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Translational invariance in critical phenomena: Ising model on a quasi-lattice

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Abstract. The Ising model on a two-dimensional quasi-crystal (the Penrose tiling) is studied. Using the correlation inequality and the duality transformation, bounds for the critical temperature are obtained as $1.82 < T_c < 7$. Monte Carlo simulations on finite lattices give an estimate of $T_c = 2.41 \pm 0.02$. Finite-size scaling analysis of the Monte Carlo data shows that the system belongs to the same universality class as the Ising model on the two-dimensional Bravais lattices. However, the finite-size scaling forms do not reproduce the asymptotic limits in the range studied whereas, in the same range, the periodic lattices are known to behave as expected.

1. Introduction

The concept of universality classes in critical phenomena (Ma 1975) suggests that the class a model should belong to is not determined by the underlying translational symmetry, provided such a symmetry exists. The last clause, though not often explicitly stated, is necessary because new types of critical behaviour emerge when such symmetries are destroyed as in lattices with randomness (McCoy and Wu 1972, Dotsenko and Dotsenko 1983). In this paper we study the critical behaviour of the Ising model on a two-dimensional quasi-lattice which is known not to have the usual Bravais lattice periodicity.

The Ising model on any lattice is defined by the Hamiltonian

$$H = -J \sum_{\langle ij \rangle} s_i s_j \tag{1.1}$$

where s_i, $s_j = \pm 1$ are the spins located at the vertices i, j of the lattice, J (>0) is the coupling constant and the sum is over the nearest neighbours only. It is well known (McCoy and Wu 1972) that, for any two-dimensional periodic lattice, the model exhibits a critical behaviour at a temperature $T = T_c$ with logarithmic divergence in the specific heat. The critical exponents‡ are known to be exactly $\alpha = 0$, $\beta = \frac{1}{8}$, $\gamma = \frac{7}{4}$ and $\nu = 1$. These exponents determine the universality class of the model. In contrast, an exact solution of a quenched random system with disorder in the coupling constant in (1.1) in one direction only (McCoy and Wu 1972) shows a much weaker singularity at a new T_c. For a homogeneously disordered Ising model, Dotsenko and Dotsenko (1983)

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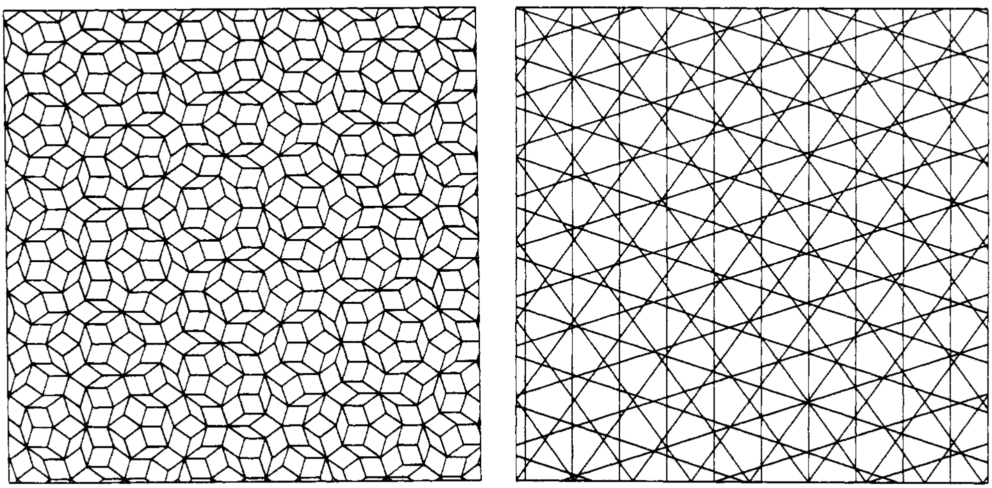
‡ The critical exponents α, β, γ and ν are defined by the relations (i) specific heat $c \sim |t|^{-\alpha}$, (ii) magnetisation $m \sim |t|^{\beta}$ ($t < 0$), (iii) susceptibility $\chi \sim |t|^{-\gamma}$, and (iv) the correlation length $\xi \sim |t|^{-\nu}$, where $t = (T - T_c)/T_c$ and $t \to 0\pm$.

found $\alpha = 0$, $\beta = 0$, $\gamma = 2$ and $\nu = 1$, with the specific heat diverging as $\ln|\ln|T - T_c||$. In this situation, it seems necessary to study other types of lattices that do not have a translational symmetry. Quasi-crystals (Penrose 1972, Gardner 1977) are an obvious choice. Moreover, since quasi-crystals can now be produced in the laboratory, it is necessary to know what type of critical behaviour is expected in such crystals.

