0.154	1.55	10.20408
q = 3	1.01	0.472	0.111	1.52	12.82051
q = 4	0.92	0.561	0.19	1.5	6.578947
q = 5	0.85	0.606	0.021	1.23	71.42857

Table 3 Critical Indices of Triangular Lattice

state	kTc/J	α	β	γ	δ
q = 2	1.85	0.299	0.16	1.39	9.615385
q = 3	1.61	0.455	0.15	1.35	9.433962
q = 4	1.46	0.502	0.07	1.35	20.83333
q = 5	1.35	0.664	0.016	1.3	83.33333

Relation between the internal energy per spin and temperature, Figure 9 are the graph show lattice site comparison of square lattice has the same state which give a result that the region where have temperature less than critical temperature the internal energy per spin is will valuable similarly. Then the temperature increase to get close critical point expansion rate goes up of the energy compares with the temperature is increase. Then lattice site increase the expansion rate of internal energy per spin increase too. That causes the slope of the graph increases and lattice site. Consider critical temperature as a result is decreases when the state increases.

Figure 16 shows triangular lattice that have same state and lattice that character graph will tend to is like square lattice but straight differently at critical point of triangular lattice the temperature are more than square lattice.

Figure 13 be the comparison spin state that have the same lattice site of square lattice and figure 20 for triangular lattice. State of spin increase cause internal energy per spin at region of temperature lower critical temperature is valuable similar in every state. When the temperature increases expansion rate of the energy compares with the temperature increase with follow the position that increase. The region where have temperature more than critical temperature when state increase the level of internal energy are follow with state.

Consider relation between specific heat per spin and temperature. Figure 10 for square lattice and Figure 17 for triangular lattice. Consider graphs that same state but different lattice site appears that the region where have temperature less than critical temperature. Specific heat per spin has value similarly. When temperature increase the expansion ratio of specific heat per spin will increase too. At critical temperature, specific heat per spin will maximum. In the region which temperature more than critical temperature specific heat per spin will decrease when the temperature increase. For the state increase expansion ratio of specific heat per spin will increase too.

Figure 14 for square lattice and figure 21 for triangular lattice that relation between specific heat per spin and temperature which same lattice site but different state. When state increase the critical point has decrease temperature and specific heat per spin increase.

Consider relation between magnetization per spin and temperature in figure 11 for square lattice and figure 18 for triangular lattice. The comparison lattice site at same state in region of temperature less than critical temperature magnetization per spin in any size has similarly value. Then temperature increase to critical temperature magnetization per spin will decrease. If lattice site is large change rate of magnetization is be down faster than small lattice site. When temperature increase pass the critical temperature, magnetization per spin will decrease to magnetization per spin divide by spin state.

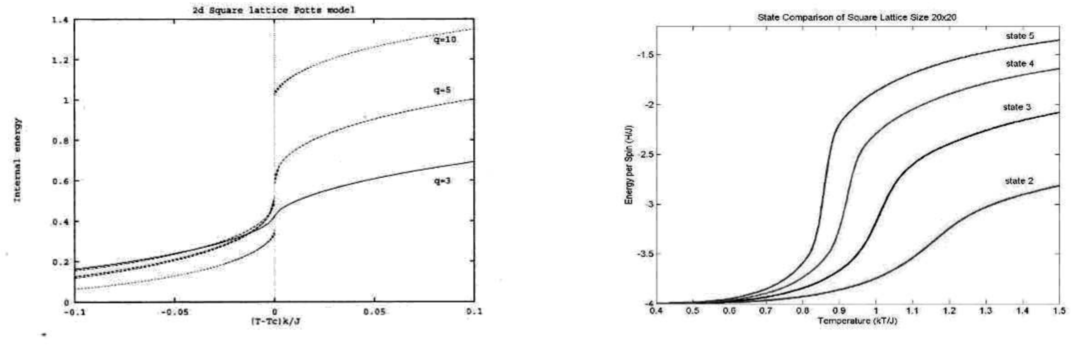
Figure 15 for square lattice and figure 22 for triangular lattice is comparison between states of spin at the same lattice site. When state increase magnetization per spin go down temperature.

