

Phase Transition & Approximate Partition Function In Ising Model and Percolation In Two Dimension: Specifically For Square Lattices

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Abstract: We study the percolation behavior of in two dimensional Ising model with spontaneous magnetization for pure and diluted lattices containing spins. Expression for partition function is calculated for pure lattice and is applied to find out the same for diluted lattices. Specific example is taken for nearest neighbor interaction in two dimensional square lattices and validity range of the calculation is checked. Behavior of partition function is studied at different temperatures and at different number of spins.

Keywords: Ising model, Percolation, Partition function, Diluted Ising Model, Critical Temperature

I. Introduction

Percolation phenomenon explains the connectedness and phase transition behavior of a physical system [1]. In a site percolation problem, sites of an empty system are occupied randomly and uniformly with occupation probability p . When this occupation probability becomes greater than a threshold value, known as percolation threshold, probability of percolation increase rapidly until it reaches $p=1$. Site percolation threshold p_t is measured to be $p_t = 0.5926$ [1 & 2]. Below percolation threshold isolated microscopic clusters exist. As occupation probability is increased these microscopic clusters merge together and grow in size. Above percolation threshold macroscopic clusters are formed that span the system. Thus a phase transition in terms of connectedness occurs. A similar type of phase transition in magnetization state of a spin system is seen in the Ising model, where temperature plays the role of occupation probability. The situation becomes broader when site dilution is also incorporated. Here site occupation probability and temperature both play their role in phase transition property of the system.

In this present work I have studied the phase transition behavior of two dimensional (2D) spin systems with and without dilution. I have tried to find an explanation for finite size effect in pure case by finding out individual probability for different number of spin flips using partition function obtained using Maxwell Boltzmann statistics. I have extended this calculation for partition function to diluted case also.

II. Phase Transition In Undiluted 2D Lattice

In absence of external field the Hamiltonian of a spin- system can be written as:

$$H = \sum_{\substack{i,j \\ i \neq j}}^N J_{ij} \sigma_i \sigma_j$$

Here J_{ij} represents the interaction strength acting between spins σ_i and σ_j , where N is total no. of spins [3].

We consider a 2D square lattice of spins at absolute zero. Now the temperature (T) is gradually increased from absolute zero and at some value of T , the magnetization changes its state from high value to a low value i.e. phase transition occurs (See figure. 1). Ideally, below critical temperature T_c magnetization (M) is ± 1 , and above T_c it is 0. We assume that out of two kind of spins (1 or -1), the one which is majority, is occupied site. Hence at $T < T_c$, $p=1$; and at $T > T_c$, $p=0.5$. So at T_c , p lies between 1 and 0.5. If we assume that T_c and p_c occurs simultaneously then at $p = p_c = 0.5926$, the value of T gives critical temperature. Near critical temperature magnetization is poorly defined, so as the occupation probability. So I have performed a number of Monte Carlo simulations [4] for 100x100 & 128x128 lattices and plotted average occupation probability vs. Temperature (Figure. 1 & 2). This graphical results show $T_c = 2.3712$ & 2.3478 for 100x100 & 128x128 lattices respectively, which are close to theoretical value 2.2603, given by Onsager. This small departure ($\delta T=0.1097, 0.0895$) in agreement between theoretical and graphical value is arising due to the following facts:

- Percolation threshold for finite lattices cannot be exactly found at the theoretical value. This is known as finite size effect.
- Critical temperature in Ising model also shows finite size effect.
- Magnetic percolation occurs earlier to site percolation in a finite sized lattice.

The third point in the above facts may be a good reason for this discrepancy. We cannot eliminate problems due to finite size effect completely, because in computer simulation we work with finite lattices. So better idea is to calibrate lattice size vs. critical temperature. I have done simulations with various lattice sizes (See figure. 3). Here we see that critical temperature curve corresponding to site percolation (Figure3: red curve) falls at a greater rate than the magnetic percolation curve (Figure3: green curve). Here I have assumed magnetic percolation to occur at $M=0.6$ i.e. $p=.8$. Although it could have been taken at any value between $p=0.5926$ to $p=1$, provided corresponding magnetization lies in the critical temperature line. Green curve in figure.3 gives a better approximation of critical temperature from theoretical view point, at $T= 2.2618$ for 128×128 lattice. Since $M-T$ curve for finite lattices is a distorted step like function, Binder gave an intellectual way to find critical temperature by calculating standard deviation in fourth power of magnetization vs. temperature at different lattice sizes and their intersection is the critical temperature [5].

