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LETTER TO THE EDITOR

# Ising model on an icosahedral quasilattice

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**Abstract.** The Ising model on the three-dimensional icosahedral quasilattice is studied by use of a Monte Carlo simulation. We treat both cases where the spins are located on the vertices of the lattice and the centres of the lattice. We investigate the critical phenomena on the basis of finite-size scaling. It is shown that the critical exponents are universal among regular lattices and quasilattices. The critical temperatures of both models are found to be higher than that of the simple cubic lattice though the (average) coordination numbers of the three lattices are all six.

The discovery of quasicrystals has brought about a growing interest in the spin statistics in quasicrystals. The spin systems on the one-dimensional (1D) quasilattice can be solved with an exact renormalisation approach (Achiam *et al* 1986), and interesting behaviour which comes from the characteristics of quasilattices was pointed out. It is more interesting to investigate the role of the quasiperiodicity and the self-similarity in phase transitions and critical phenomena. Higher-dimensional systems should be studied for such a purpose.

The Ising model on the 2D Penrose lattice was previously studied by means of an approximate renormalisation scheme (Godrèche *et al* 1986). Some special model was treated by an exact approach (Choy 1988). The Monte Carlo simulation is a powerful method to obtain precise numerical information. The present authors (Okabe and Niizeki 1988a, b, c) made the Monte Carlo simulation of the Ising the model on the Penrose lattice of a size up to 439 204 sites. Other authors (Bhattacharjee *et al* 1987, Miyajima *et al* 1988, Amarendra *et al* 1988, Oitmaa and Johnson 1989) also studied the Ising model by the Monte Carlo method for smaller systems. Quite recently, the high-temperature expansion (Abe and Dotera 1989) and the coherent anomaly method (Kinoshita and Suzuki 1989) have been applied to the study of the Ising model on the Penrose lattice. It is to be noted that the Potts model on the Penrose lattice was studied by Monte Carlo simulation (Wilson and Vause 1989a, b).

In a previous Monte Carlo study of the 2D Penrose lattice (Okabe and Niizeki 1988a, b, c), we showed the universality of critical exponents and the duality between the critical temperatures of dual lattices. We also pointed out that the critical temperature, which is a non-universal quantity, for the Penrose (dual Penrose) lattice is very close to that for the dice (Kagomé) lattice. A similar behaviour was found in the study of the percolation threshold for the bond percolation problem of the Penrose and its dual lattices (Yonezawa *et al* 1989). We can show that the high-temperature series coefficients of the Penrose lattice are numerically close to those of the dice lattice. This similarity of the local structure may give the reason for the closeness of the critical temperatures of the Penrose lattice and of the dice lattice.

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It is interesting to study spin systems on more realistic 3D quasilattices. In this letter, we report the extension of the Monte Carlo study to the 3D icosahedral quasilattice (IQL). An IQL is a 3D set of points derived from a 6D simple hypercubic lattice by the cut-and-projection method (for the structure of the IQL, see Henley (1986)). The 6D lattice naturally forms a 6D network whose coordination number is 12, where a network is composed of vertices and bonds linking them. The network is reduced, by the cut-and-projection, into a 3D one. The coordination number of the 3D network ranges from 4 to 12 and the average is 6. The 3D network gives rise to a 3D (Penrose) tiling, by which the 3D space is filled with two types (prolate and oblate) of rhombohedra; vertices and edges of a rhombohedron coincide with those of the 3D network. Note that two vertices linked by a bond in the network are not necessarily nearest to each other. We usually identify the 3D network and the 3D tiling with the IQL.

We shall call the dual network to the 3D tiling a dual IQL. A vertex of the dual IQL is located at the centre of a rhombohedron of the 3D tiling and two vertices are linked by a bond if the corresponding two rhombohedra share a surface (a rhombus). Obviously, the coordination number of the dual IQL is fixed to 6. Note that the density of the vertices of the dual IQL is exactly equal to that of the IQL, which follows from the fact that the inner solid angle of the eight vertices of a rhombohedron total to $4\pi$.

Since the icosahedral point group has ten threefold axes, a prolate (or oblate) rhombohedron can assume ten orientations and the dual IQL can be divided into 10 (or 20) sublattices if a prolate rhombohedron and an oblate one is not distinguished (or is). Two rhombohedra (of the same type of different types) never share a surface if their axes are parallel and, consequently, no bonds link two vertices belonging to the same sublattice of the dual IQL. Note that the lengths of the bonds in the dual IQL can assume three values in contrast to the case of the IQL where they are all equal.