A quasi-crystal is a lattice which is not topologically equivalent to a periodic Bravais lattice. One can possibly associate some sort of quasi-periodicity† to such lattices (and hence the name). Such a lattice was first discovered by Penrose (1972) and that particular lattice, shown in figure 1(*a*), will be called the Penrose tiling. This tiling has points with coordination number varying from 3 to 7. Its dual lattice, shown in figure 1(*b*), is a four-coordinated lattice, i.e. each point has four nearest neighbours. This is because the building blocks of the tiling are two rhombuses. Note that the dual lattice has a non-crystallographic pentagonal symmetry. In fact, the tiling of figure 1(*a*) has been constructed from the dual lattice of figure 1(*b*) using the duality transformation (see de Bruijn (1981) and Socolar *et al* (1986) for details).



(*a*) (*b*)

Figure 1. Penrose tiling (*a*) and its dual lattice (*b*).

We have used both analytical and numerical methods for studying the critical behaviour of the Ising model on the Penrose tiling. Bounds on the critical temperature are obtained in § 2. The Monte Carlo (MC) method is used in § 3 to obtain numerical values of the critical exponents. Section 4 is the summary and conclusion.

2. Bounds on the transition temperature

We shall assume the existence of a thermodynamic limit as the number of vertices of the tiling, N, goes to infinity. With this assumption, one can use Peierl's argument to show the existence of an ordered state at sufficiently low temperatures. In this section we use correlation inequalities to obtain both upper and lower bounds for the transition temperature.

† A quasi-periodic function is the sum of periodic functions with incommensurate periods.

2.1. *Upper bound on T_c*

For the Ising model, in a magnetic field h, given by

$$H = -J \sum_{ij} s_i s_j - h \sum_i s_i \tag{2.1}$$

with $J > 0$ and $h > 0$, one can use one of the Griffiths-Kelly-Sherman inequalities (Griffiths 1972) to show that

$$M \leqslant \tanh \beta h + q_m M \tanh \beta J \tag{2.2}$$

where M is the spontaneous magnetisation in the thermodynamic limit, defined as

$$M = \lim_{N \to \infty} \sum_i \langle s_i \rangle / N \tag{2.3}$$

N being the number of lattice points, q_m is the largest coordination number of the lattice and $\beta = 1/k_B T$, k_B being the Boltzmann constant. This is trivially true (since $h > 0$) if $q_m \tanh \beta J > 1$. For $q_m \tanh \beta J < 1$, (2.2) can be written as

$$M \leqslant \frac{\tanh \beta h}{(1 - q_m \tanh \beta J)}. \tag{2.4}$$

This shows that $M \to 0+$ as $h \to 0+$, provided $q_m \tanh \beta J < 1$. Hence

$$q_m \tanh \beta J = 1 \tag{2.5}$$

gives a temperature T^* above which $M = 0$ with $h = 0$. For a Penrose tiling $q_m = 7$. Therefore, an upper bound for T_c is obtained as

$$(k_B T_c / J) \leqslant (\tanh^{-1} q_m^{-1})^{-1} < q_m = 7. \tag{2.6}$$

2.2. *Lower bound on T_c*

The duality transformation for the 2D Ising model (Syozi 1972) connects the low-temperature partition function on a lattice to the high-temperature partition function on the dual lattice and vice versa. Using K for $J/k_B T$, this transformation, for large lattices, gives

$$\frac{Z(K)}{2^{N/2}(\sinh 2K)^{N/2}} = \frac{Z^*(K^*)}{2^{N^*/2}(\sinh 2K^*)^{N^*/2}} \tag{2.7}$$

where N is the number of sites on the lattice, $*$ represents the corresponding quantities on the dual lattice and (K, K^*) are connected by

$$\exp(2K^*) = \coth K. \tag{2.8}$$

Therefore, if K_c is the critical point for the tiling and K_c^* for the dual lattice in figure 1(b), they will be connected by (2.8). One can now use the inequality in (2.2) to show that

$$1/K_c^* < 4 \tag{2.9}$$

because the grid lattice is a four-coordinated lattice†. One can, in fact, get a better bound by using self-avoiding walk results (Fisher 1967); the bound is

$$1/K_c^* < 2/\ln 2 \tag{2.10}$$

† Note that (2.9) as an equality is the mean-field transition temperature (Stanley 1971) for the Ising model on the dual lattice.