2.1 Partition function in 2D Ising model:

From the theory of Maxwell- Boltzmann statistics (MBS), we know that general form of partition function (PF) can be written as,

$$Z = \sum_{\text{all states } i} g(i) \exp[-E(i)/kT] \quad \text{---- (2.1.1)}$$

Calculation of PF in Ising model (IM) is very tedious job because in this case one has to deal with 2^N possible states. Also, at a very large number of spins, degeneracy of every energy state increases very rapidly with total number of spins. Let us take an example of 2×2 lattices. Considering periodic boundary condition and nearest neighbor interaction (NNI) of ferromagnetic (FM) type, individual states with multiplicity are shown in Table 1. Hence the explicit expression of PF becomes,

$$Z(2 \times 2) = 2 \exp(16/kT) + 2 \exp(-16/kT) + 12 \exp(0)$$

Therefore,

$$Z(2 \times 2) = 2 \exp(16/kT) + 2 \exp(-16/kT) + 12 \quad \text{---- (2.1.2)}$$

Here we see 3 terms in the expression of PF containing all 16 ($2+2+12= 2^4$) states. Equation 2.1.2 can be simplified as,

$$Z(2 \times 2) = 4 \cosh(16/kT) + 12$$

Explicit expressions for PF even for 3×3 lattices becomes time consuming because it involves consideration of 2^9 states so I have not included these results [6].

In the following subsection I have calculated PF for square lattice using some assumption and checked its applicability range.

2.1.1 PF in IM:

I assume that the energy of a system containing N spins where i spins are flipped is $E(i)$ and it is non degenerate i.e. energy of the configuration is dependent on the number of up spins and downspins only.

Hence PF can be computed in the following way by allocating spins on lattice. Consider at any stage the no. of up spins is ‘ i ’ and rest is down spins. Now the no. of ways in which ‘ i ’ spins can be allocated in a lattice containing N spins, can be written as follows:

$$G(i) = \frac{N!}{i!(N-i)!} \quad \text{--- (2.1.1.1)}$$

Hence the PF is,

$$Z = \sum_{i=0}^N G(i) e^{-\frac{E(i)}{kT}} \quad \text{----- (2.1.1.2)}$$

Where k = Boltzmann constant, $E(i)$ = Energy of the system of N spins with ‘ i ’ spins flipped i.e. i spins of one kind and rest of other kind.

2.1.2 PF for Square lattice with NNI:

Partition function for square lattice can be found using equation -2.2.1, by replacing $E(i)$ with energy of the system with i spins flipped considering ferromagnetic n-n interaction. Incorporating periodic boundary condition the ground state energy at $T=0$, is $E(0)= -4NJ$.

Energy of the system with i spins flipped is $E(i)=-4NJ+8Ji$, here I have assumed that the system evolves in such a manner that isolated spins are flipped and no cluster forms.

Substituting this in equation -2.1.1.2 we get,

$$\begin{aligned} Z &= \sum_{i=0}^N G(i) e^{-\frac{(-4NJ + 8Ji)}{kT}} \quad \text{--- (2.2.2)} \\ &= e^{\frac{4NJ}{kT}} \sum_{i=0}^N G(i) e^{-\frac{8Ji}{kT}} \end{aligned}$$

Now the probability of the situation where ‘ i ’ spins are found in flipped condition is,

$$p_l = \frac{1}{Z} e^{\frac{4NJ}{kT}} G(l) e^{-\frac{8Jl}{kT}} \quad \text{---(2.2.3)}$$

We see that p_l is a function of N & T both. Condition for extremum for p_l can be written as follows,

$$\frac{dp_l}{dx} = 0 \quad \text{---(2.2.4)}$$

Where x is either N or T.