Numerical simulations are performed on finite systems; therefore, it is desired to make the size effect as small as possible. For this purpose, we employ the periodic boundary condition. Then the IQL must be modified slightly into a series of 'periodic' IQLs (Elser and Henley 1985) whose sizes, $N_i$, in the total lattice sites in a unit cell are 576, 2440, 10 336, ... (note the recursion relation, $N_{i+1} = 4N_i + N_{i-1}$); the golden ratio $\tau = (1+\sqrt{5})/2$ is approximated by a consecutive pair of Fibonacci numbers.

An Ising model is defined for the IQL (more exactly, the network associated with it) or its dual in such a way that the spins are located on the vertices and the ferromagnetic interactions between the spins are assigned to the bonds:

$$\mathscr{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \qquad (\sigma_i = \pm 1) \tag{1}$$

where the symbol $\langle i, j \rangle$ denotes the bond between $i$ and $j$ in the network. Note that the two models on the IQL and its dual are actually *not* dual to each other in the sense of the duality relation where the Euler theorem holds (for the duality relation, see Syozi (1972)). We follow the usual Metropolis method of the Monte Carlo simulation. As in the case of the 2D Penrose lattice (Okabe and Niizeki 1988a, b, c), we apply the fast algorithm of multispin coding due to Bhanot *et al* (1986a, b). For the IQL, the coordination number ranges from 4 to 12; the energy difference at a spin-update trial takes 25 values. It is straightforward to apply the multispin coding, although the logical operations become complicated. The use of a vector computer is practically efficient. The calculation is fully vectorised if the lattice is decomposed into appropriate interpenetrating sublattices; such a sublattice decomposition is simply guaranteed for the IQL because it is a bipartite lattice. On the other hand, the dual IQL can be divided into ten interpenetrating sublattices as mentioned above. With these techniques we can realise the speed of the Monte Carlo simulation of the same order as that for the regular lattice. The multispin coding of simulation is much simpler for the dual IQL because all the coordination numbers are fixed to be 6, which is the same as the simple cubic lattice.

We measured the square of the magnetisation per spin $\langle m^2 \rangle$. In figure 1, we show the temperature dependence of $\sqrt{\langle m^2 \rangle}$ for the ferromagnetic Ising model on the IQL and on its dual lattice for a wide range of temperature. The lattice sizes are shown in the inset. The largest lattice has 43 784 sites. We did two independent runs for each size and temperature, each of 10 000 sweeps. The first 2000 sweeps were excluded when taking an average. In the limit $N \to \infty$, the quantity $\sqrt{\langle m^2 \rangle}$ leads to the spontaneous magnetisation for $T < T_c$, and $\langle m^2 \rangle$ becomes the susceptibility $\chi T/N$ for $T > T_c$. We clearly see the second-order paramagnetic–ferromagnetic phase transition for both quasilattices from the figure. The critical temperature for the simple cubic lattice is shown by an arrow, which is lower than $T_c$s for both quasilattices. This point will be discussed later.

Our main focus is to investigate the critical properties. We performed high-statistics simulations for the temperatures near $T_c$. The temperature dependence of $\langle m^2 \rangle$ for $4.8 \leqslant T/J \leqslant 5.1$ for the IQL and for $5.5 \leqslant T/J \leqslant 5.8$ for the dual IQL are shown in figure 2. Simulations were made for 400 000 sweeps, and the first 80 000 sweeps were discarded when taking an average. To estimate the critical temperature and the critical exponent with these data, we use a phenomenological Monte Carlo renormalisation group analysis due to Barber and Selke (1982). We examine the ratio of the values of $\langle m^2 \rangle$ for different sizes. We plot the temperature dependence of the quantity

$$R[N, N'] = \frac{\log(\langle m^2 \rangle_L / \langle m^2 \rangle_{L'})}{\log(L/L')} + d \tag{2}$$

for both quasilattices in figure 3, where the linear size $L$ is given by $\sqrt[3]{N}$, and $d = 3$. We note that $R \to 0$, for $T \to \infty$, and $R \to d$ for $T \to 0$. All pairs $[N, N']$ are expected to intersect at a single point if corrections to finite-size scaling are negligible. The critical

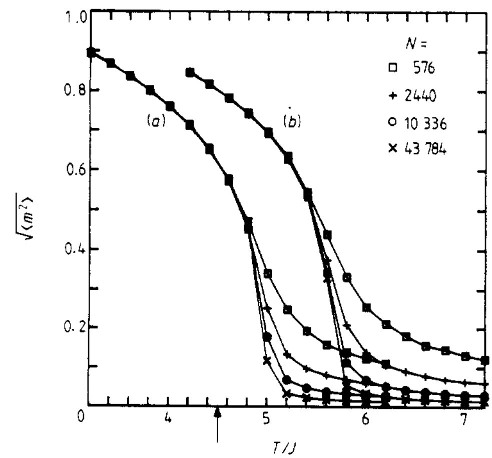


**Figure 1.** Temperature dependence of $\sqrt{\langle m^2 \rangle}$ for the ferromagnetic Ising model on the icosahedral lattice ($a$) and its dual lattice ($b$) for a wide range of temperature. The lattice sizes are shown in the inset. The arrow gives $T_c$ for the simple cubic lattice.

