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Spontaneous magnetisation of the Ising model on a 3-12 lattice

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Abstract. We have calculated exactly the spontaneous magnetisation of the Ising model on a 3-12 lattice with nine different coupling constants and six different magnetic moments. Our result is a generalisation of Huckaby's work on an isotropic 3-12 lattice with two different coupling constants and the same magnetic moment for all spins. A low-temperature series expansion is derived to check our result.

1. Introduction

The spontaneous magnetisation of the Ising model on a rectangular lattice was first obtained by Onsager (1949), although he never published his derivation. Yang (1952) was the first to publish a derivation of the spontaneous magnetisation of the Ising model on a square lattice, and his result was generalised by Chang (1952) to a rectangular lattice. Recently Huckaby (1986) derived exactly the spontaneous magnetisation of the Ising model on an isotropic 3-12 lattice with a coupling constant R between a pair of neighbouring spins on the same triangle and a coupling constant L between a pair of neighbouring spins on different triangles. The magnetic moments are assumed to be the same for all spins. His result was used by Huckaby and Shinmi (1986) to calculate the properties of a three-component system on a honeycomb lattice. The motivation of the present paper is to generalise Huckaby's work to a general 3-12 lattice with nine different coupling constants and six different magnetic moments.

2. The Ising model on a 3-12 lattice

We consider the Ising model on a 3-12 lattice with $6N$ sites as shown in figure 1. The partition function is

$$Z_{3-12} = \sum_{S_i} \exp \left(\sum_{ij} J_{ij} S_i S_j + \sum_i H m_i S_i \right) \quad (1)$$

where S_i takes the values ± 1 , J_{ij} is the coupling constant (in units of kT) between spins on sites i and j , m_i is the magnetic moment for spin on site i , and H is the magnetic field. There are nine coupling constants and six magnetic moments (see figure 1). The isotropic 3-12 lattice corresponds to the case $J_i = J'_i = R$, $J''_i = L$ and $m_i = m'_i = m$. We use the star-triangle transformation (Syozzi 1972) to relate the partition function on a 3-12 lattice to the partition function on a doubly decorated honeycomb lattice (see figure 2). We have

$$Z_{3-12} = A^N A'^N Z_{DH} \quad (2)$$

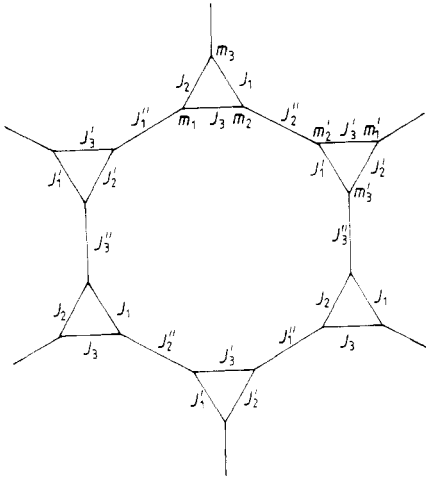


Figure 1. The unit cell of a 3-12 lattice with nine different coupling constants and six different moments.

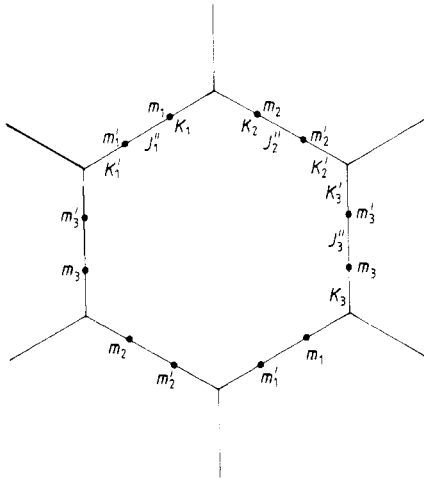


Figure 2. The unit cell of a doubly decorated honeycomb lattice.

where

$$A = (C_1 C_2 C_3 + S_1 S_2 S_3) / 2 \cosh K_1 \cosh K_2 \cosh K_3$$

$$C_i = \cosh J_i \quad S_i = \sinh J_i$$

$$\tanh^2 K_i = (C_j S_k S_i + S_j C_k C_i) (C_k S_i S_j + S_k C_i C_j) / (C_1 C_2 C_3 + S_1 S_2 S_3) (C_i S_j S_k + S_i C_j C_k)$$

K_i and K'_i are coupling constants on the doubly decorated honeycomb lattice as shown in figure 2, and (ijk) is a cyclic permutation of (123) .