Writing p_l in explicit form and simplifying we get,

$$p_l = \frac{1}{\sum_{i=0}^N \frac{(N-i)!}{(N-i)!} e^{\frac{8J(l-i)}{kT}}} \quad \text{---(2.2.5)}$$

Total probability

$$p = \sum_{l=0}^N p_l = 1$$

Putting equation -2.2.5 on 2.2.4 and simplifying for x=T, we obtain,

$$\sum_{i=0}^N \frac{(l-i)}{(N-i)!} e^{\frac{8J(l-i)}{kT}} = 0 \quad \text{---(2.2.6)}$$

Equation -2.2.6 is very tedious to solve for T. Instead of solving this equation I have plotted p_l for several l and N vs. T (See figure. 4). This way we can discuss certain properties of p_l as a function of T & l & N. p_l contains terms that are factorials of N, large exponential terms which limit our computer simulation up to N=16 only. For numerical simplification I put (8J/kT) as (1/T). From figures 4 & 5 we see that greater the total no. of spins p_l decreases for any l, more rapidly with increasing temperature. This explains finite size effect. As N increases the system get more and more scheme of spin flips keeping total probability equal to 1 and therefore individual probability of every possible no. of spin flips decreases, so during phase transition magnetization changes its state more discretely and phase transition becomes steeper. Figure 6, shows p_l vs l for N=4, and l=0(black curve), l=1(red curve), l=2(green), l=3(blue), l=4(purple).

The probability of all spin in same state is unity at T=0 and falls very quickly as T departs from absolute zero. Single spin flipping probability has a prominent maxima at T=0.9. Double, triple and four spin flip has no definite maxima. At T close to zero p_l increases as l decreases; on the other hand at large T, p_l increases as l increases. Any line parallel to p_l axis, intersect p_l vs l curves. Summation of the value of p_l at those intersections gives total probability and is equal to 1.

Using equation 2.2.6, I shall find out the maxima of p_l for N=4 at l=1. After few steps of simplification we get,

$$e^{4/T} - 6e^{2/T} - 8e^{1/T} - 3 = 0$$

Or,

$$\left(e^{\frac{1}{T}} + 1\right)^3 \left(e^{\frac{1}{T}} - 3\right) = 0$$

Hence, $e^{1/T} = -1, 3$; Relevant choice is $e^{1/T} = 3$; from this we get the temperature at which single flip probability is extremum, as $T = 1/\ln 3 = 0.91$. This is a maximum as we can see the red curve in figure 6.

2.1.2.1 Calculation of thermodynamic quantities using PF in 2D IM with NNI of FM type:

Using equation 2.1.1.1 we can write the expression for thermodynamic probability as follows

$$W = \sum_{i=0}^N \frac{N!}{i!(N-i)!} \quad \text{---(2.1.2.1.1)}$$

Hence, expression for entropy(S) becomes,

$$S = k \ln W$$

Therefore,

$$S = k \ln N! + k \ln \left(\sum_{i=0}^N \frac{1}{i!(N-i)!} \right) \quad \text{---(2.1.2.1.2)}$$

Now from equation 2.2.2 we get,

$$k \ln Z = k \ln N! + k \ln \left(\sum_{i=0}^N \frac{e^{-\frac{(-4NJ+8Ji)}{kT}}}{i!(N-i)!} \right)$$

So,

$$k \ln Z = k \ln N! + \frac{4NJ}{T} + k \ln \left(\sum_{i=0}^N \frac{e^{-\frac{8Ji}{kT}}}{i!(N-i)!} \right) \quad \text{---(2.1.2.1.3)}$$

Using equations 2.1.2.1.2 & 2.1.2.1.3 we get,

$$S = k \ln Z - \frac{4NJ}{T} + k \ln \left(\sum_{i=0}^N \frac{1}{i!(N-i)!} \right) - k \ln \left(\sum_{i=0}^N \frac{e^{-\frac{8Ji}{kT}}}{i!(N-i)!} \right) \quad \text{---(2.1.2.1.4)}$$

This is the general expression for entropy.

