CALCULATIONS OF DIFFERENT PHYSICAL PARAMETERS BY 2D SIMULATIONS OF THE ISING MODEL FOR DIFFERENT GEOMETRICAL LATTICES

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ABSTRACT

This work presents a theoretical simulation of the dependencies of different physical parameters (internal energy, magnetization, specific heat, magnetic susceptibility and others) on the temperature for a two-dimensional Ising model and for different geometrical lattices (square, triangular, rhombohedral). These different geometrical lattices allow the determination of the dependency of the critical temperature on the coordination number (number of nearest neighbors). The linear behavior of the maximum values for the specific heat and for the magnetic susceptibility as a function of different geometrical lattice dimensions was obtained.

Keywords: Ising model, phase transition, Monte Carlo method

INTRODUCTION

Nearly six decades ago, (Onsager, 1944) found an exact solution for an S=1/2 square Ising lattice. The Ising model for magnetic materials had been developed by (Ising, 1925). In this model, a phase transition at the critical temperature was found to be nonexistent for the one-dimensional lattice.

The Monte Carlo method together with the Metropolis algorithm was recently used by (Fitzpatrick, 2002) in order to study the dependence of the different physical parameters on the temperature during a magnetic phase transition. The author considered a square lattice of sizes 5, 10, 20 and 40 and averaged the results over 4000 steps. Averages over 10000 steps on a square lattice of different dimensions were done by (Sun, 1999). Monte Carlo simulations on a 100x100 square lattice were also performed by (Chien, 1995).

The work presented in this paper extends the Monte Carlo simulation of the Ising model using the Metropolis algorithm to the triangular and rhombohedral lattices. Due to the unavailability of large calculators, it was however restricted to an average over 250 steps.

THEORY

In order to calculate the different physical parameters, we use the Hamiltonian equation:

$$E = -\frac{J}{2} \sum_{\substack{<i,j>\,nearest \\ neighbors}} S_i S_j - H \sum_i S_i \tag{1}$$

where S_i = ±1 and H is the external magnetic field. Using this equation, we calculate the internal energy of the system from which we derive the specific heat, which is proportional to the variance of the internal energy and to $1/T^2$. The magnetization is written as $\sum_i S_i$ and the susceptibility is proportional to the variance of the magnetization and to 1/T.

All these parameters depend on the absolute temperature T, and also on the dimension L of the lattice. Note that the properties of a three-dimensional lattice can be figured out numerically with a certain degree of accuracy but the exact solution, using known mathematical equations, has not yet been found.

In order to calculate the physical parameters and simulate the general behavior of the lattice of spins, a sampling algorithm is needed. We use the Metropolis algorithm (Metropolis *et al*., 1953) that consists of flipping a spin and calculating the probability of accepting the new configuration, as

$$A(s \to s') = \min\left[1, \frac{\pi_i(s')}{\pi_i(s)}\right] \tag{2}$$

where π_i is the probability of the system to be in the microstate i.

The analytical expression of the internal energy and the magnetization for N spins are evaluated, for the square and triangular lattices, respectively as:

Square lattice:

$$U = -2NJ\, th\frac{2J}{kT} - NJ\frac{sh^2\frac{2J}{kT} - 1}{sh\frac{2J}{kT}}\left[\frac{2}{\pi}K(x) - 1\right] \tag{3}$$

where $K(x) = \int_0^{\pi/2} \frac{1}{\left[1 - x^2 \sin^2 \Phi\right]^{1/2}} d\Phi$ and $x = 2\frac{sh\frac{2J}{kT}}{ch^2\frac{2J}{kT}}$

J is the exchange interaction and k is the Boltzmann constant.

$$M(T) = \lim_{N\to\infty} \frac{\sum_i S_i}{N} = (1 - \frac{1}{sh^4 2J/kT})^{1/8} \quad \text{for } T \le T_C \tag{4}$$

Triangular lattice:

$$U \sim -N \coth(\frac{2J}{kT}) \quad \text{(neglecting the integral)} \tag{5}$$

$$M = (1 - K^2)^{1/8} \tag{6}$$

where $K = \frac{(1-v)^3(1+v)}{4v\sqrt{v(1-v+v^2)}}$ and $v = \tanh\frac{1}{kT}$

Whereas this simulation allows us to calculate the equilibrium physical properties as simple averages, it suffers from slowdown at the critical point. Algorithms that do not suffer from this slowdown are those that flip groups of lattice spins as a whole that is cluster algorithms (Swendsen &Wang, 1987).