Consider magnetic susceptibility per spin and temperature in figure 12 for square lattice and figure 19 for triangular lattice. In region of temperature less than critical temperature magnetic susceptibility has similar. When temperature increases close to critical temperature the change rate of magnetic susceptibility are increase follow increasing lattice site and get maximum value at critical temperature. In region more than critical temperature magnetic susceptibility will decrease with change rate follow increasing lattice site.

Figure 15 for square lattice and figure 22 for triangular lattice is comparison of spin states at same lattice site it show that small state has maximum point less than large state and critical temperature of small state are higher than large state.

Discussion

The average energy per spin of the system varies as the temperature. In the range of the temperature lower than the critical temperature, spins tend to align in the same direction. The spin alignment causes the energy per spin lower according to the equation (32). When temperature increases spins can change direction easily due to the thermal energy. The energy of spin system also increases. At critical temperature, the spin direction and the energy per spin change quickly. When the temperature is above the critical temperature and the spin turns gradually to other direction easily, the energy per spin is higher however the changing rate of the energy per spin will decrease.

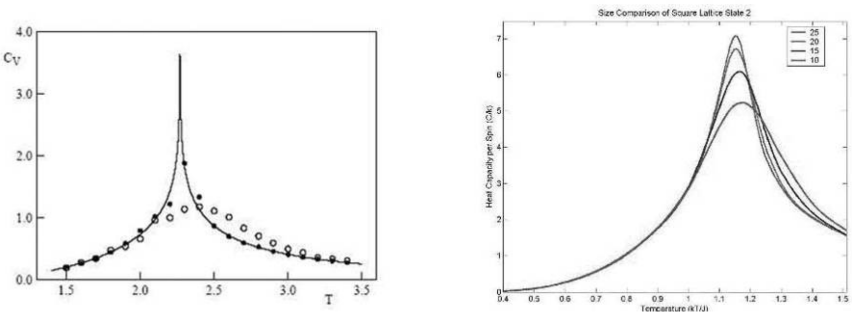


(a) (b)

Figure 26 The comparison square lattice energy per spin with K.M. Briggs' graph in (a) and graph of this thesis in (b).

Graph in Figure 26 of K M Briggs internal energy at q = 3 is lower than spin state q = 5 and q = 10. At critical temperature, the change rate of internal energy q =3 less than q = 10. Graph of K M Briggs shows when spin state increases the change rate of internal energy will increase. At lower spin state, the internal energy is lower too.

Specific heat per spin is the changing rate of energy per spin with respect to the temperature. At low temperature the specific heat per spin is low. At higher temperature the specific heat per spin is higher. At the vicinity of the critical temperature the specific heat per spin increases abruptly. At the far from the critical temperature the specific heat decreases slowly.

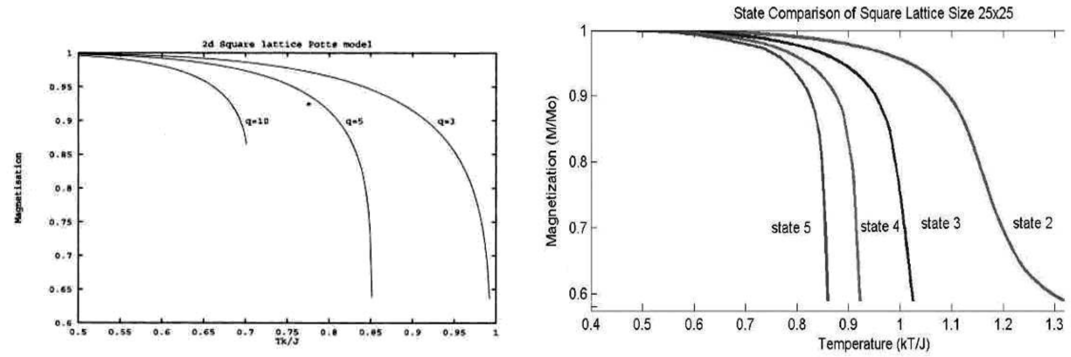


(a) (b)

Figure 27 The compare with Specific heat per spin of ising model for lattice site L = 8 and L = 16 with Harway Gould and Jan Tobochnick's graph in (a) and graph of potts model of this thesis in (b) .