Equation 2.1.2.1.4 is difficult to handle. Let us see the form of S in low T and high T limit.

In low T limit, fourth term in R.H.S. of equation 2.1.2.1.4 can be expanded as,

$$k \ln \left(\sum_{i=0}^N \frac{e^{-\frac{8Ji}{kT}}}{i!(N-i)!} \right) = \frac{k}{N!} + k \ln \left(\sum_{i=1}^N \frac{e^{-\frac{8Ji}{kT}}}{i!(N-i)!} \right)$$

Now 2nd term in R.H.S. of above equation decays as $e^{-\frac{8Ji}{kT}}$ with i, so at $T \rightarrow 0$, we can neglect them.

After some simplification, in low T limit entropy can be written as,

$$S = k \ln Z - \frac{4NJ}{T} + k \ln \left(\sum_{i=1}^N \frac{1}{i!(N-i)!} \right) \quad \text{---(2.1.2.1.5)}$$

Now, in high T limit $e^{-\frac{8Ji}{kT}} \rightarrow e^{-0} = 1$; so we get from equation 2.1.2.1.4,

$$S = k \ln Z - \frac{4NJ}{T} \quad \text{---(2.1.2.1.6)}$$

Internal energy (U) can be found out in the following way,

$$\begin{aligned} U &= \frac{1}{Z} \sum_{i=0}^N G(i) E(i) e^{-\frac{E(i)}{kT}} \\ &= \frac{1}{Z} \sum_{i=0}^N \frac{N!}{i!(N-i)!} (-4NJ + 8Ji) e^{-\frac{(-4NJ+8Ji)}{kT}} \end{aligned}$$

Hence,

$$U = -4NJ + 8J \frac{\sum_{i=1}^N \frac{N!}{(i-1)!(N-i)!} e^{-\frac{8Ji}{kT}}}{1 + \sum_{i=1}^N \frac{N!}{i!(N-i)!} e^{-\frac{8Ji}{kT}}} \quad \text{---(2.1.2.1.7)}$$

On a similar way expression for absolute magnetic moment (M) can be found as,

$$M = N - 2 \frac{\sum_{i=1}^N \frac{N!}{(i-1)!(N-i)!} e^{-\frac{8Ji}{kT}}}{1 + \sum_{i=1}^N \frac{N!}{i!(N-i)!} e^{-\frac{8Ji}{kT}}} \quad \text{---(2.1.2.1.8)}$$

Using equations 2.1.2.1.4 & 2.1.2.1.7 expression for Helmholtz free energy (F) can be found as,

$$F = U - TS$$

From equations 2.1.2.1.7 & 2.1.2.1.8 we get,

$$U/M = -4J \quad \text{---(2.1.2.1.9)}$$

2.1.2.1.1 Applicability range of PF calculated in 2.1.2.:

Present calculation of PF includes specific configurations only. So I need to check for the accuracy of this calculation and its applicability range. From the size of equations in previous subsection we see that the best way to check validity of our theory is to check the validity of equation 2.1.2.1.9 as a first attempt. In figure 10, I have plotted U/M vs T for square lattices considering $J=k=1$, at $N=25 \times 25$, 100×100 and 200×200 .

Here we see that equation 2.1.2.1.9 is well obeyed in the range $0 \leq T \leq 2.26$, by all three curves. Above $T=T_0=2.26$ all three curves depart from obeying equation 2.1.2.1.9. We see that above T_0 , U/M falls at greater rate as N is increased. This is because finite size effect is reduced as N increases. Comparing the theoretical value of critical temperature we may conclude that $T_0 = T_c = 2.2603$. So a better way to find critical temperature is found. We see our theory works in the FM phase and works until critical temperature is reached. So critical temperature is the highest temperature at which our theory remains valid.

