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Non-universality in the Ising model with nearest and next-nearest neighbour interactions

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Abstract. The critical behaviour of the Ising model on the square lattice with ferromagnetic nearest-neighbour interactions (J) and anti-ferromagnetic next-nearest neighbour interactions (J') is discussed for small $\lambda = J/|J'|$. The singular part of the free energy is calculated to second order in λ by perturbation theory. Near the critical temperature of the unperturbed system ($J = 0$), this expansion is found to have a form which may be exponentiated yielding, for non-zero λ , a non-universal critical line along which the exponents vary continuously with λ . For small λ , the specific heat exponent, $\alpha = \alpha_1 \lambda^2 + O(\lambda^2)$ with $\alpha_1 \approx 1.5$.

1. Introduction

It is becoming increasingly apparent that the critical behaviour of two-dimensional Ising spin systems has a greater richness than was previously thought. Indeed, Krinsky and Mukamel (1977) have argued that such systems (for appropriate choices of the interaction parameters) can exhibit phase transitions characterised by order parameters of dimension $n \geq 2$. In particular, they showed that the system described by the Hamiltonian ($\sigma = \pm 1$)

$$H = -J \sum_{nn} \sigma \sigma' - J' \sum_{nnn} \sigma \sigma' \quad (1.1)$$

has a two-component order parameter in the regime†

$$-J \leq 2J' < 0. \quad (1.2)$$

In (1.1), the first sum runs over the nearest-neighbour bonds of a square lattice and the second over the next-nearest-neighbour (diagonal) bonds. Krinsky and Mukamel went on to conjecture that the critical behaviour of (1.1) should belong to a universality class of the two-component vector model. Recent work (see José *et al* 1977 and references therein) has established that the critical behaviour of this model in two dimensions can be particularly rich, including non-universal critical lines (see also Kadanoff 1977).

The existence of a non-universal critical line in (1.1) in the regime (1.2) was earlier suggested by van Leeuwen (1975) from an investigation of the fixed point structure and critical surface of two-dimensional Ising systems. Subsequently, Nightingale (1977) performed approximate renormalisation group calculations on (1.1), which indicated

† This inequality differs from that quoted in Krinsky and Mukamel 1977, which is misprinted.

that the exponents varied continuously with $J/|J'|$ for negative J' . In this paper, we present an analysis which confirms these conclusions, at least for small $J/|J'|$. Specifically, we show using perturbation theory that (1.1) possesses a critical line given by

$$K'_c = K'_{c,0} + c(J/J')^2 + O[(J/J')^2], \tag{1.3}$$

where $K' = \beta|J'|$, $K'_{c,0} (= \frac{1}{2} \ln(1 + 2^{1/2}))$ is the critical temperature for $J = 0$ and c is a positive constant with the approximate value

$$c \approx 0.134. \tag{1.4}$$

Along the line, the specific heat exponent varies as

$$\alpha = \alpha_1(J/J')^2 + O[(J/J')^2], \tag{1.5}$$

where α_1 has the approximate value

$$\alpha_1 \approx 1.496. \tag{1.6}$$

Our arguments are arranged as follows. In the following section we briefly describe the possible ground states of (1.1) and the associated critical surface. This knowledge helps to elucidate the possible phase transitions of the system. § 3 specialises to the regime (1.2) and we construct a perturbation expansion of the free energy about the line $J = 0, J' < 0$. The behaviour of the leading correction term, in the vicinity of the critical temperature of the unperturbed ($J = 0$) system, is analysed in § 4. On the basis of this behaviour, we argue in § 5 that the results of § 4 can be exponentiated to yield a continuous exponent which reduces to (1.5) in the simplest limit. A concluding discussion is given in § 6.

2. Ground states

Depending on the values of the interaction parameters, J and J' , the Hamiltonian (1.1) has three possible ground states. These are depicted in figure 1, where we also show the spin configuration in each state. The state SAF (sub-lattice anti-ferromagnetic) is of special interest because of its four-fold degeneracy. It is this state that according to Krinsky and Mukamel (1977) has a two-component order parameter.