which is, incidentally, the temperature given by the Bethe-Peierls approximation. Using (2.8), (2.10) can be written in terms of K as

$$\tanh K_c \leq \tfrac{1}{2} \tag{2.11}$$

so that

$$k_B T_c / J \geq (\tanh^{-1} 0.5)^{-1} = 1.82\ldots. \tag{2.12}$$

3. Monte Carlo calculation

The standard importance-sampling Monte Carlo (MC) technique (see, e.g., Binder 1984) is used to calculate various statistical averages. In this algorithm, new spin configurations are generated by flipping the spins one at a time. Whether a spin will be flipped or not is determined by comparing the Boltzmann factor associated with the change in energy to a random number between 0 and 1. One MC step consists of one run through the whole lattice. An estimate of the statistical average of a quantity is then obtained by taking a simple average over the MC steps.

The calculations are done, for obvious reasons, on small lattices. The averages calculated are (i) the magnetisation $M = \langle |S| \rangle / N$, where $S = \Sigma_i s_i$, (ii) $\langle S^2 \rangle$, (iii) $\langle S^4 \rangle$, (iv) the average total energy $\langle E \rangle$ and (v) $\langle E^2 \rangle$. The specific heat, c, and the susceptibility, χ, are then obtained from the relations

$$c = (k_B T^2)^{-1} N^{-1} (\langle E^2 \rangle - \langle E \rangle^2) \tag{3.1a}$$

and

$$\chi = (k_B T)^{-1} N^{-1} (\langle S^2 \rangle - \langle S \rangle^2). \tag{3.1b}$$

$\langle S^4 \rangle$ is used, as described below, to determine the critical temperature T_c. Throughout this section and in the figures, the temperature is in units of J/k_B.

For each lattice size, 10^5 steps are generated, of which the first 50 are not considered ('equilibration' time) and every tenth one is taken for evaluating the averages. The whole calculation is performed twice with different random numbers. The standard random number generator RANF, supplied with the FORTRAN compiler, is used in the calculation which is done on a Cyber computer. Lattices of different sizes are extracted from different parts of a master lattice containing about 11 000 points.

3.1. *Analysis of data*

The data obtained by the MC method are analysed by the finite-size scaling method (Barber 1983). This analysis is based on the assumption of the existence of a critical point in the thermodynamic limit.

If a quantity $G(T)$, in the thermodynamic limit, shows a critical behaviour of the type

$$G(T) \approx \mathscr{G}_{\pm} |t|^{-a} \tag{3.2}$$

where $t = (T - T_c)/T_c$ and if $G_L(T)$ is the corresponding quantity for a finite system of linear dimension L, then finite-size scaling theory predicts

$$G_L(T) \approx L^{a/\nu} f_G(L^{1/\nu} t) \tag{3.3}$$

with

$$f_G(x) \approx \mathscr{G}_{\pm} x^{-a} \tag{3.4}$$

as $x \to \infty$. If G has a log divergence, i.e. if

$$G(T) \approx -\mathscr{G} \ln|t| \tag{3.5}$$

as for the specific heat for 2D periodic Ising models, then

$$G_L(T) \approx \mathscr{G} \ln L + f_G(L^{1/\nu} t) \tag{3.6}$$

with

$$f_G(x) \approx -\mathscr{G} \ln|x| \tag{3.7}$$

as $x \to \infty$. Asymptotic forms in (3.4) and (3.7) for large x is valid for systems with periodic boundary conditions. If there are free boundaries, one can still have such a scaling form but $f_G(x)$ will have a surface correction term (Landau 1976a, b).