Now I explain why our theory fails above T_c . as T_c is reached no isolated minority spins exist. Minority spins starts forming clusters and majority clusters break apart. Due to this energy of the configuration does not follow the equation, $E(i) = -4NJ + 8Ji$. Actual energy $< E(i)$. Because at this stage only the boundary spins of cluster play the role in increasing energy. So U/M becomes less than $-4J$. During phase transition as we move up from T_c , initially average cluster size of minority spins increase and the same for majority spins decrease until identification of majority and minority is possible. Thereafter cluster size of both spins reduce with increase in temperature and in $T \rightarrow \infty$ limit a configuration with isolated spins in anti FM alignment and total magnetic moment equal to zero is obtained. We can see the recovering nature of U/M in green curve for $N=200 \times 200$ as T departs far from T_c , in figure 10. So the range of validity of our theory lies in the range of temperature $T < T_c$ & $T \rightarrow \infty$.

III. Percolation And Phase Transition In Diluted Lattice

When a lattice is occupied with uniform random probability, greater than percolation threshold then at least one spanning cluster exists and rest of the clusters are small in size, isolated. This spanning cluster produces significant contribution to magnetization and other properties of the whole lattice. Magnetization can be low or high depending on the number of spanning cluster and their additive contribution. At high value of occupancy when only one percolation cluster exists contribution to magnetization is solely given by this cluster. Let us represent this mathematically,

Assume,

Magnetization of lattice = M_L

Magnetization of j'th spanning cluster = $M_s(j)$

Magnetization of k'th isolated nonspanning cluster = $M_i(k)$.

Hence, average magnetization of lattice,

$$\langle M_L \rangle = \langle \sum_j M_s(j) + \sum_k M_i(k) \rangle \quad \text{---(3.1)}$$

For large lattices, each isolated nonspanning cluster can be either positive or negative magnetization state with equal probability. So on averaging their contribution becomes negligible.

Hence we get from equation 3.1,

$$\langle M_L \rangle = \langle \sum_j M_s(j) \rangle$$

We cannot apply similar argument as we applied in nonspanning cluster to neglect their contribution. Because however large, the lattice is, the no. of spanning cluster is not very large in number. Some of those clusters may cancel each other but some of them add together. So net magnetization reduces but in most cases remains nonzero. For square lattice considering n-n interaction if the probability of occupancy is greater than $(1-1/\sqrt{N})$, then it is for sure that more than one cluster cannot exist because at this stage one row is not unoccupied, creating separated cluster. So there is no opportunity to get low value of magnetization below critical temperature. There is one more way to get macroscopic magnetization always, by biasing occupied sites for one of the spins either up or down. The amount of biasing depends on the occupation probability. Assuming occupation probability for say, up spins in the occupied islands to be p_u and probability of occupation for occupied sites as p_s , I have plotted p_u vs p_s in 100x100 lattice for which ferromagnetic phase does not show any low value in magnetization (See figure 8). Using straight line approximation, relation between p_u & p_s can be written in form of the following equation,

$$10p_s + 6p_u = 13 \quad \text{---(3.2)}$$

Equation 3.2 gives asymptotic relation between p_u & p_s .

Figure 9 also shows linear type dependence between the temperature (T) at which magnetization becomes equivalent to that of properly biased with p_u , vs p_u at different p_s for 100x100 lattice. This figure clearly shows that as p_s increases both T & p_u decreases. So in the figure we see that curves approaches to the origin at $p_u = 0.5, T = 0$, as p_s increases towards unity from percolation threshold.

3.1 Approximate partition function in diluted lattice with FM type interaction:

Partition function for diluted lattice can be found in a similar way like undiluted case. With a similar argument as given in subsection 2.1.2.1.1 it can be said that our calculation of PF remains valid in FM phase in percolated phase only. Now, assume that at a certain configuration probability of occupation is p. If total no. of sites is N, then no. of occupied sites is approximately Np and the no. of unoccupied sites is (N-Np). The number of ways in which Np occupied sites can be accommodated in N sites is,

$$G(Np) = \frac{N!}{Np!(N-Np)!} \quad \text{---(3.3)}$$

Among the 'Np' occupied sites, the no. of ways of occupying l flipped spins is,

$$G(l) = \frac{Np!}{l!(Np-l)!} \quad \text{---(3.4)}$$

Now the no. of ways of distribution of l flipped spins in N lattice points with probability of occupancy p is,

