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1977 J. Phys. A: Math. Gen. 10 L67

(http://iopscience.iop.org/0305-4470/10/4/004)

J. Phys. A: Math. Gen., Vol. 10, No. 4, 1977. Printed in Great Britain. © 1977

LETTER TO THE EDITOR

Numerical evidence for two critical points in a triplet Ising model

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Received 25 January 1977

Abstract. It is shown that numerical data recently used to evaluate the residual entropy of Kagomé ice can be adapted to form an expansion for the zero field free energy of a three-spin Ising model on a triangulated dice lattice. The expansion is used to test a recent conjecture of Wu, that this model should exhibit two phase transitions.

Recently the authors (Wood and Pegg 1977, to be referred to as I) have shown that in the thermodynamic limit the zero field free energy per site, f, of a large class of planar triplet Ising models satisfies the duality relation

$$f(K) = \ln \sinh 2K + f(K^*), \tag{1}$$

where $K = \beta J$ and K^* is the usual dual temperature defined by

$$\sinh 2K \sinh 2K^* = 1. \tag{2}$$

In the two cases where such triplet models are defined on the Union Jack lattice (Hintermann and Merlini 1972) and the triangular lattice (Baxter and Wu 1973, 1974) f is known exactly, and both triplet models exhibit one phase transition point which is therefore located at the temperature predicted by using (1) and the uniqueness postulate of Wannier (1945). The duality relation (1) holds for any plane triangulation which is a maximal plane graph containing an even number of triangles incident at each vertex. Wu (1977) has recently argued that triplet models on such triangulations may exhibit two phase transitions, and considers in detail the dice lattice triangulation introduced in I and shown in figure 1. Wu reduces this triplet model to an equivalent

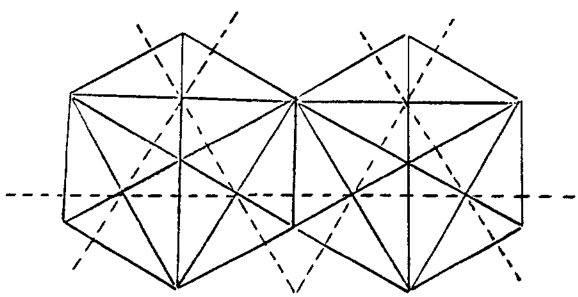

Figure 1. The triangulated dice lattice shown by the full lines, the Kagomé sublattice relating to the expansions (5) and (8) is shown by the broken lines.

Ashkin–Teller (AT) model on the triangular lattice (Ashkin and Teller 1943). We mention in passing that this triplet model can also be reduced to two other equivalent AT models, one on the honeycomb lattice with Boltzmann weights

$$\sqrt{\omega_1} = \tanh 2K, \qquad \sqrt{\omega_2} = 1/\cosh 2K, \qquad \omega_3 = 0, \tag{3}$$

and the other on the Kagomé lattice with weights

$$\omega_1 = \tanh 2K, \qquad \omega_2 = 1/\cosh 2K, \qquad \omega_3 = 0 \tag{4}$$

where the notation of Wu (1977) is used.

Following the earlier procedure of Wu and Lin (1974) Wu constructs the expected form of the critical surface of the AT model on the triangular lattice, and concludes that the thermodynamic path given by (3) ($\omega_1 + \omega_2 = 1$) will intersect the critical surface at two points yielding two critical temperatures which are probably associated with sublattice order parameters which become zero at different temperatures. Wu raises the question of seeking evidence for two transition temperatures from a series expansion of f, and in this letter we show that a recent numerical study of the residual entropy of Kagomé lattice ice (Lin and Tang 1976) can be used in conjunction with results obtained in I to form a low temperature series expansion of f.