3.2. *Determination of T_c*

The critical temperature T_c is determined by calculating the fourth cumulant (Binder 1981)

$$U_L = 1 - \frac{\langle s^4 \rangle}{3\langle s^2 \rangle^2} \tag{3.8}$$

which is zero for a Gaussian distribution. U_L has the finite-size scaling form

$$U_L(T) = f_U(L^{1/\nu} t). \tag{3.9}$$

It is known (Binder 1981) that for a finite lattice

$$\begin{aligned} U_L(T) &\to \tfrac{2}{3} && \text{as } T \to 0 \\ &\to 0 && \text{as } T \to \infty \\ &= U^* \equiv f_U(0) && \text{at } T = T_c \text{ (i.e. } t = 0) \end{aligned} \tag{3.10}$$

so that the ratio

$$R_{L_1 L_2}(T) \equiv \frac{U_{L_1}(T)}{U_{L_2}(T)} = 1 \tag{3.11}$$

as $T \to 0$, $T \to \infty$ and $T = T_c$. Therefore, a plot of $R_{L_1 L_2}(T)$ as a function of T will give T_c without any adjustable parameters.

The results of our simulation are shown in figure 2 where $1 - R_{L_1 L_2}$ (L_2 here refers to the smallest lattice of 96 vertices) is plotted against T. From these curves, we determine $T_c = 2.41 \pm 0.02$ where the error is more of a measure of the spread than a rigorous statistical error.

3.2.1. Exponent ν. From (3.9), it follows that plotting U_L against $L^{1/\nu} t$ will give a universal curve for the right choice of ν. In the absence of a good measure of the linear size of the lattices, we take

$$L = N^{1/2}$$

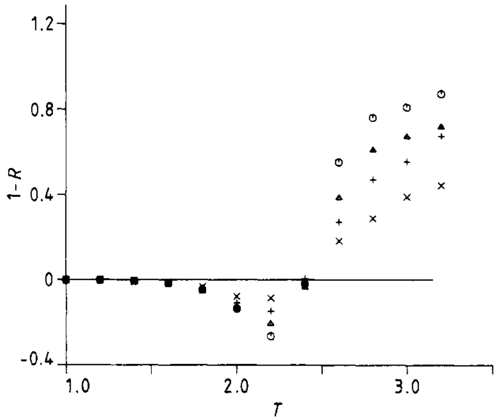


Figure 2. The critical temperature T_c is obtained by plotting $1-R_{L_1L_2}(T)$ (3.11) against T. L_2, for all the data points, stands for the smallest lattice with $N=96$ vertices. The four sets are for $N=228(\times)$, $N=414(+)$, $N=642(\triangle)$ and $N=1232(\bigcirc)$. Note that in this plot and in all the following figures, the temperature is in units of J/k_B.

as the linear size. Figure 3 shows a scaling plot with $\nu=1$. We find a better collapse of data when $\dot{t}=(T-T_c)/T$ is used instead of the usual $t=(T-T_c)/T_c$ for reduced temperature. Note that, once T_c is determined, this plot involves only one adjustable parameter, namely ν. The plot is rather insensitive to small variations in T_c and ν because of the inherent error in the simulation.

3.2.2. Exponents β and γ. Figures 4 and 5 show the scaling plots for magnetisation M and susceptibility χ. In figure 4, $ML^{\beta/\nu}$ is plotted against $\dot{x}=L^{1/\nu}\dot{t}$ ($\dot{t}=(T-T_c)/T$) with $\beta=\frac{1}{8}$ and $\nu=1$. In figure 5, $\chi L^{-\gamma/\nu}$ is plotted against $\dot{x}$ with $\gamma=\frac{7}{4}$ and $\nu=1$. In both cases, the good collapse of the data is an indication of the right choice of the exponents. The data can, as well, be fitted by slightly lower values of the exponents of β and γ, which, if necessary, can be used as a measure of the error for the exponents.