We next use a decoration transformation (Naya 1954, Huckaby 1986) to relate Z_{DH} to the partition function on a honeycomb lattice. We define

$$h_i = Hm_i \quad h'_i = Hm'_i. \tag{3}$$

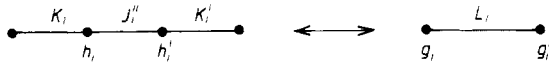


Figure 3. The decoration transformation.

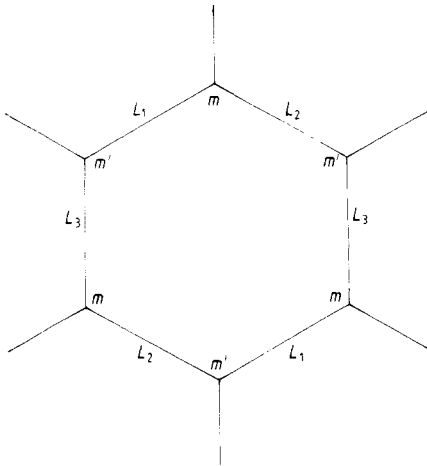


Figure 4. The unit cell of a honeycomb lattice with three different coupling constants and two different magnetic moments.

The decoration transformation (see figure 3) is

$$\begin{aligned}
 e^{J''} \cosh(h + h' + K + K') + e^{-J''} \cosh(h - h' + K - K') \\
 &= (B/2) \exp(L + g + g') \\
 e^{J''} \cosh(h + h' - K - K') + e^{-J''} \cosh(h - h' - K + K') \\
 &= (B/2) \exp(L - g - g') \\
 e^{J''} \cosh(h + h' + K - K') + e^{-J''} \cosh(h - h' + K + K') \\
 &= (B/2) \exp(-L + g - g') \\
 e^{J''} \cosh(h + h' - K + K') + e^{-J''} \cosh(h - h' - K - K') \\
 &= (B/2) \exp(-L - g + g').
 \end{aligned} \tag{4}$$

We have

$$Z_{DH} = (B_1 B_2 B_3)^N Z_H \tag{5}$$

where Z_H is the partition function on a honeycomb lattice (see figure 4) with coupling constants L_1, L_2, L_3 and magnetic moments m and m' such that

$$\begin{aligned}
 m &= (g_1 + g_2 + g_3) / H \\
 m' &= (g'_1 + g'_2 + g'_3) / H.
 \end{aligned} \tag{6}$$

3. Spontaneous magnetisation on a 3-12 lattice

The spontaneous magnetisation on a 3-12 lattice is given by

$$I_{3-12} = \partial \lim_{N \rightarrow \infty} [(6N)^{-1} \ln Z_{3-12}] / \partial H |_{H=0}. \tag{7}$$

When $H = 0$, we have

$$\partial \ln B_i / \partial H = \partial \ln A / \partial H = \partial \ln A' / \partial H = \partial L_i / \partial H = 0$$

$$\exp(2L_i) = \frac{\exp(2J_i'') \cosh(K_i + K_i') + \cosh(K_i - K_i')}{\exp(2J_i'') \cosh(K_i - K_i') + \cosh(K_i + K_i')}$$

$$m + m' = \frac{\sum_{i=1}^3 [(m_i + m_i') \sinh(K_i + K_i') + (m_i - m_i') \exp(-2J_i'') \sinh(K_i - K_i')]}{[\cosh(K_i + K_i') + \exp(-2J_i'') \cosh(K_i - K_i')]} \tag{8}$$

It follows from equations (7) and (8) that

$$I_{3-12} = I_H / 3 \tag{9}$$

where I_H is the spontaneous magnetisation per spin on a honeycomb lattice in which one of the two triangular sublattices consists of spins with magnetic moment m , and the other consists of spins with magnetic moment m' as shown in figure 4. The special case of $m' = 0$ was considered by Naya (1954), who called such a lattice a semiferromagnetic lattice. Naya showed that the spontaneous magnetisation of the semiferromagnetic honeycomb lattice was exactly half that of the normal ferromagnetic honeycomb lattice. Naya's argument can be generalised to arbitrary m' such that

$$I_H(m, m') = \frac{1}{2}(m + m')I_H(1, 1). \tag{10}$$

Therefore finally we get

$$I_{3-12} = 6^{-1}(m + m')(1 - k^2)^{1/8} \tag{11}$$

where

$$k^2 = 16(1 + x_1 x_2 x_3)(x_1 + x_2 x_3)(x_2 + x_1 x_3)(x_3 + x_1 x_2)[(1 - x_1^2)(1 - x_2^2)(1 - x_3^2)]^{-2}$$