In I it was shown possible to develop a *low* temperature series expansion of f for any plane triangulation in the form of a weak graph expansion (Nagle 1968), but one in which only the *polygonal* subgraphs contribute to the expansion. The expansion parameters for these expansions can be expressed as simple functions of the usual low temperature variable $u = \exp(-4K)$ but depend upon lattice structure. In particular the expansion of F_{6N} on the dice lattice model (assumed to have $6N$ sites) can be written in the form

$$\exp(-\beta F_{6N}) = 2^{3N} \cosh^{3N} 4K \sum_{g(p)} \omega^{n_2} \tag{5}$$

where $g(p)$ defines the set of polygonal subgraphs on the $3N$ site Kagomé sublattice shown in figure 1, n_2 is the number of degree 2 vertices in $g(p)$, and

$$\omega = 2u/(1+u^2). \tag{6}$$

At $\omega = \frac{1}{3}$ which is also the dual point ($K = K^*$, $\sqrt{u} = \sqrt{2} - 1$) the expansion (6) is identical with Nagle's weak graph expansion for the residual entropy of Kagomé ice (Nagle 1968). This version of the ice problem has been examined numerically by Lin and Tang (1976) who evaluated the coefficients in the series

$$W_{3N} = (\tfrac{3}{2})^{3N}\Big(1 + \sum_{g(p)} 3^{-n_2}\Big), \tag{7}$$

and

$$W = (\tfrac{3}{2})^{3}\Big(1 + \sum_{m} \phi_m 3^{-m}\Big) \tag{8}$$

up to the coefficient ϕ_{12}. In (8) the thermodynamic limit has been taken, and we can see from (5) that the coefficients can be used to form an expansion for f. For the present purpose it is more convenient to use the usual low temperature variable u, in terms of which we find that the free energy of the dice lattice is given by

$$-\beta f = 3\ln(u+u^{-1})+16u^3+48u^4+144u^5+576u^6+2976u^7+15456u^8$$
$$+75509\tfrac{1}{3}u^9+371520u^{10}+1944240u^{11}+9484432u^{12}+\ldots. \quad (9)$$

While it may not be possible to determine the radius of convergence of (9) with much accuracy it might be possible to test Wu's conjecture of two critical points, since if $u_c^{1/2} \neq \sqrt{2}-1$ we must have at least two singularities in f. Although the coefficients in (9) remain positive the terms are much too irregular to use any ratio method, and we have obtained numerical estimates of u_c from the Padé approximants to the logarithmic derivative of the specific heat series formed from (9). The results are summarized in the form of a pole–residue plot (here the residue is the low temperature specific heat exponent α') shown in figure 2. Earlier experience with such pole–residue plots (Ritchie

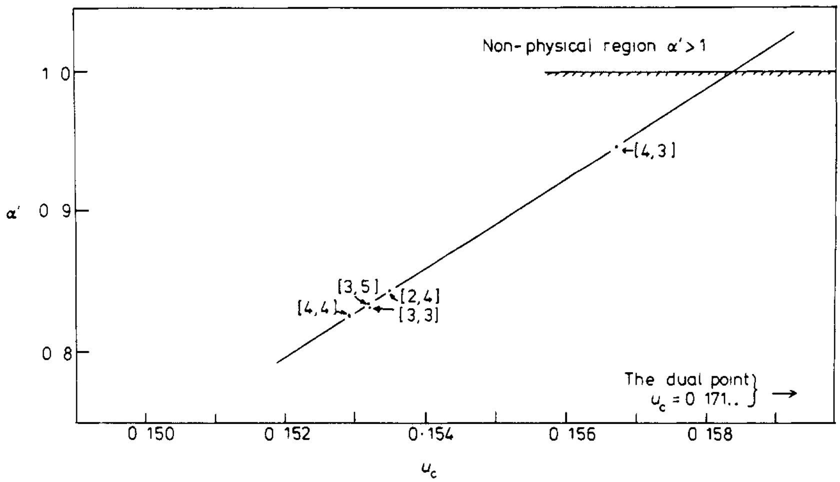

Figure 2. A pole–residue plot of the singularities u_c and the exponent α' obtained from the Padé approximants to the logarithmic derivative of the specific heat series formed from (9).

and Essam 1975, Wood and Griffiths 1976, Essam *et al* 1976) indicates that the exact location of the singularity is commonly found to be sufficiently close to the pole–residue curve to be able to rule out a single phase transition in this case. In addition we are aided by being able to reject the unphysical domain $\alpha' > 1$, which would yield a divergence in the internal energy function. The pole–residue plot for the specific heat function strongly suggests that

$$u_c^{1/2} < \sqrt{2}-1 \quad (10)$$

thus supporting Wu's prediction of two phase transitions in this triplet model.

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