SIMULATIONS AND RESULTS

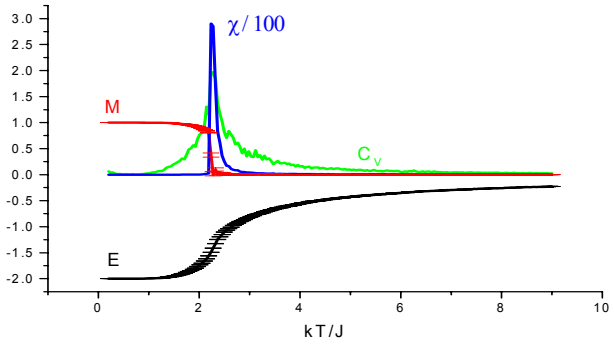
To resolve the statistical problem of N spins in interaction on a two-dimensional lattice, the Metropolis algorithm was implemented for L*3 equilibrium steps (for L=4, 5, 10, 13, 16, 32 and 40) and 250 iterations (each iteration includes a sweep through all spins), from which we extracted the averages $\overline{E}, \overline{M}, \overline{C}_v, \overline{\chi}$ (internal energy, magnetization, specific heat, magnetic susceptibility) per spin respectively. These 250 iterations are repeated for different temperatures kT/J and applied to the square, triangular and rhombohedral lattices (4, 6 and 2 nearest neighbors respectively). For L=40, the curves corresponding to the square and triangular lattices are shown in Figure 1 (traced with error bars for $\overline{E}, |\overline{M}|$).

The critical temperature T_C was extracted from the curves of the square and triangular lattices using the analytical expressions of the internal energy and the magnetization presented in the second paragraph (equations (3), (4), (5) and (6)) and the approximation

J/k=1. This T_C corresponds also to the maximum values of $\overline{C}_v$ and $\overline{\chi}$. These maximum values were deduced using an integral method.

Analytical expressions were not found for the rhombohedral (or trigonal) lattice. Large errors were observed in the results for this lattice type especially at large dimensions; the magnetization was less than 1.0 at small temperatures and the width of the susceptibility and heat capacity peaks increased with the dimension L instead of decreasing. In addition, the number of fluctuations was large. This behavior was attributed to the small number of nearest neighbors (n=2) and to the distortion of the lattice at high temperatures.

a) Square Lattice



b) Triangular Lattice

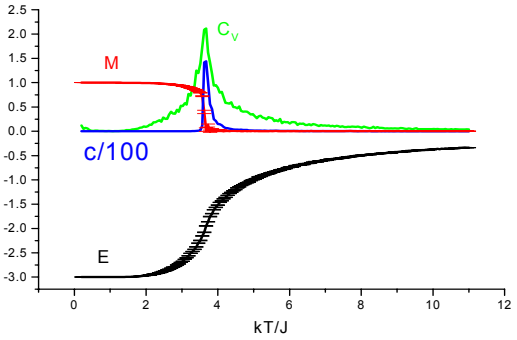


Figure 1. Variation of $\overline{E}, |\overline{M}|, \overline{C}_v$ and $\overline{\chi}$ /100 per spin as a function of the temperature for the a) Square lattice and b) Triangular lattice of dimension L=40.

Because of these errors at large L, the study of variation of the physical parameters as a function of kT/J was restricted to a lattice of dimension L=3 (this was done with 280 steps and L*10 equilibrium steps); and $\overline{C}_v$ was used to extract T_C for this lattice type.

