

Critical Behaviour of the Ising $S=1/2$ and $S=1$ Model on $(3,4,6,4)$ and $(3,3,3,3,6)$ Archimedean Lattices

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Abstract. We investigate the critical properties of the Ising $S=1/2$ and $S=1$ model on $(3,4,6,4)$ and $(3^4,6)$ Archimedean lattices. The system is studied through the extensive Monte Carlo simulations. We calculate the critical temperature as well as the critical point exponents γ/ν , β/ν , and ν basing on finite size scaling analysis. The calculated values of the critical temperature for $S=1$ are $k_B T_C/J=1.590(3)$, and $k_B T_C/J=2.100(4)$ for $(3,4,6,4)$ and $(3^4,6)$ Archimedean lattices, respectively. The critical exponents β/ν , γ/ν , and $1/\nu$, for $S=1$ are $\beta/\nu=0.180(20)$, $\gamma/\nu=1.46(8)$, and $1/\nu=0.83(5)$, for $(3,4,6,4)$ and $0.103(8)$, $1.44(8)$, and $0.94(5)$, for $(3^4,6)$ Archimedean lattices. Obtained results differ from the Ising $S=1/2$ model on $(3,4,6,4)$, $(3^4,6)$ and square lattice. The evaluated effective dimensionality of the system for $S=1$ are $D_{\text{eff}}=1.82(4)$, for $(3,4,6,4)$, and $D_{\text{eff}}=1.64(5)$ for $(3^4,6)$.

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Key words: Monte Carlo simulation, Ising model, critical exponents.

1 Introduction

The Ising model [1,2] has been used during long time as a "toy model" for diverse objectives, as to test and to improve new algorithms and methods of high precision for calculation of critical exponents in Equilibrium Statistical Mechanics using the Monte Carlo method as Metropolis [3], Swendsen-Wang [4], Wang-Landau [5] algorithms, Single histogram [6] and Broad histogram [7] methods. The Ising model was already applied

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decades ago to explain how a school of fish aligns into one direction for swimming [8] or how workers decide whether or not to go on strike [9]. In the Latané model of Social Impact [10] the Ising model has been used to give a consensus, a fragmentation into many different opinions, or a leadership effect when a few people change the opinion of lots of others. To some extent the voter model of Liggett [11] is an Ising-type model: opinions follow the majority of the neighbourhood, similar to Schelling [12], all these cited model and others can be found in [13]. Recently, Zaklan et al. [14, 15] developed an economics model to study the problem of tax evasion dynamics using the Ising model through Monte-Carlo simulations with the Glauber and heatbath algorithms (that obey detailed balance-equilibrium) to study the proposed model.

The beauty and the popularity of this model lies in both its simplicity and possible applications from pure and applied physics, via life sciences to social sciences. In the way similar to the percolation phenomenon, the Ising model is one of the most convenient way of numerical investigations of second order phase transitions.

In the simplest case, the Ising model may be used to simulate the system of interacting spins which are placed at the nodes of graphs or regular lattices. In its basic version only two values of the spin variable are available, i.e., $S = -1/2$ and $S = +1/2$. This is the classical Ising $S = 1/2$ model. For a square lattice this model defines the universality class of phase transitions with analytically known critical exponents which describe the system behaviour near the critical point. The critical point separates two-ordered and disordered-phases.

One of possible generalization of the Ising model is to enlarge the set of possible spin values (like in the Potts model [16, 17]). The Ising $S = 1$ model corresponds to three possible spin values, i.e., $S \in \{-1, 0, +1\}$, Ising $S = 3/2$ allows for four spin variables $S \in \{\pm 3/2, \pm 1/2\}$, etc. The Ising $S \neq 1/2$ model on various networks and lattices may form universality classes other than the classical square lattice Ising model.

The spin models for $S=1$ were extensively studied by several approximate techniques in two and three dimensions and their phase diagrams are well known [18–24]. The case $S > 1$ has also been investigated according to several procedures [25–31]. The Ising model $S = 1$ on directed Barabási-Albert network was studied by Lima in 2006 [32]. It was shown, that the system exhibits a first-order phase transition. The result is qualitatively different from the results for this model on a square lattice, where a second-order phase transition is observed.

The Archimedean lattices are the vertex transitive graphs that can be embedded in the plane such that every face is a regular polygon. A polygon is regular if all edges have the same length and all interior angles are the same. Kepler [33] showed that there exist exactly 11 such graphs. The lattices are given names according to the sizes (number of sides of the polygon) of faces incident to a given vertex. The face sizes are listed in order, starting with a face such that the list is the smallest possible in lexicographical order. The square lattice thus gets the name $(4, 4, 4, 4)$, abbreviated to (4^4) , triangular (3^6) , honeycomb (6^3) and the Kagomé lattice the name $(3, 6, 3, 6)$.

