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Magnetization of the three-spin triangular Ising model

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Abstract. Below its critical temperature, the triangular Ising model with pure three-spin interactions has a spontaneous magnetization M. The first 13 terms of a series expansion for M are known. Here these are re-arranged into a form which can be extrapolated to all terms in a natural way. Thus a conjecture is obtained for M. It fits the scaling prediction $\beta = 1/12$.

Another order parameter is similarly discussed, together with the difficulties encountered in applying the technique to the two-spin Ising model susceptibility.

1. Introduction and summary

The free energy f has now been obtained exactly for several two-dimensional lattice models in statistical mechanics, and it is possible to see common properties in the mathematical solutions. In particular, there appear to be 'natural parameters' (here denoted simply by x) that occur in the working, such that if we use these rather than the original interaction energies or Boltzmann weights, then the free energy can be written as the logarithm of a fairly simple infinite product. (The F and KDP models in their disordered states are exceptions.)

The order parameter, ie the spontaneous magnetization M or polarization P, has been calculated for only some of these models, but in each case can be written as a very simple infinite product in terms of the natural parameters.

In this paper we first illustrate these remarks by considering the normal two-spin Ising model on the square lattice, and the F model. For these both f and M (or P) are known.

We then consider the triangular Ising model with pure three-spin interactions, for which f is known, but not M or P. (Both order parameters can be defined for this model.) From the working for f we know how to construct the 'natural parameter' x for the model. We then take the available low-temperature series expansions for P and M (which we have obtained to twelfth order), express them in terms of x and remark that the series simplify enormously. Further, by comparing these series with the exact results for the other models, we are led to conjecture what the infinite series may be, ie to conjecture expressions for M and P.

The expression for M agrees with the scaling predictions for the critical exponent β_M.

Finally, we try to apply similar ideas to the high-temperature susceptibility of the two-spin square lattice Ising model, but are not able to find any simple function of x that fits the available series expansions.

2. Two-spin square lattice Ising model

As Onsager showed in 1944, the free energy of this model can be expressed in terms of elliptic functions. Here we use the notation developed by one of us (Baxter 1972) by noting that the isotropic Ising model with two-spin interaction $-J\sigma_1\sigma_2$ between nearest neighbours is equivalent to an eight-vertex model with weights

$$c = d^{-1} = e^{2\beta J}, \qquad a = b = 1, \tag{1}$$

where $\beta = 1/kT$ is the Boltzmann factor.

From equation (5.7), with b negated, of Baxter (1972), we are led to introduce elliptic functions of modulus k (*not* Boltzmann's constant), given by $0 < k \leqslant 1$ and

$$k^{1/2}+k^{-1/2} = 2\sinh^2(2\beta J). \tag{2}$$

Here we consider the low-temperature regime, when $\sinh 2\beta J \geqslant 1$.

If K, K' are the associated complete elliptic integrals of the first kind, then we find from this equation (5.7) that $v = 0$, $\eta = iK'/4$, and

$$e^{-2\beta J} = -ik^{1/2}\,\mathrm{sn}(iK'/4). \tag{3}$$

From equation (8.146.23) of Gradshteyn and Ryzhik (1965 to be referred to as GR) it follows that

$$e^{-2\beta J} = x^{1/2}\prod_{n=1}^{\infty}\frac{(1-x^{8n-7})(1-x^{8n-1})}{(1-x^{8n-5})(1-x^{8n-3})}, \tag{4}$$

where $x = \exp(-\pi K'/4K)$ and $0 < x < 1$. Setting $q = x^4$, $z = 1$ in equation (D.37) of Baxter (1972), we find the free energy per site f is given by

$$-\beta f = 2\beta J + \sum_{n=1}^{\infty}\frac{x^{2n}(1-x^n)^2(1-x^{2n})^2}{n(1+x^{2n})(1-x^{8n})}. \tag{5}$$

Here x is the 'natural parameter', and can be regarded as defined by equation (4). The free energy is then given by (5). At low temperatures x is small, so these equations are suitable for comparison with series expansions. As the temperature T increases from 0 to the critical temperature T_c, x increases from 0 to 1.

By Taylor-expanding the summand in (5) and performing the n summation for each term, we can write $\exp[-\beta(f+2J)]$ as an infinite product of the form

$$\prod_{n=1}^{\infty}(1-x^n)^{c_n}, \tag{6}$$

where the exponents c_n are integers. In this case they appear to be somewhat complicated.