Using the results extracted from these three lattice types and using T_C=1.52 for the honeycomb lattice characterized by three nearest neighbors per spin (Meyer, 1999), the critical temperature as a function of the number of nearest neighbors n was obtained (Figure 2). A linear fit for n=3, 4 and 6 gives: $T_C \sim (0.71 \pm 0.01)\, n + (-0.59 \pm 0.04)$

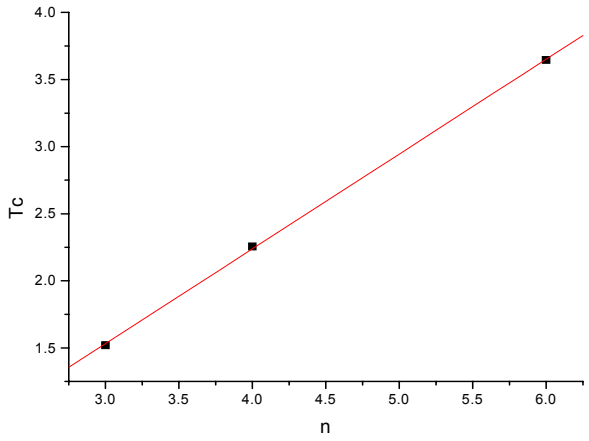


Figure 2. Variation of the critical temperature as a function of the number of nearest neighbors n for the square, triangular and honeycomb lattices.

As for (n=2, T_C=1.22), it is far from the linear fit as is shown in Figure 3.

It is conclude that the linearity of T_C(n) is only valid above a threshold value of n=2.

The maximum values of C_v and χ at the critical temperature were obtained as a function of $\log_{10} L$ for the square and triangular lattices. The following results were found (Figures 4 and 5):

Square Lattice:

$\overline{C}_{v\max} \sim (1.31 \pm 0.03) \log_{10} L$ or $\overline{C}_{v\max} \sim L^{(0.15\pm0.03)}$ (the exact value being $\overline{C}_{v\max} = L^{\alpha/\upsilon} = L^0$ where α and υ are critical exponents) and $\overline{\chi}_{\max} \sim L^{(1.56\pm0.02)}$ (the exact result is $\overline{\chi}_{\max} = L^{\gamma/\upsilon} = L^{1.75}$).

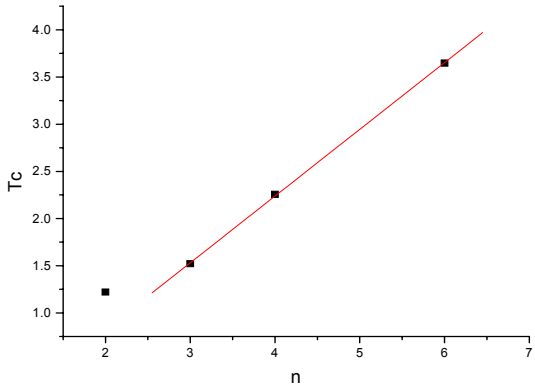


Figure 3. The critical temperatures corresponding to n=2,3 4 and 6 with a linear fit for the last three points.

Triangular Lattice:

$\overline{C}_{v\max} \sim (1.36 \pm 0.03)\ \log_{10} L$ and $\overline{\chi}_{\max} \sim L^{(1.37\pm0.01)}$. A small deviation was observed in the result for $\overline{C}_{v\max}$. However one would expect the same result, due to the universality of the critical exponents. This discrepancy indicates that a larger number of Monte Carlo steps should be used for this lattice type.

The results for different lattice types are summarized in the Table 1.

TABLE 1

Numerical Results and Comparison with Other Results

Lattice type	$\overline{C}_{v\max}$	$\overline{\chi}_{\max}$	numerical results (7,9)
Square	$\overline{C}_{v\max} \sim (1.31 \pm 0.03) \log_{10} L$	$\overline{\chi}_{\max} \sim L^{(1.56\pm0.02)}$	$\overline{C}_{v\max} = L^0$, $\overline{\chi}_{\max} = L^{1.75}$
Triangular	$\overline{C}_{v\max} \sim (1.36 \pm 0.03) \log_{10} L$	$\overline{\chi}_{\max} \sim L^{(1.37\pm0.01)}$	$\overline{C}_{v\max} = L^0$, $\overline{\chi}_{\max} = L^{1.75}$
Rhombohe-dral	$\overline{C}_{v\max} \sim (-0.33 \pm 0.09) \log_{10} L + (0.47 \pm 0.06)$	$\overline{\chi}_{\max} \sim L^{(1.11\pm0.17)}$	$\overline{C}_{v\max} = L^0$, $\overline{\chi}_{\max} = L^{1.75}$
Tc (n)	$T_C \sim (0.71 \pm 0.01)\ n + (-0.59 \pm 0.04)$		T_C =0.7n-0.57