The striking feature of these plots is the limiting behaviour. For large $\dot{x}$, one can fit straight lines through these plots but the slopes *do not* reproduce the values of β

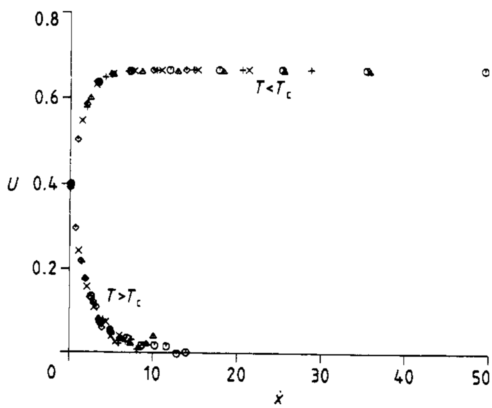


Figure 3. Scaling plot of the cumulant U_L (3.8) against $\dot{x}=L^{1/\nu}\dot{t}$, where $L=\sqrt{N}$, $\dot{t}=(T-T_c)/T$ and N is the number of vertices. For this plot, $\nu=1$ and $T_c=2.41$. The data points are for $N=96(\diamond)$, $N=228(\times)$, $N=414(+)$, $N=642(\triangle)$ and $N=1232(\bigcirc)$.

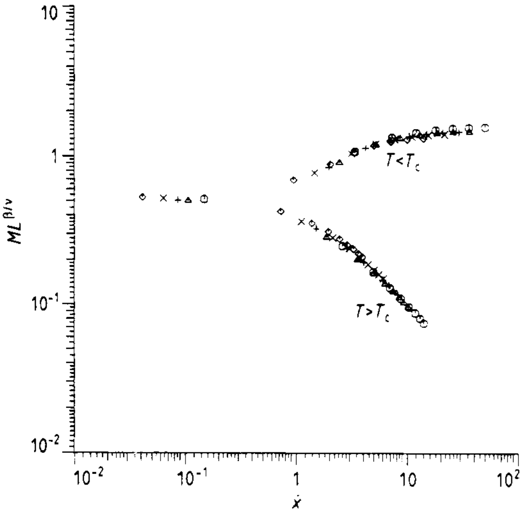


Figure 4. Scaling plot of the magnetisation. $ML^{\beta/\nu}$ is plotted against $\dot{x}$ with $\beta = \frac{1}{8}$ and $\nu = 1$. The symbols are the same as in figure 3. The limiting slopes are 0.09 ($T < T_c$) and 0.77 ($T > T_c$).

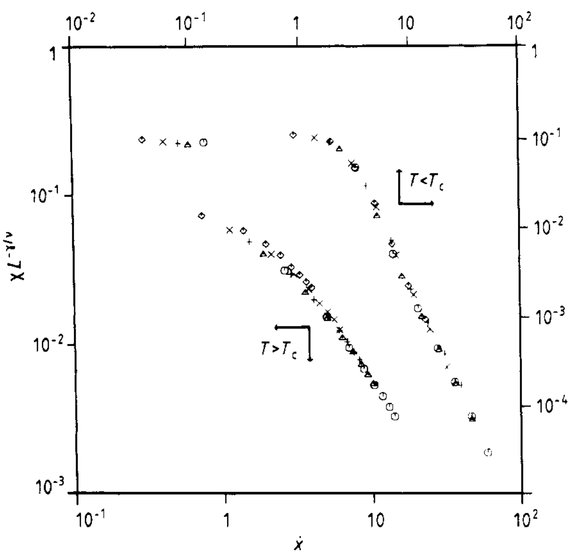


Figure 5. Scaling plot of the susceptibility. $\chi L^{-\gamma/\nu}$ is plotted against $\dot{x}$ with $\gamma = \frac{7}{4}$ and $\nu = 1$. See figure 3 for the meaning of the symbols. The limiting slopes are 2.7 ($T < T_c$) and 1.6 ($T > T_c$).

and γ as they should according to (3.4). (For $T > T_c$, the slope of the magnetisation curve should be $1 - \beta$ (Landau 1976).) In contrast, for the square lattice Ising model, asymptotic slopes are observed in the same range of the variable. In view of this, no estimate for the amplitudes (i.e. the coefficients in (3.2)) can be obtained.

In figure 6, χ at $T = 2.4$ ($\approx T_c$) is plotted against N (set a), the total number of vertices. This can be fitted to a straight line very well, giving an estimate of $\gamma = 1.73$. This reiterates the form (3.3) with $f_\chi(0) \approx 0.9$ as estimated from figure 5.

