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A direct high-temperature star graph expansion for the fourth-field derivative of the Ising free energy

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Abstract. It is shown that the fourth-field derivative, $\chi_0^{(2)}$, of the free energy of the Ising model above the critical temperature can be expressed as an expansion in terms of two-connected graphs or stars. The contribution of any star graph to the expansion is expressed in terms of the weak lattice constant of the graph, and a weight, the latter being a property of the star graph only. The method is used to derive series expansions for $\chi_0^{(2)}$ on the four-dimensional hyper-simple cubic, hyper-body-centred cubic and hyper-face-centred cubic lattices to order 16, 11 and 9 respectively.

1. Introduction

The existence of star graph expansions for the zero-field Ising partition function and the reciprocal of the zero-field susceptibility (χ_0^{-1}) is well known (Domb and Hiley 1962, Rapaport 1974, McKenzie 1975a, b). The existence of star graph expansions for higher-field derivatives has been demonstrated (Domb 1974). We show that, in the limit $H \to 0$,

$$\frac{\partial^3 \ln Z(\rho, v)}{\partial \rho^3}\bigg|_{\rho=1/2} = -8\frac{\partial^4 \ln Z/\partial H^4}{\chi_0^4} = -8\frac{\chi_0^{(2)}}{\chi_0^4}, \tag{1.1}$$

where Z is the partition function of the Ising model, and ρ is the density of overturned spins; v $(=\tanh(J/kT))$ is the usual high-temperature variable, and H is the magnetic field. We also show that, for a lattice $\mathscr{L}$, (1.1) can be expressed in the form

$$\partial^3 \ln Z/\partial \rho^3\,|_{\rho=1/2} = \sum_G (G; \mathscr{L}) W_G(v). \tag{1.2}$$

The sum runs over all star graphs G. Also included in the set are the isolated vertex and the bond. $(G; \mathscr{L})$ is the weak lattice constant of G on $\mathscr{L}$, defined per site. $W_G(v)$ is the weight of G, and is a function of v.

To derive an exact series expansion for (1.2), correct to order v^n, one has to consider all star graphs G with up to n edges. For each G, one expands $W_G(v)$ as a power series in v and retains terms to order v^n. Substitution in (1.2) gives the required series. Equation (1.2) applies to finite clusters as well as to infinite lattices. Thus $W_G(v)$ for a finite star cluster, G, can be calculated by applying (1.1) and (1.2) to G and subtracting off the weights of all star subgraphs of G.

For inhomogeneous clusters, namely those whose vertices are not all equivalent from considerations of symmetry, the calculation of $W_G(v)$ is complicated by the fact that the different classes of vertex have different overturned spin densities ρ_i associated with them. This distinction has to be preserved until one has calculated (1.2) for the cluster. One then takes the high-temperature limit of $H \to 0$ and $\rho_i \to \frac{1}{2}$ for all i. In practice it is simpler to treat all the vertices of the cluster as being distinct.

In a recent study, Baker (1977) derived the fourth-field derivative series for the cubic lattices to order v^9 in arbitrary dimension d. The method used was that of Rushbrooke and Scoins (1962), which involves the calculation of the low-temperature partition function in a field (as a series in the magnetisation variable), followed by differentiation and transformation to high-temperature variables. Using this series, together with a revised estimate for the exponent ν pertaining to the correlation length ξ, Baker obtained, for $d = 4$,

$$2\Delta - d\nu - \gamma = -0{\cdot}302 \pm 0{\cdot}038. \tag{1.3}$$

This result is in conflict with the renormalisation group (RG) approach (see e.g., Brézin *et al* 1976), which assumes the hyperscaling relation

$$2\Delta - d\nu - \gamma = 0 \tag{1.4}$$

for $2 \leqslant d \leqslant 4$. Also, RG calculations predict, in four dimensions, the existence of confluent logarithmic terms modifying the dominant algebraic singularities in χ_0, ξ and $\chi_0^{(2)}$.

Gaunt *et al* (1979) investigated the presence of logarithmic terms in the χ_0 and $\chi_0^{(2)}$ series for the hyper-simple cubic (HSC) lattice in four dimensions. Using 17-term expansions, they concluded that the series data were consistent with the presence of logarithmic correction terms. Their analysis was confined to the HSC lattice.

We have used the direct high-temperature star graph expansion method to calculate series expansions for $\chi_0^{(2)}/\chi_0^4$ for the four-dimensional HSC, hyper-body-centred cubic (HBCC) and hyper-face-centred cubic (HFCC) lattices to order 16, 11 and 9 respectively. Our series for the HSC lattice are in agreement with Gaunt *et al* (1979). The series for the other two lattices are new.