$$x_i = \exp(-2L_i).$$

A low-temperature series expansion has been calculated to check our result. We define

$$y_i = \exp(-2J_i) \quad y_i' = \exp(-2J_i') \quad z_i = \exp(-2J_i'')$$

$$\sum f(i, j) = f(1, 2) + f(1, 3) + f(2, 3) \tag{12}$$

$$\sum g(i, j, k) = g(1, 2, 3) + g(2, 3, 1) + g(3, 1, 2).$$

The series expansion is

$$I_{3-12} = [m_1 M(y_1, y_2, y_3, y_1', y_2', y_3', z_1, z_2, z_3) + m_2 M(y_2, y_1, y_3, y_2', y_1', y_3', z_2, z_1, z_3)$$

$$+ m_3 M(y_3, y_1, y_2, y_3', y_1', y_2', z_3, z_1, z_2)$$

$$+ m_1' M(y_1', y_3', y_2', y_1, y_3, y_2, z_1, z_3, z_2)$$

$$+ m_2' M(y_2', y_3', y_1', y_2, y_3, y_1, z_2, z_3, z_1)$$

$$+ m_3' M(y_3', y_2', y_1', y_3, y_2, y_1, z_3, z_2, z_1)] / 6 \tag{13}$$

where

$$M(y_1, y_2, y_3, y_1', y_2', y_3', z_1, z_2, z_3) = 1 + \sum_{i=3}^{\infty} M_i$$

$$M_3 = -2z_1(z_2 z_3 + y_2 y_3)$$

$$M_4 = -2y_2 y_3 y'_2 y'_3 - 2 \sum z_i z_j (z_i z_j + y_i y_j + y'_i y'_j)$$

$$M_5 = 2z_1 y_1^2 y_2 y_3 - 6z_1 z_2 z_3 (z_1^2 + z_2^2 + z_3^2) - 2 \sum z_i (y_i y_j + y'_i y'_j) (y_i y_k + y'_i y'_k) \\ - 4 \sum z_i (z_j^2 + z_k^2) (y_j y_k + y'_j y'_k)$$

$$M_6 = 2(z_1 y_2 y_3)^2 - 30(z_1 z_2 z_3)^2 + 4z_1^2 z_2 z_3 y_2 y_3 + 2(z_1^2 + y_1^2 + y_1'^2) y_2 y_3 y'_2 y'_3 \\ - 4 \sum z_i^4 (z_j^2 + z_k^2) - 2(y_1 y_2 + y'_1 y'_2) (y_1 y_3 + y'_1 y'_3) (y_2 y_3 + y'_2 y'_3) \\ - 2 \sum (z_i^2 + z_j^2) (y_i y_j + y'_i y'_j)^2 - 6 \sum (y_i^2 y_j y_k + y_i'^2 y'_j y'_k) z_j z_k \\ - 8 \sum z_i z_j y_k y'_k (y_i y'_j + y'_i y_j) - 16z_1 z_2 z_3 \sum z_i (y_j y_k + y'_j y'_k) \\ - 6 \sum (z_i^3 z_j + z_i z_j^3) (y_i y_j + y'_i y'_j)$$

$$M_7 = 4z_1 z_2 z_3 y_2 y_3 y'_2 y'_3 + 4z_1 y_2 y_3 \sum z_i z_j (z_i z_j + y_i y_j + y'_i y'_j) \\ + 2z_1 y_2 y_3 [(y'_2 y'_3)^2 - y_1^2 (y_2^2 + y_3^2) + 2y_2 y_3 y'_2 y'_3] \\ - 10z_1 z_2 z_3 (z_1^4 + z_2^4 + z_3^4) - 46z_1 z_2 z_3 \sum (z_i z_j)^2 \\ - \sum z_i [8(z_j^4 + z_k^4) + 12z_i^2 (z_j^2 + z_k^2) + 60z_j^2 z_k^2] (y_j y_k + y'_j y'_k) \\ - \sum z_i [6z_i^2 + 16(z_j^2 + z_k^2)] (y_i y_j + y'_i y'_j) (y_i y_k + y'_i y'_k) \\ + 2 \sum [2z_i (z_j^2 + z_k^2) + z_j (y_i y_j + y'_i y'_j) + z_k (y_i y_k + y'_i y'_k)] (y_i^2 y_j y_k + y_i'^2 y'_j y'_k) \\ - 4 \sum [4z_1 z_2 z_3 + z_i (y_j y_k + y'_j y'_k) + z_j (y_i y_k + y'_i y'_k)] (y_i y_j + y'_i y'_j)^2.$$

The low-temperature series expansion agrees with the exact formula (11) up to the seventh order.

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