In this paper we study the Ising $S = 1$ model on two Archimedean lattices (AL),

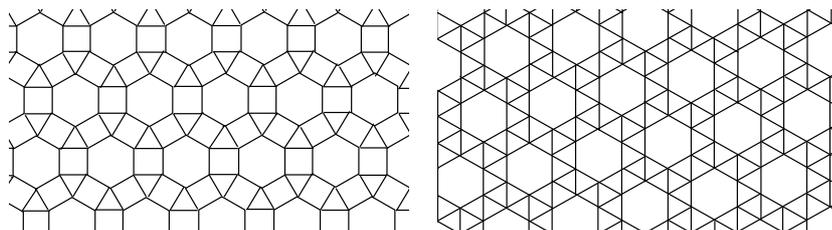


Figure 1: Topology of (3,4,6,4) (left) and (3⁴,6) (right) AL.

namely on (3,4,6,4) and (3⁴,6). The topologies of (3,4,6,4) and (3⁴,6) AL are presented in Fig. 1. Critical properties of these lattices were investigated in terms of site percolation in [34]. Topologies of all eleven existing AL are given there as well. Also the critical temperatures for Ising $S = 1/2$ model [35] and voter model [36] on those AL were estimated numerically.

Here, with extensive Monte Carlo simulations we show that the Ising $S = 1$ model on (3,4,6,4) and (3⁴,6) AL exhibits a second-order phase transition with critical exponents that *do not* fall into universality class of the square lattice Ising $S = 1/2$ model.

2 Model and simulation

We consider the two-dimensional Ising $S = 1$ model on (3,4,6,4) and (3⁴,6) AL lattices. The Hamiltonian of the system can be written as

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j, \quad (2.1)$$

where spin variable S_i takes values $-1, 0, +1$ and decorates every $N = 6L^2$ vertex of the AL. In Eq. (2.1) J is the magnetic exchange coupling parameter and sum runs on nearest neighbour sites.

The simulations have been performed for different lattice sizes $L = 8, 16, 32, 64$ and 128 . For each system with $N = 6L^2$ spins and given temperature T we performed Monte Carlo simulation in order to evaluate the system magnetization m . The simulations start with a uniform configuration of spins ($S_i = +1$, but the results are independent on the initial configuration). It takes 10^5 Monte Carlo steps (MCS) per spin for reaching the steady state, and then the time average over the next 10^5 MCS are estimated. One MCS is accomplished when all N spins are investigated whether they should flip or not. We carried out $N_{\text{run}} = 20$ to 50 independent simulations for each lattice and for given set of parameters (N, T) . We have employed the heat bath algorithm for the spin dynamics.

We evaluate the average magnetization M , the susceptibility χ , and the magnetic 4-th order cumulant U :

$$M(T, L) = \langle |m| \rangle, \quad (2.2a)$$

$$\frac{k_B T}{J} \cdot \chi(T, L) = N(\langle m^2 \rangle - \langle |m| \rangle^2), \quad (2.2b)$$

$$U(T, L) = 1 - \frac{\langle m^4 \rangle}{3\langle |m| \rangle^2}, \quad (2.2c)$$

where $m = \sum_i S_i / N$ and k_B is the Boltzmann constant. In the above equations, $\langle \dots \rangle$ stands for thermodynamic average.

In the infinite-volume limit these quantities (2.2) exhibit singularities at the transition point T_C . In finite systems the singularities are smeared out and scale in the critical region according to

$$M = L^{-\frac{\beta}{\nu}} f_M(x), \quad (2.3a)$$

$$\chi = L^{-\frac{\gamma}{\nu}} f_\chi(x), \quad (2.3b)$$

where ν , β and γ are the usual critical exponents, and $f_i(x)$ are finite size scaling (FSS) functions with $x = (T - T_C)L^{1/\nu}$ being the scaling variable. Therefore, from the size dependence of M and χ one can obtain the exponents β/ν and γ/ν , respectively.

The maximum value of susceptibility also scales as $L^{\gamma/\nu}$. Moreover, the value of temperature T^* for which χ has a maximum, is expected to scale with the system size as

$$T^*(L) = T_C + bL^{-\frac{1}{\nu}}, \quad (2.4)$$

where the constant b is close to unity [37]. Therefore, the Eq. (2.4) may be used to determine the exponent $1/\nu$. We have checked also if the calculated exponents satisfy the hyper-scaling hypothesis

$$\frac{2\beta}{\nu} + \frac{\gamma}{\nu} = D_{\text{eff}} \quad (2.5)$$

in order to get the effective dimensionality, D_{eff} , for both investigated AL lattices.