The advantages of the star graph method as implemented here are twofold. Greater flexibility is achieved by separating the problem into two parts, namely the determination of star lattice constants (see e.g. Martin 1974), and the calculation of weights (see equation (1.2)). The lattice constant data can be used to derive series expansions for other properties, such as specific heat, self-avoiding walks and susceptibility, by using different sets of weights. The weights $W_G(v)$ depend only on the graphs G, and can be used to derive series on any lattice.

The other advantage of this method is that it is not necessary to retain the field variable, in explicit form, throughout the calculation. By eliminating it at an earlier stage, one is able to derive longer series than would otherwise be possible. The method in this form is admittedly not capable of yielding the complete expansion for the free energy in a field (Baker 1977, Sykes *et al* 1973), but for purposes of estimating the exponent Δ, the fourth-field derivative $\chi_0^{(2)}$ is adequate.

In the next two sections, we show the validity of equation (1.1), and discuss briefly the procedure for calculating $W_G(v)$ for any star cluster G. The series coefficients, together with results of series extrapolation, are presented in McKenzie and Gaunt (1980), the accompanying paper.

2. Density expansion for the Ising model

The work of Rushbrooke and Scoins (1955) and Domb and Hiley (1962) has shown that the partition function of the Ising model can be expressed as a series expansion in the variables ρ (the density of overturned spins) and u ($=\exp(-4J/kT)$). In this form, the expansion is analogous to the virial expansion for the imperfect gas. The coefficients of the series are made up of contributions from star graphs alone. Thus there exists a star graph expansion for

$$\ln Z(\rho, u), \tag{2.1}$$

where

$$\rho = \mu \partial \ln Z/\partial\mu \tag{2.2}$$

and

$$\mu = \exp(-2mH/kT).$$

It then follows that all derivatives of $\ln Z$ with respect to ρ have star graph expansions. At temperatures above the critical point ($T > T_c$), the partition function per spin can be written down as (Domb 1974)

$$\ln Z = \ln 2 + (q/2)\ln(1+v) - \ln(1+\tau) + \ln[1 + X^{(0)} + \tau^2 X^{(2)} + \tau^4 X^{(4)} + \dots], \tag{2.3}$$

where

$$\tau = (1-\mu)/(1+\mu) \tag{2.4}$$

and

$$X^{(r)} = \sum_{l=1}^{\infty} d_l^{(r)} v^l. \tag{2.5}$$

$d_l^{(r)}$ represents the sum of weak lattice constants per site of all graphs with l edges and r vertices of odd degree. q is the coordination number of the lattice.

The overturned spin density ρ is defined as

$$\rho = -[(1-\tau^2)/2]\partial \ln Z/\partial\tau. \tag{2.6}$$

Denoting the expression in square brackets in (2.3) by F, and defining

$$\partial^r F/\partial\tau^r \Big|_{\tau=0} = F^{(r)}, \tag{2.7}$$

it can be shown that, in the limit $\tau \to 0$,

$$\begin{aligned} &\partial \ln Z/\partial\tau = -1, && \partial^2 \ln Z/\partial\tau^2 = 1 + F^{(2)}/F^{(0)}, \\ &\partial^3 \ln Z/\partial\tau^3 = -2, && \partial^4 \ln Z/\partial\tau^4 = 6 - 3(F^{(2)}/F^{(0)})^2 + F^{(4)}/F^{(0)}. \end{aligned} \tag{2.8}$$

From (2.2), (2.4), (2.6) and (2.8), we see that $H \to 0$ implies $\mu \to 1$, $\tau \to 0$ and $\rho \to \frac{1}{2}$.

From (2.6), it follows that

$$\begin{aligned} \partial/\partial\rho &= [-\tfrac{1}{2}(1-\tau^2)\partial^2 \ln Z/\partial\tau^2 + \tau\partial \ln Z/\partial\tau]^{-1}\, \partial/\partial\tau \\ &= A^{-1}\partial/\partial\tau. \end{aligned} \tag{2.9}$$

Also, in the limit $\tau \to 0$, $\rho \to \frac{1}{2}$,

$$\frac{\partial^3 \ln Z}{\partial \rho^3} = -8\left(\frac{\partial^4 \ln Z}{\partial \tau^4} - 8\frac{\partial^2 \ln Z}{\partial \tau^2}\right) \Big/ \left(\frac{\partial^2 \ln Z}{\partial \tau^2}\right)^4$$

$$= -8(\beta m)^4 \frac{\partial^4 \ln Z/\partial H^4}{(\partial^2 \ln Z/\partial H^2)^4}. \tag{2.10}$$