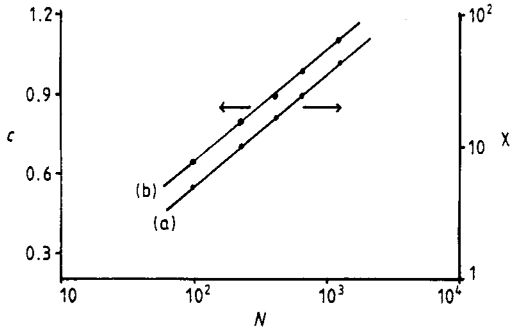


Figure 6. Plots of χ (set a) and c (set b) at $T = 2.4$ ($\approx T_c$) against N. The log-log plot for χ can be fitted to a straight line giving an estimate of $\gamma = 1.73$. The semilog plot of c can also be fitted to a straight line $c = \mathscr{C}_0 \log N + A$ with $\mathscr{C}_0 = 0.85$ and $A = -0.2$.

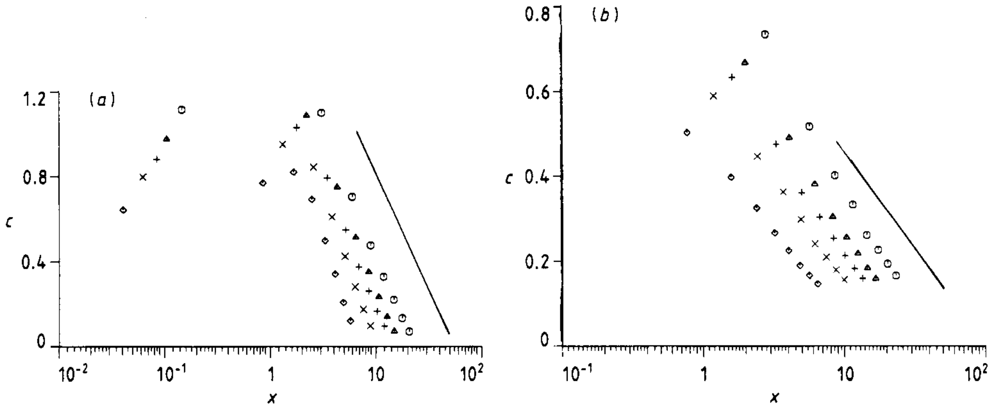


Figure 7. Specific heat c is plotted against $x = Lt$ where $t = (T - T_c)/T$, with $T_c = 2.41$, for (*a*) $T < T_c$ and (*b*) $T > T_c$. The data points ($N = 96(\Diamond)$, $N = 228(\times)$, $N = 414(+)$, $N = 642(\triangle)$ and $N = 1232(\bigcirc)$) for large x can be fitted to parallel lines (shown by the full lines) with slopes $\bar{\mathscr{C}}_- = 0.5$ ($T < T_c$) and $\bar{\mathscr{C}}_+ = 1.09$ ($T > T_c$).

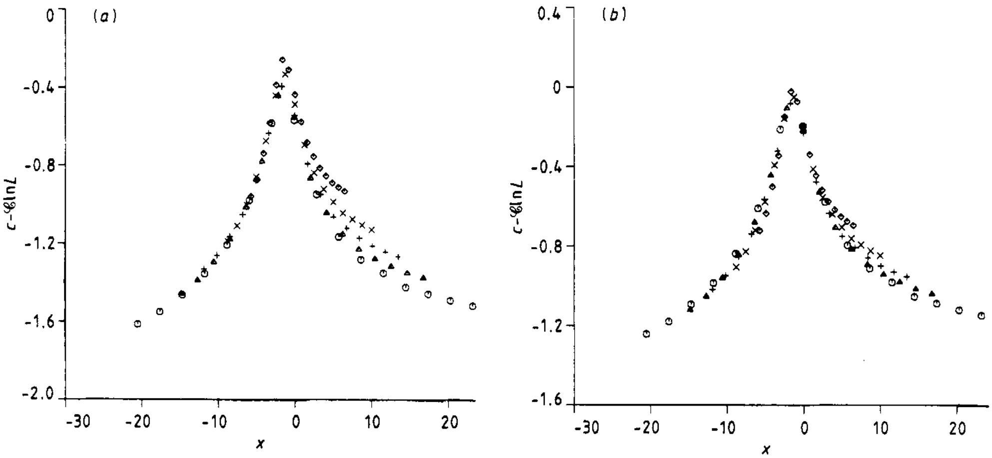


Figure 8. Plots of $c - \mathscr{C} \ln L$ against x. (*a*) $\mathscr{C} = \bar{\mathscr{C}}_- \ln 10$ and (*b*) $\mathscr{C} = \mathscr{C}_0 \ln 10$.