However, the spontaneous magnetization M can be expressed very simply as such an infinite product. From Yang (1952) and equation (2),

$$M = \left(\frac{1-k}{1+k}\right)^{1/4} \tag{7}$$

$$= \prod_{n=1}^{\infty}\frac{1-x^{4n-2}}{1+x^{4n-2}} \tag{8}$$

$$= 1-2x^2+2x^4-4x^6+6x^8+\dots \tag{9}$$

(using (8.197.4) of GR).

Note that here the definition (4) of the natural parameter x involves elliptic functions, or more precisely the sort of infinite products that occur in the expansion of elliptic functions. This appears to be generally true, though there are exceptions, such as the following example.

3. F Model

The free energy of this model was obtained by Lieb (1967). Baxter (1971, 1973a, b) showed that if one introduces a parameter x (or t), defined by

$$x+x^{-1} = e^{2\beta\epsilon}-2 = (c/a)^2-2, \tag{10}$$

then below T_c we can define $0 < x < 1$, and the free energy f and spontaneous staggered polarization P are given by:

$$\exp(-\beta f) = \frac{1}{1-x^2}\prod_{n=1}^{\infty}\left(\frac{1-x^{4n-1}}{1-x^{4n+1}}\right)^2, \tag{11}$$

$$P = \prod_{n=1}^{\infty}\left(\frac{1-x^{2n}}{1+x^{2n}}\right)^2. \tag{12}$$

Thus again we can define a 'natural' parameter x such that $\exp(-\beta f)$ and the order parameter are infinite products of the general type (6). In this case x is simply an algebraic function of the Boltzmann weights; it increases from 0 to 1 as T increases from 0 to T_c.

One can also think of the F model as a limiting case of the eight-vertex model, and the eight-vertex model as an Ising model with two- and four-spin interactions (Wu 1971, Kadanoff and Wegner 1971). Then one can define a spontaneous magnetization for the F model. This has been evaluated by one of us (RJB) and found to be given by

$$M = \prod_{n=1}^{\infty}\frac{1-x^{4n-2}}{1+x^{4n-2}}. \tag{13}$$

Note that the expression is the same as that, (8), for the Ising model (but the x's are different). This was part of the evidence used by Barber and Baxter (1973) in conjecturing that (8) is valid for all zero-field eight-vertex models, with an appropriate natural definition of x.

4. Triangular Ising model with pure three-spin interactions

This model has been discussed by Wood and Griffiths (1972), Merlini *et al* (1973), Merlini (1973), Griffiths and Wood (1973), Sykes *et al* (1973) and Watts (1974). The free energy has been obtained exactly by Baxter and Wu (1973, 1974), but the spontaneous magnetization is not yet known.

The model differs from the previous two in that it is presumably not a special case of the square lattice eight-vertex model. Nevertheless, its free energy has a similar form. For $T < T_c$, Baxter and Wu (1974) introduce elliptic functions of modulus k (or m), where

$$k = \sinh^{-2}(2\beta J_3). \tag{14}$$

Thus

$$u_3 = e^{-4\beta J_3} = \frac{(k+1)^{1/2}-1}{(k+1)^{1/2}+1} = x\prod_{n=1}^{\infty}\left(\frac{(1-x^{8n-7})(1-x^{8n-1})}{(1-x^{8n-5})(1-x^{8n-3})}\right)^2, \tag{15}$$

where $x = \exp(-\pi K'/2K)$. (This follows from equation (8.155.1) of GR with $u = \mathrm{i}K'/4$, together with (8.151.3) and (8.146.23–25).)

It is interesting to note, comparing (4) and (15), that the relation between x and J_3 is the same as that between x and J for the normal two-spin Ising model.

The exact result of Baxter and Wu (1974) for the free energy can be written in the form

$$u_3^{1/2}\,e^{-\beta f} = \prod_{n=1}^{\infty}\frac{(1-x^{8n-4})^3(1-x^{8n})(1-x^{6n-3})}{(1-x^{8n-5})^2(1-x^{8n-3})^2(1-x^{6n})}. \tag{16}$$

We can regard x as defined by (15) and f by (16). At low temperatures u_3 and x are small, so these expressions can readily be compared with the low-temperature expansions of Griffiths and Wood (1973), as modified by Sykes *et al* (1973). They of course agree. As T increases from 0 to T_c, x increases from 0 to 1.