Equation (2.10) applies to finite homogeneous clusters as well as to infinite regular lattices. For finite clusters, it is more convenient to define the $X^{(r)}$ in (2.5) in terms of total number of embeddings, rather than lattice constants per site. Using this definition and making the necessary modifications to (2.3) and (2.8), we obtain, for a cluster with N sites,

$$\frac{\partial^3 \ln Z}{\partial \rho^3} = -8\,\frac{-2-(3/N)(F^{(2)}/F^{(0)})^2-(8/N)(F^{(2)}/F^{(0)})+(1/N)(F^{(4)}/F^{(0)})}{[1+(1/N)F^{(2)}/F^{(0)}]^4}. \tag{2.11}$$

From (2.3) and (2.7), it can be seen that

$$F^{(0)} = 1 + \sum d_l^{(0)} v^l, \qquad F^{(2)} = 2\sum_{l\geqslant 1}^{\infty} d_l^{(2)} v^l, \qquad F^{(4)} = 24\sum_{l\geqslant 2} d_l^{(4)} v^l, \tag{2.12}$$

where the $d_l^{(r)}$ now represent the total number of embeddings, not lattice constants per site. Thus (2.11) can be calculated for a cluster G, from a knowledge of its subgraphs with zero, two and four odd vertices. Substitution of (2.12) in (2.11) gives $\partial^3 \ln Z/\partial\rho^3$. Use of (1.2) gives $W_G(v)$. We shall now consider the examples of the isolated vertex ($\cdot$) and the bond ($\bullet\!-\!\bullet$). For the former, $F^{(0)}$ is simply one, and $F^{(2)}$ and $F^{(4)}$ are both zero. Substitution in (2.11) gives

$$-\tfrac{1}{8}\,\partial^3 \ln Z/\partial\rho^3 = -2, \tag{2.13}$$

which is also the weight of the isolated vertex.

For the bond, it can be seen that

$$F^{(0)} = 1, \qquad F^{(2)} = 2v, \qquad F^{(4)} = 0. \tag{2.14}$$

Substitution in (2.11) gives

$$-\tfrac{1}{8}\,\partial^3 \ln Z/\partial\rho^3 = -2(1+3v)/(1+v)^3. \tag{2.15}$$

Expanding (2.15) as a power series in v, we obtain

$$-\tfrac{1}{8}\,\partial^3 \ln Z/\partial\rho^3 = -2(1-3v^2+8v^3-15v^4+24v^5+\ldots)$$

$$= -2 + \tfrac{1}{2}W(\bullet\!-\!\bullet). \tag{2.16}$$

Subtracting off the weight of ($\cdot$), we obtain the weight series for the bond, which is

$$W(\bullet\!-\!\bullet) = -4(-3v^2+8v^3-15v^4+24v^5\ldots). \tag{2.17}$$

For the square (p_4), equation (2.11) gives

$$-\tfrac{1}{8}\,\partial^3 \ln Z/\partial\rho^3 = -2(1-6v^2+16v^3-48v^4+144v^5). \tag{2.18}$$

Subtracting off the contributions due to the vertex and the bond, we derive

$$W(p_4) = 144v^4 - 768v^5 + \ldots. \tag{2.19}$$

It can be verified that substitution of (2.13), (2.17) and (2.19) in (1.2), with appropriate lattice constants, gives the $(\partial^4 \ln Z/\partial H^4)/\chi_0^4$ series correct to order v^5 for any cubic lattice.

3. Finite inhomogeneous clusters

The calculation of $\partial^3 \ln Z/\partial \rho^3$ for inhomogeneous clusters is complicated by the fact that one has to work with a set of ρ_i's, one for each class of site (Domb and Hiley 1962). In practice, it is simpler to treat all sites of the cluster as being distinct. Thus for a cluster G with R sites, the partition function takes the form

$$\ln Z = -\frac{1}{R}\sum_{i=1}^{R} \ln(1+\tau_i) + \frac{1}{R}\ln F_R(v, \underline{\tau_i}), \tag{3.1}$$

where $\underline{\tau_i}$ denotes the set $(\tau_1, \tau_2 \ldots \tau_R)$. The overturned spin densities are defined by

$$\rho_i = -\tfrac{1}{2}(1-\tau_i^2)\partial \ln Z/\partial \tau_i \qquad \text{for } i = 1 \text{ to } R. \tag{3.2}$$