3.2.3. Specific heat. Plots for specific heat are shown in figures 7 and 8. In figure 7, c is plotted against $x = Lt$ where, for large x, one can see parallel lines. For $T < T_c$, in figure 7(a) the slope is $\bar{\mathscr{C}}_- = 1.09$ whereas it is $\bar{\mathscr{C}}_+ = 0.5$ for $T > T_c$ (figure 7(b)). $\bar{\mathscr{C}}_\pm$ are the amplitudes in (3.5) when the logarithm is in base 10.) This is in contradiction to the scaling prediction of (3.7) because the scaling theory for the bulk predicts that the amplitude in (3.5) has to be the same on both sides of T_c (Widom 1965). From (3.6), it follows that plots of $c - \mathscr{C} \ln L$ against x will be a universal one. Figure 8(a) shows these plots for $\mathscr{C}_- = \bar{\mathscr{C}}_- \ln 10$. Good collapse is observed with $\mathscr{C}_-$ only for $T < T_c$ whereas with $\mathscr{C}_+ = \bar{\mathscr{C}}_+ \ln 10$, it is observed only in the region $T > T_c$ (not shown).

Figure 6 (set b) shows the N dependence of c at $T = 2.4$ ($\approx T_c$) and from the semilog plot we get a slope of $\bar{\mathscr{C}}_0 = 0.85$ which, incidentally, is the mean of the two slopes in figure 7. In figure 8(b) we plot $c - \mathscr{C}_0 \ln L$ against x ($\mathscr{C}_0 = \bar{\mathscr{C}}_0 \ln 10$). As expected, the collapse is not totally satisfactory.

4. Discussions

We have shown that the critical temperature for the Ising model on the Penrose tiling lies between 1.82 and 7. The mean-field transition temperature for the dual lattice of figure 1(b) is $k_B T_c = 4J$ and a naive estimate for the Penrose tiling would be $k_B T_c = \bar{q}J$ where $\bar{q}$ is the average coordination number for the tiling (also close to 4). Monte Carlo simulations give $k_B T_c / J = 2.41 \pm 0.02$. From the duality transformation of (2.8), the transition temperature for the grid lattice is 1.07.

Finite-size scaling analysis of the Monte Carlo data is consistent with the exponents $\alpha = 0$, $\beta = \frac{1}{8}$, $\gamma = \frac{7}{4}$ and $\nu = 1$ which are the exponents for a pure translationally invariant 2D lattice. However, the scaling plots in figures 5 and 6 *do not* reproduce the asymptotic scaling forms of (3.4). That this is not an indication of a crossover to a new critical behaviour is checked by the behaviour right at T_c as in figure 6. We have found similar behaviour on another non-Penrose quasi-crystal. We therefore tend to believe that this delay in the approach to the limiting behaviour is a characteristic of the quasi-crystals in general. We made no attempt to analyse the data in terms of surface effects and/or corrections to scaling, because their contributions introduce curvature in the plots for large values of x. Scaling plots like figures 4 and 5 generally give estimates for amplitudes in the bulk (Landau 1976a, b) but such predictions cannot be made for quasi-crystals. Why this is so remains unexplained. This behaviour is also reflected in the scaling plot of specific heat as shown in figures 8(a) and (b). Figure 6 suggests that the bulk behaviour is like

$$c \approx -\mathscr{C} \ln|t|$$

with $\mathscr{C} = 1.7$. Even though the scaling plot in figure 8(b) is not that impressive, one cannot rule out the possibility of a systematic size-dependent correction to the scaling plots since at least one exactly solvable case like that is known (Bhattacharjee and Nagle 1985).

The conclusion is that the Ising model on a 2D quasi-crystal belongs to the same universality class as the pure translationally invariant Ising model but significant differences exist in the finite-size scaling behaviour.

Acknowledgments

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