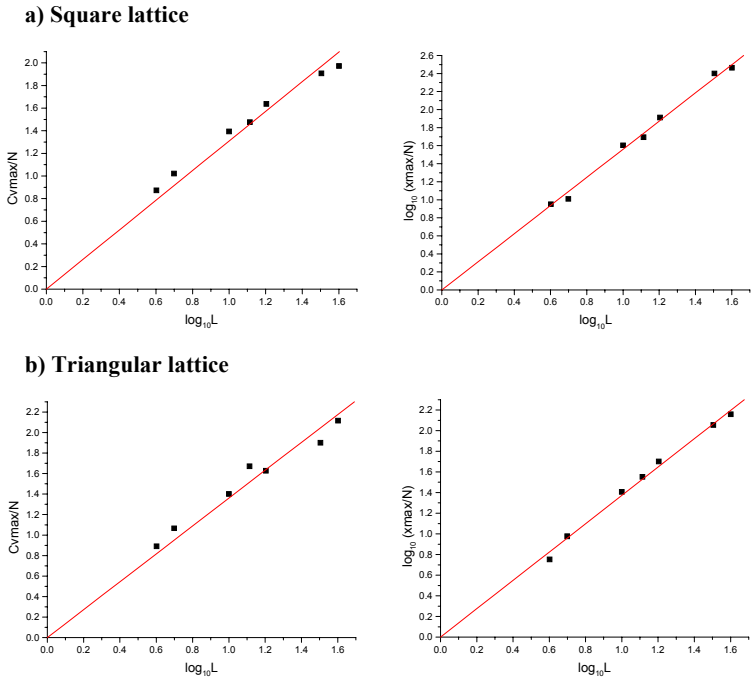


Figure 4. Variation of $\overline{C}_{v\max}$ /N and $\log_{10}$ ($\overline{\chi}_{\max}$ /N) as a function of $\log_{10} L$ for the a) Square lattice and b) Triangular lattice.

A comparison with the numerical results of reference (Fitzpatrick, 2002) shows a good compatibility with the linear relation of $\overline{C}_{v\max}$, as a function of $\log_{10}$ L. Also the critical temperatures extracted for the square and triangular lattices present relatively small errors by comparison with the analytical results of 2.27 and 3.64 respectively. As for the linear relation found describing the dependence of the critical temperature on the number of nearest neighbors (above a threshold of n=2), it compares well with that obtained by (Meyer, 1999).

CONCLUSION

This paper presents a study on the variation of different physical parameters with temperature and lattice dimension. The study reports a linear dependency of the critical temperature versus the number of coordination for a value of n greater than 2. This result provides a way to deduce the critical temperature knowing the geometrical structure of the

lattice. This work allows to deduce the critical exponents which are constants whatever the geometrical structure of the lattice (square, triangle and rhombohedral). It is shown that the maximum values of the specific heat and susceptibility are proportional to the dimension of the lattice. Thus, despite the fact that the simulations were restricted to 250 Monte Carlo steps, results were obtained that are compatible with those found numerically for a much larger number of steps. However the algorithm shows instability near the critical temperature where the dynamics is too slow, this instability explains the increasing deviation in the values of magnetic susceptibility and specific heat in comparison by numerical values (Meyer, 1999; Sun, 1999). This is mainly due to the restriction of the algorithm on the interaction of nearest neighbors (n=4 square, n=3 triangle, n=2 rhombohedral) as well as the dimension of the lattice**.** In fact more work is driven in order to improve the instability of the algorithm.

This work can be further extended to the study of antiferromagnetic materials and the magnetisation of ferromagnetic nanoparticles characterised by uniaxial anisotropy.

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