For figure 27 left graph, Specific heat per spin of ising model (Harway Gould and Jan Tobochnick) For lattice site L = 8 and L = 16 show that when lattice site increase specific heat increase too however critical temperature will decrease.

In the range of the temperature lower than the critical temperature, spin tends to align in the same direction. This alignment makes magnetization be high value. When the temperature increases, the spin can change direction and make magnetization decrease and it decreases more quickly at the vicinity of the critical temperature. When the temperature is above the critical temperature, magnetization decreases and it is the lowest at the temperature far from the critical temperature.

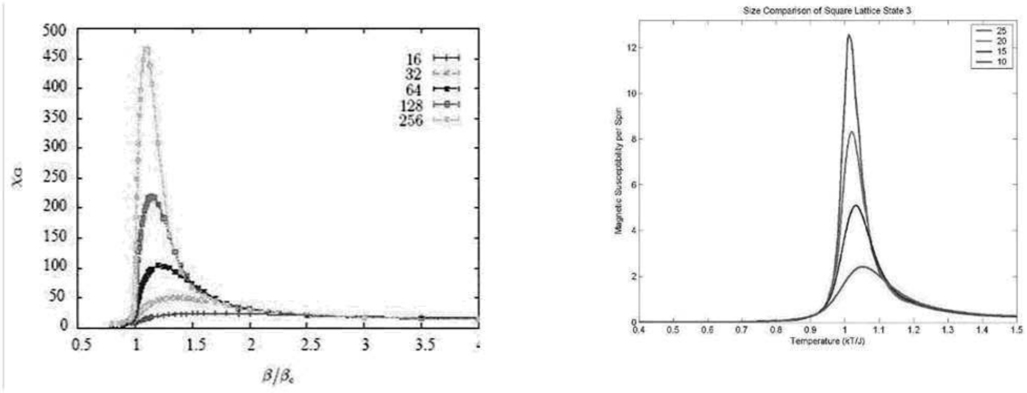


(a) (b)

Figure 28 The comparison square lattice magnetization per spin with K.M. Briggs' graph in (a) and this thesis in (b)

Figure 28 graph of K.M Briggs and his coworker show that critical temperature of spin state q = 3 is higher than q = 5 and critical temperature at spin state q = 5 is higher than q =10. This graph show when the spin state increases the critical temperature will decrease.

Magnetic susceptibility is a change of magnetization with respect to the external magnetic field. At low temperature the magnetic susceptibility is low. At higher temperature the magnetic susceptibility is higher. At the vicinity of the critical temperature the magnetic susceptibility increases abruptly. At the temperature far from the critical temperature the magnetic susceptibility decreases slowly.



(a) (b)

Figure 29 The comparison q = 3 of lattice site 16, 32, 64, 128 and 256 square lattice magnetic susceptibility per spin from dilute model with Katarina uzelac and coworker's graph in (a) and q = 3 potts model in (b)

Figure 29, when lattice site increase magnetic susceptibility at critical temperature will increase however critical temperature will decrease.

For a given lattice site, there are four different spin states. The spin state is labeled by the *q* value of 2, 3, 4 and 5. The Potts spin states give more spin directions than the Ising spin. At spin state of lower *q* value, the critical temperature is higher than the state of higher *q* value because of the spin has less direction.

The critical phenomena occur when the spin system is infinite. The finite system can treated as infinite by using periodic boundary condition. In figure 7, for 5x5 lattice site, the critical temperature is higher than critical temperature of bigger square lattice site.

The same state of spin, the size of lattice is different. Lattice site are 10x10, 15x15, 20x20 and 25x25 respectively. At small lattice site, the critical temperature is high. At larger lattice site, the critical temperature is lower.