3 Results and discussion

The dependence of the magnetization M on the temperature T , obtained from simulations on (3,4,6,4) and (3⁴,6) AL with $N = 6L^2$ ranging from 384 to 98304 sites is presented in Fig. 2. The shape of magnetization curve versus temperature, for a given value of N , suggests the presents of the second-order transition phase in the system. The phase transition occurs at the critical value T_C of temperature.

In order to estimate the critical temperature T_C we calculate the fourth-order Binder cumulants given by Eq. (2.2c). It is well known that these quantities are independent of the system size at T_C and should intercept there [38].

In Fig. 3 the corresponding behaviour of the susceptibility χ is presented.

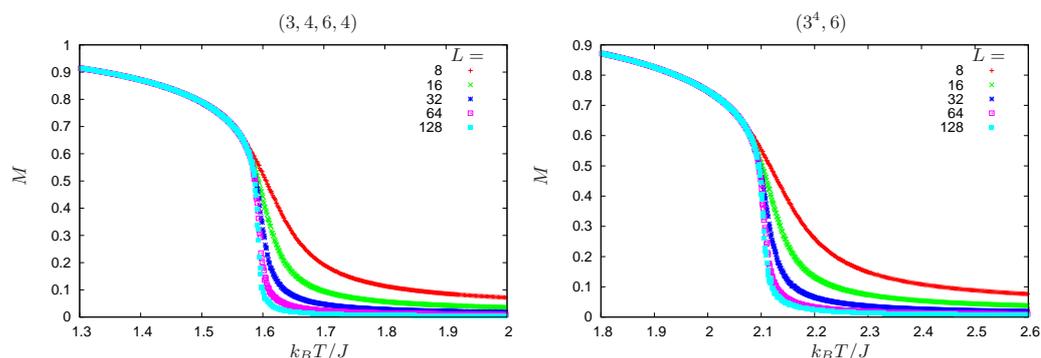


Figure 2: The magnetization M as a function of the temperature T , for $L=8,16,32,64$, and 128 and for $(3,4,6,4)$ and $(3^4,6)$ AL.

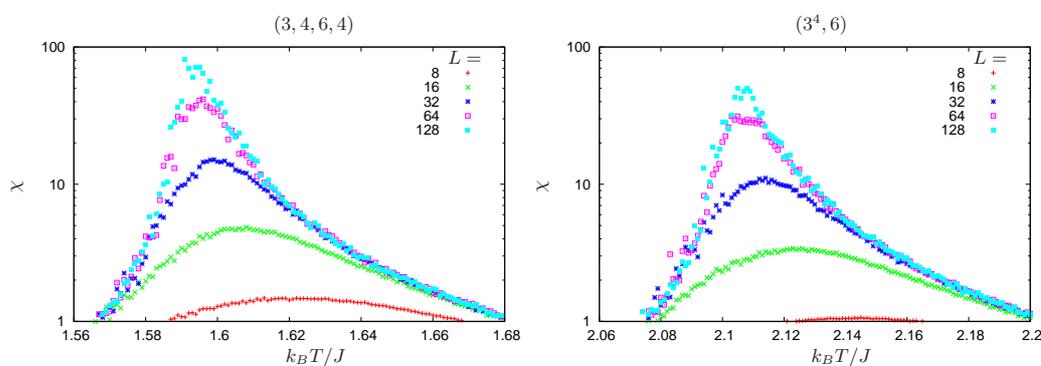


Figure 3: The susceptibility χ versus temperature T , for $(3,4,6,4)$ and $(3^4,6)$ AL.

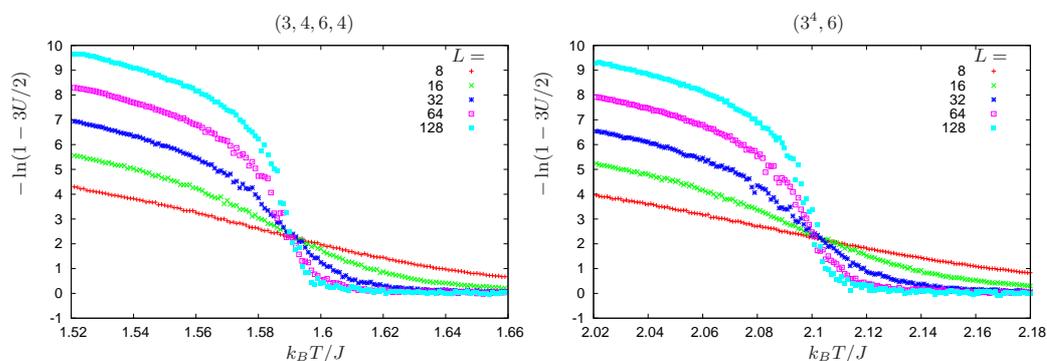


Figure 4: The reduced Binder's fourth-order cumulant U as a function of the temperature T , for $(3,4,6,4)$ and $(3^4,6)$ AL.