5. Conjectured forms for M and P

We now come to the main point of this paper. No exact result is at present available for the spontaneous magnetization M of this model, but Griffiths and Wood (1973) and Sykes *et al* (1973) have obtained the low-temperature series to order u_3^{10}. This has recently been extended to twelfth order (Watts 1974), but unfortunately the last coefficient given therein is in error. We have verified that the correct series is

$$M = 1-2u_3^3-12u_3^4-66u_3^5-350u_3^6-1848u_3^7-9\,780u_3^8-52\,012u_3^9-278\,118u_3^{10} \\ -1\,495\,092u_3^{11}-8\,077\,274u_3^{12}-\ldots. \tag{17}$$

Let us use (15) so as to write this series as an expansion in powers of x, rather than u_3. We obtain, to the same order,

$$M = 1-2x^3+0x^4+0x^5+2x^6+0x^7+0x^8-4x^9+0x^{10}+0x^{11}+6x^{12}+\ldots. \tag{18}$$

Some remarkable simplifications have obviously occurred. Most of the coefficients have vanished, leaving only x^3, x^6, x^9 and x^{12} with non-zero coefficients. Further, the series is now the same as the expansion (9) of the two-spin Ising model magnetization, except that x^3 replaces x^2. Since we already have evidence that $M(x)$ is a 'universal' function, at least for exactly soluble two-dimensional models, this suggests that M is given by (8) or (13), with x^3 replacing x^2, ie

$$M = \prod_{n=1}^{\infty}\frac{1-x^{6n-3}}{1+x^{6n-3}}. \tag{19}$$

We *conjecture* that this is the exact expression for M.

If we wish, we can use various elliptic function identities to eliminate x between (15) and (19). It turns out that M is an algebraic function of u_3, given by

$$M = \left[1 - k_1^2\left(\frac{k_1 y - 1}{y - k_1}\right)^4\right]^{1/8}, \tag{20}$$

where

$$k_1 = \frac{2k^{1/2}}{1+k} = 2\sinh 2\beta J_3 \operatorname{sech}^2 2\beta J_3, \tag{21}$$

and y is the solution of the equation

$$(y-1)^3(1+3y)/y^3 = 2(1-k^{1/2})^4/k^{1/2}(1+k) \tag{22}$$

such that $y \geqslant 1$. (This is the same y as occurs in the result of Baxter and Wu (1973) for the free energy.)

Near T_c we find that

$$k^{1/2} = 1 - C(T_c - T) + O(T_c - T)^2, \tag{23}$$

where C is a positive constant. Hence

$$\begin{aligned} y &= 1 + 2^{-2/3}[C(T_c - T)]^{4/3} + O(T_c - T)^{7/3}, \\ M &= 2^{1/3}[C(T_c - T)]^{1/12} + \text{smaller terms}. \end{aligned} \tag{24}$$

Thus our conjecture (19) predicts that the critical exponent β_M should be 1/12. This agrees with the Padé approximant prediction (Watts 1974) and the 'new universality' hypothesis of Suzuki (1974).

One can define another order parameter for this model by applying a two-spin interaction $-J_2\sigma_i\sigma_j$ to all adjacent pairs of spins. Regarding such pairs as dipoles, one can think of this as an applied electric field. Then below T_c one expects there to be a spontaneous non-zero polarization

$$P = -\frac{1}{3}\left(\frac{\partial f}{\partial J_2}\right)_{J_2=0} \tag{25}$$

(taking the derivative through positive values of J_2).

We have expanded this to order u_3^{12} and obtain

$$\begin{aligned} P = 1 - 4(&u_3^3 + 5u_3^4 + 25u_3^5 + 123u_3^6 + 616u_3^7 + 3\,133u_3^8 + 16\,160u_3^9 + 84\,335u_3^{10} \\ &+ 444\,472u_3^{11} + 2\,362\,028u_3^{12} + \ldots). \end{aligned} \tag{26}$$

Using (15) to write this as an expansion in powers of x, we find

$$P = 1 - 4x^3 + 4x^4 + 0x^5 + 4x^6 - 16x^7 + 12x^8 + 0x^9 + 16x^{10} - 48x^{11} + 36x^{12} + \ldots. \tag{27}$$