$$G(l, p) = G(Np)G(l) = \frac{N!}{Np!(N-Np)!} * \frac{Np!}{l!(Np-l)!}$$

$$G(l, p) = \frac{N!}{l!(N-Np)!(Np-l)!} \quad \text{---(3.5)}$$

If energy of the system for this configuration is E(p,l), then we get the expression for partition function for occupation probability p, as follows,

$$Z(p) = \sum_{l=0}^{Np} G(l, p) e^{-\frac{E(p,l)}{kT}} \quad \text{---(3.6)}$$

3.1.1 Approximate partition function for square lattice with n-n interaction in diluted case:

We consider a square lattice occupied with magnetic lattice points with occupation probability p. Considering ferromagnetic n-n interaction ground state energy of the system can approximately be written as, $E(0)=-4NJp$. Similarly a state where l spin is flipped can be written as, bearing energy $E(l)=-4pJ(N-2l)$. Hence partition function becomes,

$$Z(p) = \sum_{l=0}^{Np} G(l, p) e^{\frac{4pJ(N-2l)}{kT}} \quad \text{---(3.7)}$$

Writing equation 3.7, in explicit form we get,

$$Z(p) = \sum_{l=0}^{Np} \frac{N!}{l!(N-Np)!(Np-l)!} e^{\frac{4pJ(N-2l)}{kT}}$$

$$= \frac{N!}{Np!(N-Np)!} \sum_{l=0}^{Np} \frac{Np!}{l!(Np-l)!} e^{\frac{4pJN-2pJl}{kT}}$$

$$Z(p) = \frac{N!}{Np!(N-Np)!} z(Np) \quad \text{---(3.8)}$$

Where,
$$z(Np) = \sum_{l=0}^{Np} \frac{Np!}{l!(Np-l)!} e^{\frac{4pJN-2pJl}{kT}}$$

Taking logarithm of equation 3.8 we obtain,

$$\ln Z(p) = \ln z(p) + \ln N! - \ln Np! - \ln(N - Np)!$$

$$\begin{aligned} \ln(Z(p)/z(p)) &= N \ln N - N - Np \ln Np + Np - \ln(N(1-p))! \\ &= N \ln N - Np \ln Np - \ln(N(1-p))! - N(1-p) \end{aligned}$$

Now as $p \rightarrow 1$, the third and fourth terms in above equation can be neglected. Again as logarithmic function of a variable varies much slowly in comparison with the variable, we can write $Np=N$, in the logarithmic expression as $p \rightarrow 1$. Now above equation becomes,

$$\begin{aligned} \ln(Z(p)/z(p)) &= N \ln N - Np \ln N \\ \ln(Z(p)/z(p)) &= N(1-p) \ln N \\ &= \ln N^{N(1-p)} \\ Z(p) &= z(p) N^{N(1-p)} \quad \text{---(3.9)} \end{aligned}$$

At p close to unity $Z(p)$ can be said to be equivalent to partition function for undiluted system i.e. $Z(p=1)$ and $z(p)$ can be said to be partition function where occupation probability p . Hence we get from equation 3.9,

$$\begin{aligned} z(p) &\propto Z(p=1) N^{-N(1-p)} \\ \text{Hence, } z(p) &\propto N^{-N(1-p)} \quad \text{---(3.10)} \end{aligned}$$

From equation 3.10 one can study the behavior of partition function with occupation probability and total no. of sites where p is close to unity.

IV. Conclusion

In this paper phase transition behavior of spin system in Ising model is considered to be equivalent to percolation problem. Partition function is calculated for undiluted lattice using Maxwell- Boltzmann statistics. Beauty of this partition function is that the calculation does not require shape and dimension information of the lattice but it comes with a limitation of applicability range in percolated phase only. In specific cases shape and dimension of the lattice appears in the energy term present in the expression for partition function. Using simple mathematical tricks, partition function for diluted lattice is calculated. Special effort to find an expression for partition function is given because it is the key thing for calculating all the thermodynamic quantities associated with the system, such as free energy, entropy etc. Finite size effect and phase transition behavior of spins is easily understood from the nature of partition function. A new way to find critical temperature is found in the theoretical analysis. Specific examples (like one I have done for square lattice) can be taken to study phase transition behavior or measurement of any thermodynamic quantity using partition function. This can be taken as a scope for future work.