In Fig. 4, the fourth-order Binder cumulant is shown as a function of the temperature for several values of L . Taking two largest lattices (for $L=64$ and $L=128$), we have $T_C=1.590(3)$ and $T_C=2.100(3)$, for $(3,4,6,4)$ and $(3^4,6)$ AL, respectively.

In order to go further in our analysis we also computed the modulus of the magnetization at the inflection $M^* = M(T_C)$. The estimated exponents β/ν values are 0.180(20) and 0.103(7), for (3,4,6,4) and (3⁴,6) AL, respectively.

Basing on the dependence $\ln\chi$ on $\ln L$, we estimated $\gamma/\nu = 1.46(8)$ and $\gamma/\nu = 1.44(8)$, for (3,4,6,4) and (3⁴,6) AL, respectively.

To obtain the critical exponent $1/\nu$, we used the scaling relation (2.4). The calculated values of the exponents $1/\nu$ are 0.83(5) for (3,4,6,4), and $1/\nu = 0.94(5)$ for (3⁴,6). Eq. (2.5) yields effective dimensionality of the systems $D_{\text{eff}} = 1.82(4)$ for (3,4,6,4), and $D_{\text{eff}} = 1.64(5)$ for (3⁴,6).

H. W. J. Blöte and M. P. Nightingale [39] used finitesize scaling and transfer matrix techniques to calculate accurately the critical exponents of three- and two-dimensional Isinglike models for which no exact solution is available and also studying the spin-1 Ising model a two-dimensional. The results for the temperature and magnetic exponents are very close to the exact results for exactly solvable models which were assumed to be in the same universality class, but within numerical uncertainties. They also presented an estimate of the critical point of the spin-1 model, and some preliminary results concerning universal properties of critical amplitudes.

The above results, indicate that the Ising $S = 1$ model on (3,4,6,4) and (3⁴,6) AL *does not fall* in the same universality class as the square lattice Ising model, but also with numerical uncertainties, for which the critical exponents are known analytically, i.e., $\beta = 1/8 = 0.125$, $\gamma = 7/4 = 1.75$, and $\nu = 1$. The independence of exponents on S is believed numerically since a few decades [39]. Improving the statistics would reduce the statistical errors but presumably if our conclusion (violation of universality) is wrong it is due to systematic errors like system sizes. The violation of universality is surprising, but other such surprises have been found out long ago. For example, a second-order phase transition can change to tricritical behavior and then to first-order transition by continuously increasing one real parameter which is not the lattice dimensionality nor the spin symmetry, as in the Blume-Capel model. We don't think one should make a hypothesis now; first one should wait for others to check our results. We have checked numerically, that Ising $S = 1/2$ model reproduces these critical exponents with reasonable accuracy for both studied lattices [40]. We improved the value of the critical temperature T_C for these two lattices and $S = 1/2$ as well, with respect to [35].

The results are collected in Table 1.

Table 1: Critical points and critical points exponents for (3,4,6,4) and (3⁴,6) AL. For comparison, the exact values for the square lattice Ising $S = 1/2$ model are included as well.

	S	$k_B T_C / J$	β/ν	γ/ν	$1/\nu$	D_{eff}
(3,4,6,4)	1	1.590(3)	0.180(20)	1.46(8)	0.83(5)	1.82(4)
(3 ⁴ ,6)	1	2.100(3)	0.103(8)	1.44(8)	0.94(5)	1.64(5)
(3,4,6,4)	1/2	2.145(3)	0.123(17)	1.680(74)	1.066(44)	1.926(84)
(3 ⁴ ,6)	1/2	2.784(3)	0.113(10)	1.726(8)	1.25(13)	1.952(22)
square (4 ⁴)	1/2	2/arcsinh(1)	1/8	7/4	1	2

Except the exponent ν , all critical exponents for $S = 1$ differ for more than three numerically estimated uncertainties from those given analytically.

Note added in the proof

Very recently A. Codello [41] has found exact values of the Curie temperatures for Ising $S = \frac{1}{2}$ model for all AL. Our estimations of T_C agree, within errors, with these exact values.

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