Along the line $J = 0, J' < 0$, the system (1.1) decouples into two independent anti-ferromagnetic Ising models on square lattices with *nearest*-neighbour interactions J' . Hence along this line, (1.1) exhibits a conventional Ising anti-ferromagnetic

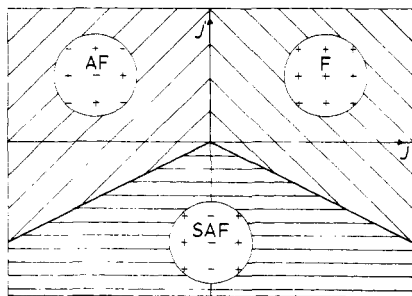


Figure 1. Possible ground states of Hamiltonian (1.1) as a function of J and J' .

transition at a temperature

$$T_c = |J'|/k_B K'_{c,0}, \quad K'_{c,0} = \frac{1}{2} \ln(1 + 2^{1/2}). \tag{2.1}$$

The fixed points and associated critical surfaces of (1.1) have been investigated using renormalisation group techniques (see e.g. Nauenberg and Nienhuis 1974, van Leeuwen 1975, Nightingale 1977). The intercept of this surface with the K - K' plane ($K' = \beta J, K' = \beta J'$) consists of two branches passing through the points ($K = 0, K' = +K'_{c,0}$) and ($K = 0, K' = -K'_{c,0}$) respectively. Van Leeuwen (1975) has argued on the basis of symmetry that this surface is cusped at the first point but smooth and analytic at the latter, which is the point of interest here.

Figure 1 indicates that there is no change in the nature of the ground state if J' is fixed at a negative value and a sufficiently small nearest-neighbour interaction J switched on to couple the two sub-lattices. In view of this observation and van Leeuwen's conjectured analyticity of the critical surface, we make the crucial assumption that at any finite temperature we can treat the thermodynamics for $J' < 0$ and J small by perturbation theory.

3. Perturbation expansion of the free energy

We will, therefore, expand the partition function

$$Z_N(K, K') = \sum_{\{\sigma\}} \exp\left(K \sum_{nn} \sigma\sigma' - K' \sum_{nnn} \sigma\sigma'\right) \tag{3.1}$$

in powers of K , where

$$K = \beta J > 0, \quad K' = \beta |J'| > 0. \tag{3.2}$$

As is usual in Ising problems, we write

$$\exp\left(K \sum_{nn} \sigma\sigma'\right) = (\cosh K)^{2N} \prod_{\langle ij \rangle} (1 + v\sigma_i\sigma_j), \tag{3.3}$$

where $\langle ij \rangle$ denotes a nearest-neighbour pair, and

$$v = \tanh K. \tag{3.4}$$

Expanding the product in (3.3) yields

$$Z_N(K, K') = (\cosh K)^{2N} Z_N(0, K') \left(1 + v \sum_{ij} \langle \sigma_i\sigma_j \rangle_0 + v^2 \sum_{\substack{\langle ij \rangle \\ \langle ij \rangle \neq \langle kl \rangle}} \sum_{\langle kl \rangle} \langle \sigma_i\sigma_j\sigma_k\sigma_l \rangle_0 + O(v^3)\right), \tag{3.5}$$

where the ensemble averages $\langle \dots \rangle_0$ are to be taken with respect to (1.1) with $J = 0$.

As observed above for $K = 0$ the system decouples into two independent nearest-neighbour Ising anti-ferromagnets; one on each of the sub-lattices of the original lattice. Hence if i and j are nearest-neighbour sites on the original lattice, they will be decoupled for $K = 0$. Thus we have

$$\sum_{\langle ij \rangle} \langle \sigma_i\sigma_j \rangle_0 = \sum_{\langle ij \rangle} \langle \sigma_i \rangle_0 \langle \sigma_j \rangle_0 = 0 \tag{3.6}$$

for all $T \geq 0$, since each sub-lattice is an anti-ferromagnet. The free energy per spin is

consequently to order v^2 given by

$$\beta f(K, K') = \beta f(0, K') - 2 \ln(\cosh K) + v^2[2 - f_1(K')] + O(v^3), \tag{3.7}$$

where

$$f_1(K') = \lim_{N \rightarrow \infty} N^{-1} \sum_{\langle ij \rangle} \sum_{\langle kl \rangle} \langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle_0. \tag{3.8}$$

Note that we have removed the restriction that the bond $\langle ij \rangle$ should not equal the bond $\langle kl \rangle$.