List of figures & Tables

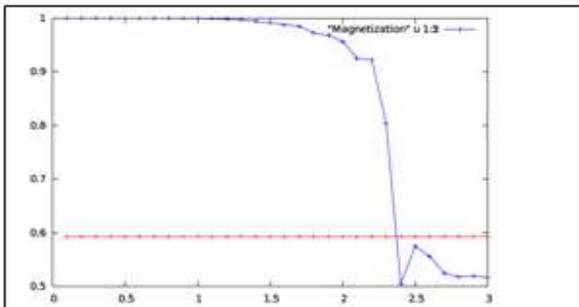


Figure 1: M vs. T for 100x100 lattice. Critical temperature=2.37

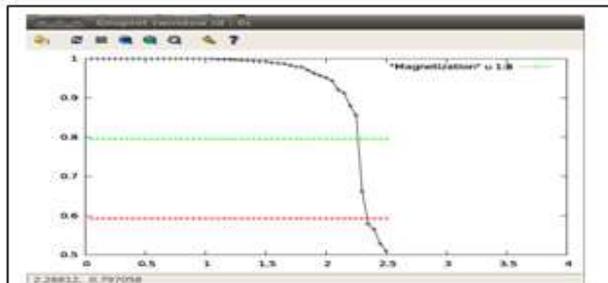


Figure 2: M vs. T for 128x128 lattice $T_c=2.3478$; at $p=0.5926$; $T_c=2.2618$; at $M=0.5926$

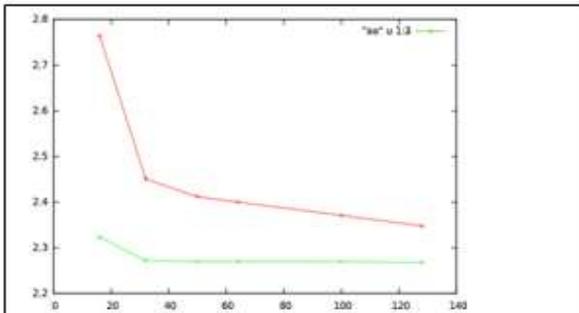


Figure 3: T_c vs vN
Red curve assuming site percolation threshold. Green one is for magnetic percolation.