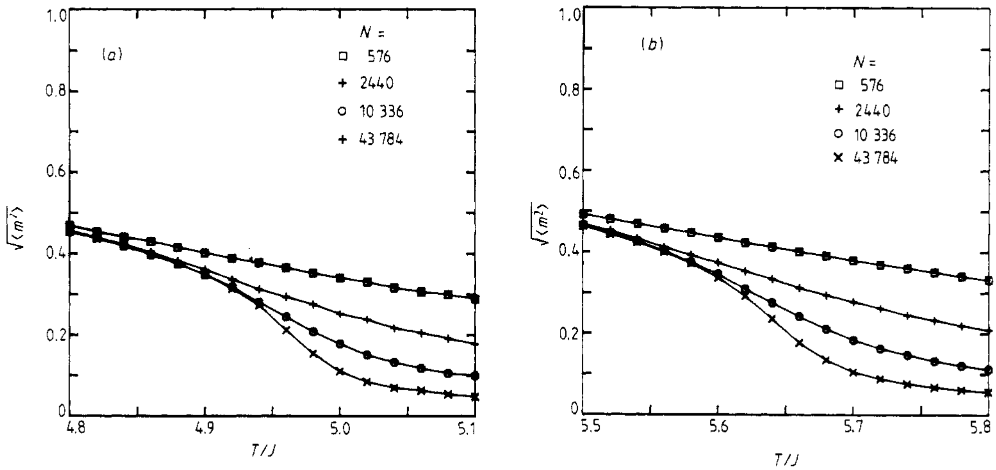


**Figure 2.** Temperature dependence of $\sqrt{\langle m^2 \rangle}$ for the ferromagnetic Ising model on the icosahedral lattice ($a$) and its dual lattice ($b$); the results of the high statistics simulations near the critical temperature. The lattice sizes are shown in the inset.

temperature $T_c$ and the magnetic exponent $2y_H - d(=\gamma/\nu)$ are given by the abscissa and the ordinate of the crossing point, respectively. From figure 3, we may estimate the critical temperature and the magnetic exponent for both quasilattices. In table 1, the estimated $T_c$ and $2y_H - d$ are tabulated.

We emphasise that the obtained critical exponent $y_H$ is no different from that of the 3D regular lattices within the errors of simulation. We confirmed the universality of critical exponents for 3D quasilattices, which is the same conclusion as obtained for 2D quasilattices. The estimated $T_c$s for both quasilattices are higher than that of the simple cubic lattice, $T_c/J = 4.512$, although the average coordination numbers of these

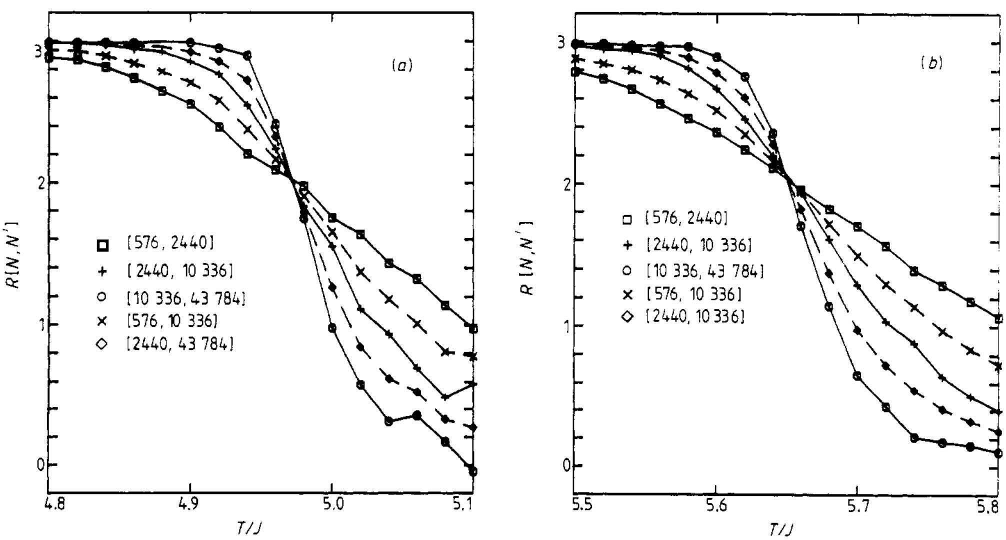


**Figure 3.** Temperature dependence of the ratio of $\langle m^2 \rangle$ for the icosahedral lattice ($a$) and the dual icosahedral lattice ($b$). The quantity $R[N, N']$ is defined by (2). The sizes of pairs, $[N, N']$, are given in the inset.