The leading term $\beta f(0, K')$ in (3.7) is simply the Onsager free energy and thus its singular part varies as

$$\beta f_s(0, K') \approx A(\Delta K')^2 \ln|\Delta K'| + \dots, \Delta K' \rightarrow 0, \tag{3.9}$$

where

$$\Delta K' = K' - K'_{c,0} \tag{3.10}$$

with $K'_{c,0}$ given by (2.1), and

$$A = 4/\pi. \tag{3.11}$$

4. Analysis of $f_1(K')$

We turn now to an analysis of $f_1(K')$, particularly near $K'_{c,0}$. To simplify the evaluation of $f_1(K')$, let us change notation as follows:

(a) Decompose the original lattice Ω into its two sub-lattices Ω_a and Ω_b . Label the sites of Ω_a by position vectors r . The sites of Ω_b are then located at positions $r \pm e_1$ and $r \pm e_2$ relative to r , where e_1 and e_2 are the unit lattice vectors of Ω .

(b) Denote the spin at site $r \in \Omega_a$ by $\sigma(r)$ and that at $r' \in \Omega_b$ by $\mu(r')$.

With this notation

$$\sum_{\langle ij \rangle} \sigma_i \sigma_j \Rightarrow \sum_{r \in \Omega_a} \sigma(r) [\mu(r + e_1) + \mu(r - e_1) + \mu(r + e_2) + \mu(r - e_2)]. \tag{4.1}$$

Substitution of this result in (3.8) allows an easy decoupling of the four-spin correlation into two-spin correlations on Ω_a and Ω_b . Explicitly we find that

$$\begin{aligned} & \sum_{\langle ij \rangle} \sum_{\langle kl \rangle} \langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle_0 \\ &= \sum_{r \in \Omega_a} \sum_{r' \in \Omega_a} \Gamma(r - r') [4\Gamma(r - r') \\ & \quad + \Gamma(r - r' + 2e_1) + 2\Gamma(r - r' + e_1 - e_2) + 2\Gamma(r - r' - e_1 + e_2) \\ & \quad + \Gamma(r - r' - 2e_1) + \Gamma(r - r' + 2e_2) + \Gamma(r - r' - 2e_2) \\ & \quad + 2\Gamma(r - r' + e_1 + e_2) + 2\Gamma(r - r' - e_1 - e_2)], \end{aligned} \tag{4.2}$$

where

$$\Gamma(r - r') = \langle \sigma(r) \sigma(r') \rangle_0 = \langle \mu(r) \mu(r') \rangle_0 \tag{4.3}$$

is the correlation between two spins at sites r and r' of a nearest-neighbour Ising anti-ferromagnet on a square lattice. All terms in (4.2) can now be regarded as referring to the *same* lattice specified by the unit vectors

$$\delta_1 = e_1 + e_2 \quad \text{and} \quad \delta_2 = e_1 - e_2. \tag{4.4}$$

Equation (4.2) immediately reveals the crucial role of anti-ferromagnetic coupling J' . If J' were positive, all terms in (4.2) would be positive and the sum would *diverge* at T_c . However, for an anti-ferromagnet $\Gamma(r - r')$ is negative if the sites r and r' lie on different sub-lattices. With this in mind, we can determine the signs of the various terms in (4.2).

Assume r and r' belong to the same sub-lattice so that $\Gamma(r - r')$ is positive. Then the sites r' and $r \pm \delta_2$ belong to different sub-lattices so that $\Gamma(r - r' \pm \delta_2)$ is negative. Conversely sites r' and $r \pm (\delta_1 \pm \delta_2)$ ($= r \pm 2e_i$) will belong to the same sub-lattice implying that $\Gamma(r - r' \pm 2e_i)$ is positive. If r and r' belong to different sub-lattices so that $\Gamma(r - r')$ is negative, the same argument goes through but with all signs reversed.