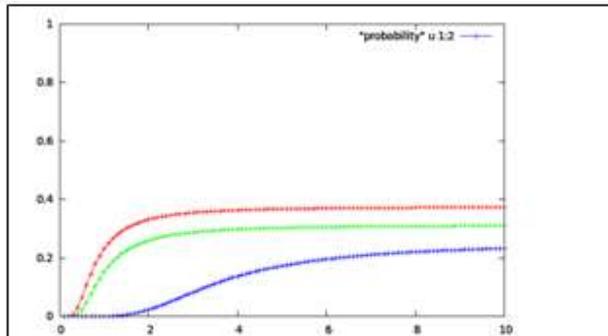


Figure 4: p_l vs l for $l=N/2$
Curves: red $N=4$; green $N=6$; blue $N=16$

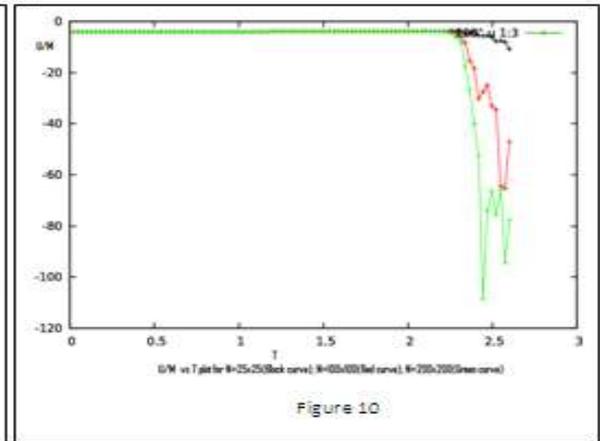
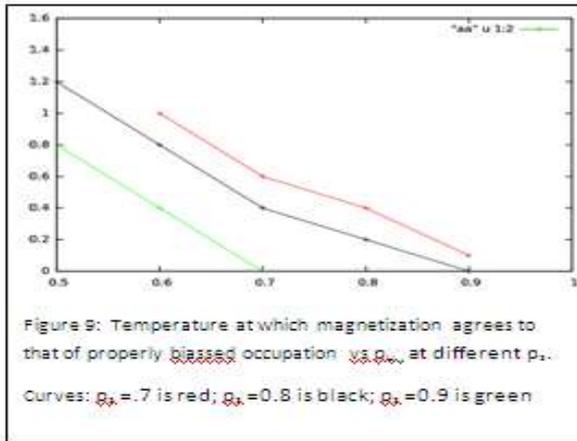
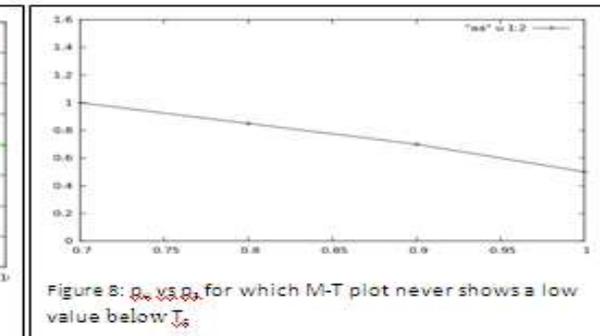
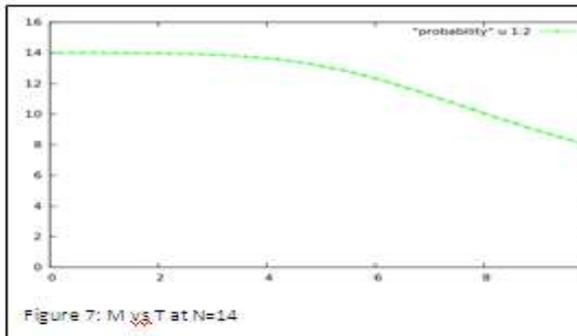
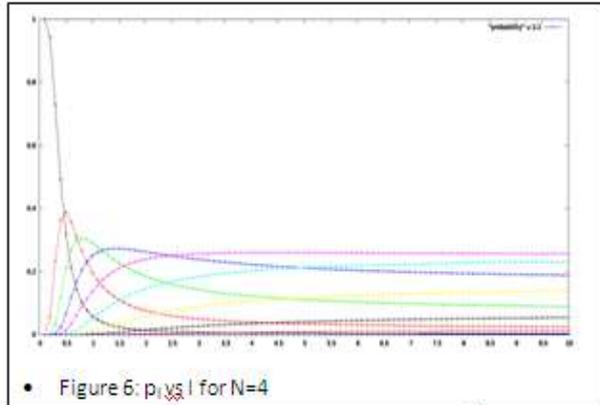
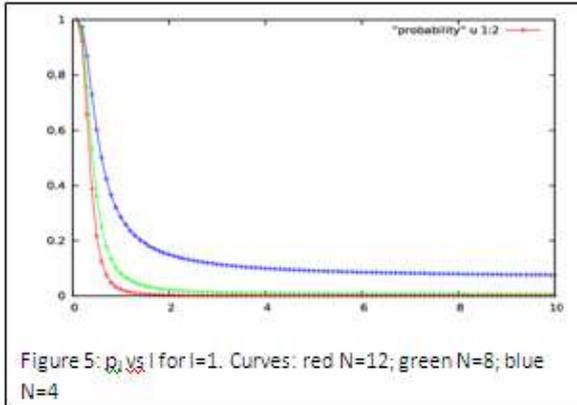


Table 1

Energy	Absolute magnetization	Multiplicity
-16	1	2
0	0.5	8
0	0	4
16	0	2

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