**Table 1.** The estimated $T_c$ and $2y_H - d$ for the icosahedral lattice and the dual icosahedral lattice. For comparison we also give the data for the simple cubic lattice.

| Lattice | $T_c$ | $2y_H - d$ |
|---|---|---|
| Icosahedral | $4.972 \pm 0.06$ | $2.00 \pm 0.05$ |
| Dual icosahedral | $5.650 \pm 0.08$ | $2.01 \pm 0.05$ |
| Simple cubic | 4.512 | 1.97 |

three lattices are the same. In the 2D case, the critical temperature for the square lattice is in the middle of the Penrose lattice and the dual Penrose lattice because of the duality relation,

$$\sinh(2J/T_c)\sinh(2J/T_c^*) = 1. \tag{3}$$

In the present 3D case, this duality relation is *not* satisfied because the Euler theorem does not hold in the present dual lattice. There was a conjecture that the lattice which has a distribution in the coordination number $z$ has a higher $T_c$ than the homogeneous lattice with the same $z$ for 2D lattices (Syozi 1972). It is *not* the case for 3D lattices because the $T_c$ for the dual IQL is higher than that for the IQL. The high-temperature series may help the study of the local structure of the lattice, i.e, the critical temperature.

In figure 4, we show a finite-size scaling plot

$$\langle m^2\rangle_L L^{2(d-y_H)} = f(tL^{y_T}) \qquad t = (T - T_c)/T_c. \tag{4}$$

The thermal exponent $y_T$ is the inverse of the correlation length exponent; $y_T = 1/\nu$. Figure 3 shows that choosing $T_c = 4.975$, $y_H = 2.485$ and $y_T = 1.59$ gives a fairly good scaling plot for the IQL, where we have used the critical exponents of 3D regular lattices. In the case of dual IQL, we chose $T_c = 5.655$ and the same parameters for critical exponents.

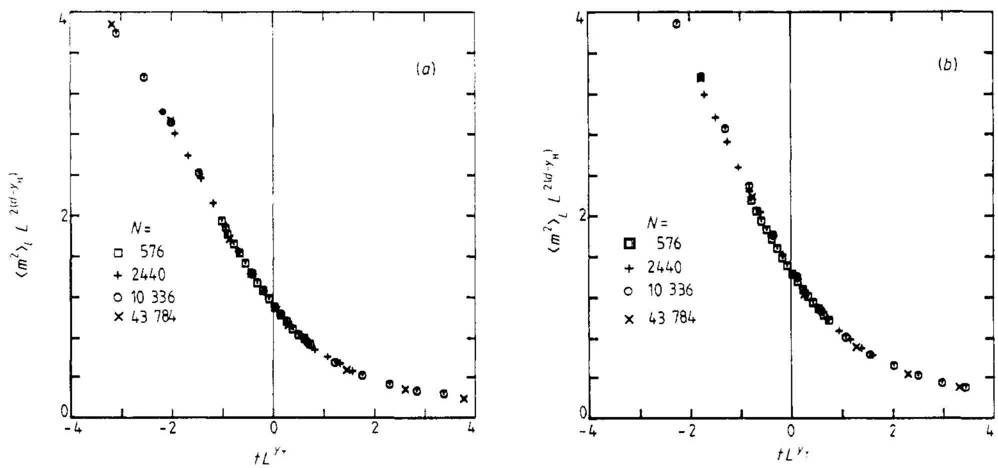


**Figure 4.** Finite-size scaling plot; $\langle m^2\rangle_L L^{2(d-y_H)}$ against $tL^{y_T}$ with $t = (T - T_c)/T_c$. The three parameters are chosen as $T_c = 4.975$, $y_H = 2.487$ and $y_T = 1.51$ for the icosahedral lattice ($a$) and $T_c = 5.655$, $y_H = 2.487$ and $y_T = 1.51$ for the dual icosahedral lattice ($b$). The critical exponents are those of the 3D regular lattices.

In summary, we have studied the critical phenomena of the Ising spins on the 3D icosahedral lattice by use of a Monte Carlo method. It has been shown that the critical exponents are universal among regular crystals and quasicrystals. We have also discussed the critical temperatures for the icosahedral quasilattice and its dual lattice. We finally remark that the antiferromagnetic spin systems on the dual icosahedral lattice are interesting subjects because of a frustration.

The preliminary result of this study was reported at the Taniguchi Symposium on Quasicrystals, November 14-18, 1989 (Okabe and Niizeki 1990).

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