The same state of spin and the same lattice site, square lattice has 4 coordination numbers, neighboring spin, and triangular lattice has 6 coordination numbers. The critical temperature of square lattice is lower than triangular lattice because of the coordination number complicate to change spin direction.

table 4 critical indices from other people

State	Owner	method	α	β	γ	δ
q = 2	F.Y.Wu		0	0.125	1.75	15
	thesis	metropolis	0.299	0.154	1.55	10.20408
		metropolis	0.299	0.16	1.39	9.615385
q = 3	F.Y.Wu		0.333333	0.111111	1.444444	14
	Zwansig and Rawshaw	series expansion	0.296		1.42	
	Burkhardt	Kadanoff Variation RG	0.3365	0.1061	1.451	14.68
	H J Herman	(cubic 45x45x45)	0.52			
	thesis	metropolis	0.472	0.111	1.52	12.82051
		metropolis	0.455	0.15	1.35	9.433962
q = 4	F.Y.Wu		0.666667	0.083333	1.166667	15
	Dasgupta	Kadanoff Variation RG	0.488	0.091	1.33	15.53
	Hu	Duality Invariant	0.487			
	thesis	metropolis	0.561	0.19	1.5	6.578947
		metropolis	0.502	0.07	1.35	20.83333

From above table show critical indict from other people by analytical and other method compare with this thesis

CONCLUSION

Potts model is the model to explain the magnetic behavior of the substance. When the temperature is lower than the critical temperature, the spin direction tends to align that is the property of ferromagnetism. It makes energy minimum and magnetization maximum. This gives the spontaneous magnetization.

When temperature increases, below critical temperature, internal energy per spin will increase rapidly that causes specific heat per spin increase too. Then spin arrangement begins to turn away from alignment resulting in lower magnetization. Magnetization per spin will decrease and magnetic susceptibility per spin will increase.

At the critical temperature, the change of internal energy per spin will make specific heat per spin reach the maximum and there exists phase transition from ferromagnetism to paramagnetism. The spin direction will be random. The magnetization will decrease rapidly.

At the temperature higher than the critical temperature, the internal energy per spin is high and the small change rate causes lower specific heat per spin. The randomization of spin will give minimum magnetization per spin.

LITERATURE CITED

Akira, O. 2002. **Phase Transition Dynamics.** Cambridge University Press, New York.

Briggs, K.M., I.G. Enting and A.J. Guttmann. 1994. Series Study of the Potts Model:Bulk Series for the Square Lattice. **J. Phys. A.** 27: 1503-1504.

Droz, M., A.L. Ferreira and A. Lipowski. 2003. Splitting the Vector Potts Model Critical Point. **Phys. Rev. E.** 67: 056108.

Foster, D.P. and C. Gerrard. 2002. The Ferro/Antiferromagnetic q-State Potts Model. **J. Phys. A.** 35: 75-80.

Gould, H. and J. Tobochnick. 2003. **Thermal and Statistical Physics.** Kalama zoo College, Michigan.

Griener, W., L. Neise and H. Stocker. 1994. **Thermodynamics and Statistical Mechanics.** Columbia University, New York.

Herrmam, H.J. 1979. Monte Carlo Simulation of the Three dimention Potts Model. **Z. physik B.** 35: 171-175.

Kaufmann, E.T. 2003. **Characterization of Materials.** N.J. John Wiley & Son,inc, United State.

Kleman, M. and O.D. Lavrentovich. 2003. **Soft Matter Physics : An Introduction.** New York Springer Verlag New York, New York.

Leff, H.S. and A.F. Rex. 2003. **Maxwell Demon 2:Entropy, Classical and Quantum information, Computing.** Bristol institute of physics publishing, Philadenphia.

Meyer, P. 2000. **Computational Studies of Phase and Dilute Spin Model.** M.S. thesis, University of Derby.

Newmamm, M.E.J. and G.T. Barkema. 1999. **Monte Carlo Methods in Statistical Physics.** Oxford University Press, New York.

Park, H. 1994. Three State Potts Model on a Triangular Lattice. **Phys. Rev. B.** 1994 (49): 881-887.

Uzelac, K. and his coworker. 1999. Second-Order Phase Transition Induced by The Quencehd Random Dilution in 3D. **Fizika. A.** 4: 369-382.

Velytsky, A. 2004. **A Model study of the Deconfining Phase Transition.** Florida State University, United State.