This argument allows (4.2) to be reduced to

$$f_1(K') = \sum_r \Gamma(r) \Delta_r^2 \Gamma(r), \tag{4.4}$$

where $\Gamma(r) = \langle \sigma(0)\sigma(r) \rangle$ is now the correlation function in a *ferromagnetic* Ising model with coupling $-J' > 0$. These have been extensively investigated and calculated by several authors (see e.g. Kaufman and Onsager 1949, Fisher and Burford 1969, Wu *et al* 1976). The operator Δ_r^2 appearing in (4.4) is a lattice difference operator defined by

$$\begin{aligned} \Delta_r^2 g(r) = & 4g(r) - 2g(r + \delta_1) - 2g(r - \delta_1) - 2g(r + \delta_2) \\ & - 2g(r - \delta_2) + g(r + \delta_1 + \delta_2) + g(r - \delta_1 - \delta_2) \\ & + g(r + \delta_1 - \delta_2) + g(r - \delta_1 + \delta_2). \end{aligned} \tag{4.5}$$

For future reference, we note that if (4.5) is expanded in the lattice spacing a , we can approximate Δ_r^2 by

$$\Delta_r^2 g(r) = a^4 \frac{\partial^4}{\partial x^2 \partial y^2} g(x, y) + O(a^6). \tag{4.6}$$

An alternative expression for $f_1(K')$ follows if we Fourier transform. Defining

$$\hat{\Gamma}(q) = \frac{1}{\sqrt{N}} \sum_r \Gamma(r) \exp(iq \cdot r) \tag{4.7}$$

we obtain

$$f_1(K') = 2 \sum_q |\hat{\Gamma}(q)|^2 [2 - 2 \cos q_x a - 2 \cos q_y a + \cos(q_x + q_y) a + \cos(q_x - q_y) a], \tag{4.8}$$

where a is the lattice spacing. Near the critical temperature, the summand behaves as $q^{-4+1/2} q_x^2 q_y^2 \sim q^{1/2}$ for small q , and hence $f_1(K')$ converges.

The required asymptotic behaviour of $f_1(K')$ near $K'_{c,0}$ now follows from known results for $\Gamma(r)$. In particular, since (see e.g. Fisher and Burford 1967)

$$\Gamma(r) = \Gamma_c(r) - E(r) \Delta K' \ln |\Delta K'| \dots \tag{4.9}$$

as $\Delta K' \rightarrow 0$ for all r , we obtain

$$f_1(K') = f_{1,c} - p\Delta K' \ln|\Delta K'| + q(\Delta K')^2(\ln|\Delta K'|)^2 + O[(\Delta K')^2 \ln|\Delta K'|] \tag{4.10}$$

The coefficients appearing in this expression are given by

$$f_{1,c} = \sum_r \Gamma_c(r)\Delta_r^2\Gamma_c(r), \tag{4.11}$$

$$p = \sum_r (\Gamma_c(r)\Delta_r^2E(r) + E(r)\Delta_r^2\Gamma_c(r)) \tag{4.12}$$

and

$$q = \sum_r E(r)\Delta_r^2E(r). \tag{4.13}$$

For large $r = |r|$, we have (see e.g. Wu *et al* 1976),

$$\Gamma_c(r) \approx D_0(a/r)^{1/4} \tag{4.14}$$

$$E(r) \approx 2D_0(r/a)^{3/4}, \tag{4.15}$$

where

$$D_0 = 0.703380 \dots \tag{4.16}$$

Whilst (4.5) implies that $E(r)$ diverges for large r , it is straightforward to check using the integral test and (4.6) that all sums in (4.11)–(4.13) converge for all $T \geq 0$.

5. Specific heat exponent for small J

Substituting the expansion (4.10) in (3.7) and making use of (3.9) implies that the singular part of $f(K, K')$ varies, near the critical temperature $K'_{c,0}$ of the unperturbed system ($J = 0$), as

$$\beta f_s(K, K') \approx A(\Delta K')^2 \ln|\Delta K'| + pv^2\Delta K' \ln|\Delta K'| - qv^2(\Delta K')^2[\ln|\Delta K'|]^2 + \dots \tag{5.1}$$

The correction terms in this expansion are of $O[v^2(\Delta K')^2 \ln|\Delta K'|]$ from $f_1(K')$ and $O[(\Delta K')^2 \ln|\Delta K'|]$ from $f_s(0, K')$ and we have absorbed all non-singular terms into the regular part of $f(K, K')$.