Guided by (8), (12) and (13), we now write this in the form

$$P = \prod_{n=1}^{\infty}\left(\frac{1-x^n}{1+x^n}\right)^{2c_n}, \tag{28}$$

where the exponents c_n are to be chosen to match the series expansion. This determines $c_1, \ldots, c_{12}$ uniquely, giving

$$c_1, \ldots, c_{12} = 0, 0, 1, -1, 0, 1, 0, -1, 1, 0, 0, 0. \tag{29}$$

Thus to order x^{12} we can take P to be given by

$$P^{1/2} = \frac{1-x^3}{1+x^3}\frac{1-x^6}{1+x^6}\frac{1-x^9}{1+x^9}\frac{1-x^{12}}{1+x^{12}}\cdots\frac{1+x^4}{1-x^4}\frac{1+x^8}{1-x^8}\frac{1+x^{12}}{1-x^{12}}\cdots. \tag{30}$$

In this case P therefore appears to be the ratio of two products of type (12), and we *conjecture* that

$$P = \prod_{n=1}^{\infty}\left(\frac{1-x^{3n}}{1+x^{3n}}\frac{1+x^{4n}}{1-x^{4n}}\right)^2. \tag{31}$$

Again we can eliminate x and express P as an algebraic function of u_3. Using various elliptic function identities, we obtain

$$P = \frac{2}{3}\frac{y^3}{(y^2-1)^2}\frac{(1-k)^{11/4}}{k^{1/2}(1+k)^{5/4}}, \tag{32}$$

where k, y are defined by (14), (22). Thus near T_c, using (23),

$$P = \tfrac{4}{3}[C(T_c-T)/4]^{1/12} + \text{smaller terms}, \tag{33}$$

so that our conjecture implies that the critical exponent β_P for this order parameter is also 1/12. (The authors know of no proof that β_M and β_P should be the same for this model.)

6. Susceptibility of the square lattice two-spin Ising model

It is tempting to apply similar ideas to the zero-field susceptibility χ of these models. In particular, the high-temperature series expansion of χ for the normal two-spin square lattice Ising model has been obtained by Sykes *et al* (1972) to order v^{21}, where $v = \tanh \beta J$. In the high-temperature regime the 'natural parameter' x is given by (4), with $\exp(-2\beta J)$ replaced by v. Thus

$$v = x^{1/2}(1-x+x^3-x^4+\ldots). \tag{34}$$

Substituting the expression (4) for v into the series for χ, setting $x = t^2$, we obtain

$$\begin{aligned}\chi = {}& 1+4t+12t^2+32t^3+76t^4+168t^5+352t^6+704t^7+1356t^8+2516t^9+4552t^{10}\\ &+8048t^{11}+13\,872t^{12}+23\,512t^{13}+39\,184t^{14}+64\,048t^{15}+103\,516t^{16}\\ &+165\,208t^{17}+259\,484t^{18}+404\,544t^{19}+623\,896t^{20}+948\,304t^{21}+\ldots.\end{aligned} \tag{35}$$

This seems to be an improvement on the original series, in that the coefficients are still positive but much smaller. We tried writing this series as a product of the form (28), or more precisely as

$$\chi = \prod_{n=1}^{\infty}\left(\frac{1+t^n}{1-t^n}\right)^{2c_n}. \tag{36}$$

The first 21 exponents c_n are uniquely defined by (35), giving

$$\begin{aligned}(c_1, c_2, \ldots, c_{21}) = {}& (1, 1, 1, 1, 1, 1, 1, 1, -3, 5, 5, -11, 13, 5, -51, 85, 21,\\ &-275, 441, -87, -1275).\end{aligned} \tag{37}$$

This is an incredible sequence. The first eight exponents are all unity, then they appear to be completely irregular.

It is tempting to assume the ninth and higher are in error and should all be unity. However, the resulting expression for χ predicts a critical exponent γ of 2, instead of the accepted value of 7/4. Also, the authors have checked one another's calculations of (37), and to the best of our knowledge it is correct.

This illustrates well the dangers of this sort of series analysis, and may be regarded as casting doubt on our previous conjectures. However, we know that for some models the order parameters can be expressed as simple infinite products, so it seems likely that this is also true for the three-spin triangular Ising model, whereas we have no such guideline for susceptibilities.

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