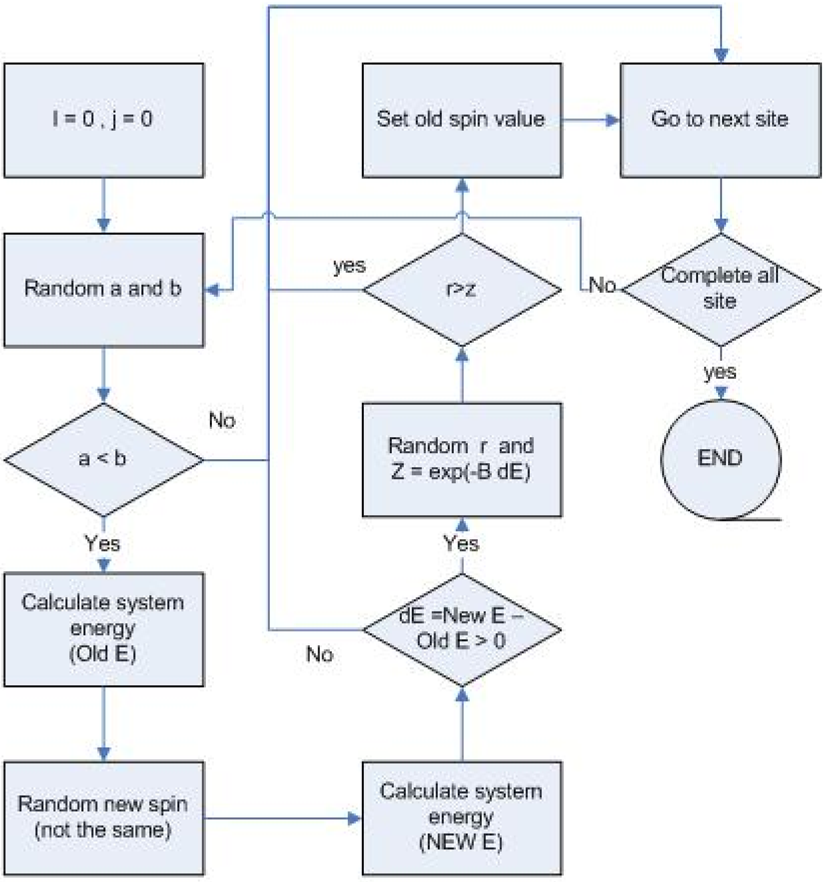
Wu, F.Y. 1982. The Potts Model. **Rev. Mod. Phys.** 54: 235-268.

Yamakuchi, C. 2003. **Application of Monte Carlo Methods to Calculate the Density of States for Classical Spin System.** M.S. thesis, Tokyo Metropolis University.

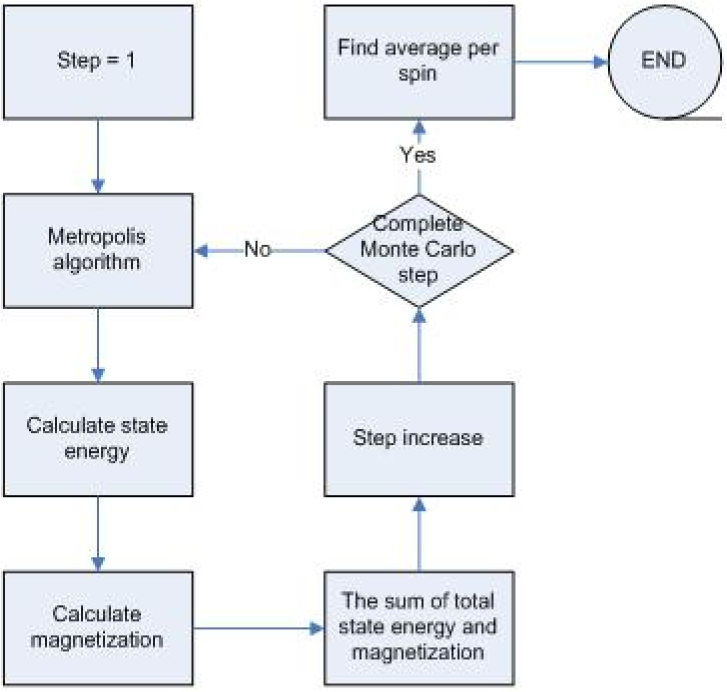
Yeomans, J.M. 1992. **Statitistical Mechanics of Phase Transitions.** Oxford University Press, New York.

Appendix

Metropolis Algorithm for each Monte Carlo Step



Data Collection



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