The structure of (5.1) is very suggestive. Indeed, Kadanoff and Wegner (1971), in their discussion of the eight-vertex model (Baxter 1972), argued that the appearance of logarithmic factors in a perturbation expansion, such as (5.1), could be an indication of a marginal operator. The existence of such an operator, in turn, implies the possibility of non-universal behaviour. Thus we compare (5.1) with the expansion for small v of

$$\beta f_s(K, K') \approx A(\Delta K')^2([1 - |\Delta K'|^{-\alpha(v^2)}]/\alpha(v^2)), \tag{5.2}$$

where

$$\Delta K' = \Delta K' + \epsilon(v^2) \tag{5.3}$$

In (5.2) and (5.3) both $\alpha(v^2)$ and $\epsilon(v^2)$ are assumed to tend smoothly to zero as v goes to zero. Expanding (5.2) to first order in α and ϵ reproduces (5.1) if

$$\alpha(v^2) = (2q/A)v^2 + O(v^2) \tag{5.4}$$

and

$$\epsilon(v^2) = (p/2A)v^2 + O(v^2) \tag{5.5}$$

To evaluate these results quantitatively, we require estimates of the constants p and q defined by (4.12) and (4.13). Unfortunately, exact values of $\Gamma_c(\mathbf{r})$ and $E(\mathbf{r})$ are known for only a few lattice vectors \mathbf{r} with $|\mathbf{r}|$ relatively small. Indeed, $E(\mathbf{r})$ appears only to have been evaluated for $r/a \leq 5^{1/2}$ (see e.g. Fisher and Burford 1967). Thus to estimate p and q we make the following approximations:

(a) For $r/a > 5^{1/2}$, we approximate $\Gamma_c(\mathbf{r})$ and $E(\mathbf{r})$ by their asymptotic expressions (4.14) and (4.15) respectively.

(b) The sums in (4.12) and (4.13) are then performed numerically out to $|\mathbf{r}| = r_0$, with the remainder approximated by an integral, in which Δ^2 is replaced by the continuum approximation (4.6).

In this way, we estimate

$$p \approx -1.759 \quad q \approx 4.903 \tag{5.6}$$

The main source of error is presumably the first approximation. However, comparison of the asymptotic formulae with the exact values tabulated by Fisher and Burford (1967) indicates that even at $r/a = 5^{1/2}$, the error is 1% or so. Hence the estimates (5.6) can be considered as reasonable, with an error of probably no more than a few percent. We shall use these values in the remainder of the paper.

6. Conclusion

In the preceding section, we showed that it is possible to adsorb the second-order perturbation theory corrections for small J into a shift in the critical temperature and a *continuous* non-universal exponent. At this stage, it is convenient to rewrite the above results in a more natural form. To do so, we take $K' = \beta|J'|$ as our basic temperature variable and define

$$\lambda = J/|J'|. \tag{6.1}$$

For finite λ , the critical temperature $K'_c = K'_c(\lambda)$ is determined by

$$\Delta \dot{K}' = 0. \tag{6.2}$$

Hence from (5.5), we find that K'_c is the solution of

$$K'_c = K'_{c,0} - (p/2A) \tanh^2 \lambda K'_c + O(\lambda^2) \tag{6.3}$$

The specific heat exponent α can now be expressed as

$$\alpha(\lambda) = (2q/A) \tanh^2 \lambda K'_c + O(\lambda^2) \tag{6.4}$$

The solution of (6.3) for $K'_c(\lambda)$ is plotted in figure 2 for $0 \leq \lambda \leq 0.8$. A similar plot of $\alpha(\lambda)$ is given in figure 3. Note that these curves should only be considered as schematic since they are based on results valid only to second order in $\tanh \lambda K'_c$. If $\tanh \lambda K'_c$ is replaced by $\lambda K'_{c,0}$, (6.3) and (6.4) reduce to the results, (1.3) and (1.5), quoted in the Introduction. These approximations are indicated in the figures by the broken curves.

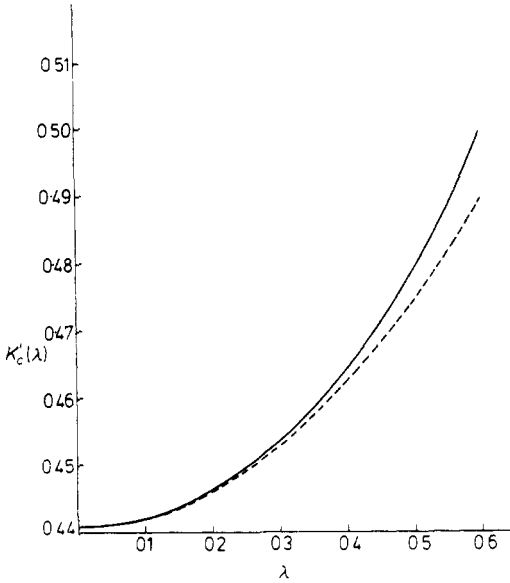


Figure 2. Variation of the critical temperature K'_c with $\lambda = J/|J'|$. The full curve represents the solution of (6.3), while the broken curve is the simpler approximation (1.3).

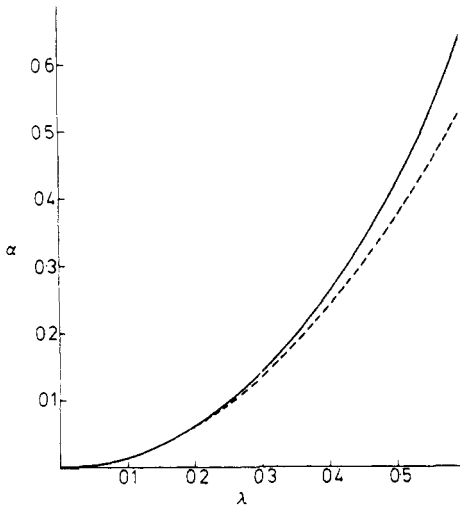


Figure 3. Variation of the specific heat exponent α with $\lambda = J/|J'|$. The full curve represents (6.4), while the broken curve is the simpler approximation (1.5).

The crucial assumption underlying this perturbation calculation (recall § 2) concerns the analyticity of the critical parameters for $J' < 0$ and small λ . This has certainly not been established. However, if a similar argument is applied (Kadanoff and Wegner 1971) to the eight vertex model, Baxter's exact results are recovered to leading order in the four-spin interaction. This success gives us confidence that the analysis described in this paper is valid.

As noted earlier, Nightingale (1977) has performed approximate renormalisation group calculations on (1.1). Unfortunately, the smallest value of λ considered was $\lambda \approx 0.44$ [$K = 0.2$] for which he estimated

$$\alpha \approx 0.07 \quad K'_c \approx 0.448. \quad (6.5)$$

These values are considerably smaller than those predicted by (6.3) and (6.4) which give

$$\alpha \approx 0.3 \quad K'_c \approx 0.47. \quad (6.6)$$

This discrepancy is, however, of little significance in view of the large value of λ involved. On the other hand, Nightingale's results do show a definite curvature as a function of K which could be consistent with the quadratic predictions of (6.3) and (6.4).

Plischke and Oitmaa (1978) have recently generated high-temperature series expansions for the staggered susceptibility of (1.1) and a three-dimensional analogue. Unfortunately, the two dimensional series are too short for any definite conclusions to be reached. Additional renormalisation group and/or series investigations would be highly desirable.

Despite the unsatisfactory situation described in the preceding paragraphs, the argument of van Leeuwen (1975) and Nightingale's results suggest that the square lattice Ising model with competing nearest and next-nearest interactions does possess a non-universal critical line beyond the regime in which the analysis described here is valid. In view of the argument of Krinsky and Mukamel (1977) it seems reasonable to conjecture that this line is one of the critical lines which emerge from the two-dimensional planar model's multi-critical point (José *et al* 1977). The four-fold degeneracy of the ground state (see § 2) suggests that the line may be isomorphic to that analysed by Kadanoff (1977). If this is so, and we accept Kadanoff's arguments, then along the non-universal line (1.1) should be in the same universality class as the Ahskin-Teller and eight-vertex models. It would be very interesting if this relationship could be exhibited more explicitly.

A final very intriguing question concerns the behaviour as the system crosses the boundaries between the SAF and A or F phases (see figure 1). If $J = -2J'$, it seems certain that there is no long-range order, since the ground-state energy remains invariant to the spin-flip of alternating rows (or columns). Does this imply that $T_c = 0$? Or is it possible that the model still possesses a finite transition temperature isomorphic to the planar model's multicritical point? It is hoped to return to these questions in a later publication.

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