It now follows that

$$\frac{\partial}{\partial \tau_r} = \sum_{i=1}^{R} \frac{\partial \rho_i}{\partial \tau_r}\frac{\partial}{\partial \rho_i}. \tag{3.3}$$

We define a matrix A, whose elements a_{ij} are given by

$$a_{ij} = \partial \rho_j/\partial \tau_i. \tag{3.4}$$

We also define the matrix $B(=A^{-1})$, with elements b_{ij}, and write

$$\partial/\underline{\partial \rho_i} = B\partial/\underline{\partial \tau_i}, \tag{3.5}$$

where $\partial/\underline{\partial \rho_i}$ and $\partial/\underline{\partial \tau_i}$ are R-component vectors. It then follows that

$$\frac{\partial}{\partial \rho} = \sum_{i=1}^{R}\frac{\partial}{\partial \rho_i} = \sum_{r=1}^{R}\sum_{i=1}^{R} b_{ir}\frac{\partial}{\partial \tau_r} = \sum_{r=1}^{R}\frac{\partial}{\partial \tau_r}\sum_{i=1}^{R} b_{ir}. \tag{3.6}$$

Denoting $\Sigma_{i=1}^{R} b_{ir}$ by B_r, the operation $\partial/\partial\rho$ can be replaced by

$$\sum_{i=1}^{R} B_i \frac{\partial}{\partial \tau_i}. \tag{3.7}$$

It can then be shown that, in the limit $\rho_i \to \frac{1}{2}R$, $\tau_i \to 0$, for $i = 1$ to R,

$$\begin{aligned}\frac{\partial^3 \ln Z}{\partial \rho^3} = \sum_{i,j,k=1}^{R}\bigg(&B_k\frac{\partial B_j}{\partial \tau_k}B_i\frac{\partial^2 \ln Z}{\partial \tau_i\,\partial \tau_j} + B_k\frac{\partial B_j}{\partial \tau_k}\frac{\partial B_i}{\partial \tau_j}\frac{\partial \ln Z}{\partial \tau_i} + B_kB_jB_i\frac{\partial^3 \ln Z}{\partial \tau_i\,\partial \tau_j\,\partial \tau_k}\\ &+ B_kB_j\frac{\partial B_i}{\partial \tau_k}\frac{\partial^2 \ln Z}{\partial \tau_i\,\partial \tau_j} + B_kB_j\frac{\partial B_i}{\partial \tau_j}\frac{\partial^2 \ln Z}{\partial \tau_i\,\partial \tau_k} + B_kB_j\frac{\partial^2 B_i}{\partial \tau_k\,\partial \tau_j}\frac{\partial \ln Z}{\partial \tau_i}\bigg).\end{aligned} \tag{3.8}$$

Since we are only interested in deriving a series expansion and not a closed-form expression for (3.8) we can calculate B by using

$$B = A^{-1} = 2\sum_{n\geq 0}(-1)^n C^n, \tag{3.9}$$

where $C = 2A - I$. The elements of A, B and C are polynomials in v and τ. If (3.9) is truncated at $n = N$, the expansion for B will be correct to order v^N. The factor of 2 in (3.9) is omitted in our subsequent treatment. It can be re-introduced at the end.

Using (3.9), it can be shown that

$$\partial B/\partial\tau_i = -B\, C_i B \tag{3.10}$$

and

$$\partial^2 B/\partial\tau_i\, \partial\tau_j = -BC_{ij}B + BC_iBC_jB + BC_jBC_iB,$$

where C_i is a matrix whose elements are obtained by differentiation with respect to τ_i of the corresponding elements of C. C_{ij} is similarly defined.

From (3.2) and (3.4) it can be shown that, in the zero-field limit,

$$\partial B/\partial\tau_i = 0, \qquad \partial^2 B/\partial\tau_i\, \partial\, \tau_j = -BC_{ij}B. \tag{3.11}$$

Thus (3.8) takes the form

$$\frac{\partial^3 \ln Z}{\partial\rho^3} = -2 \sum_{i=1}^{R} B_i^3 + \sum_{j,k} B_k B_j\, \mathbf{1}^{\mathrm{T}} [BC_{jk}B]\mathbf{1}, \tag{3.12}$$

where $\mathbf{1}^{\mathrm{T}}$ and $\mathbf{1}$ are R-component row and column vectors, all of whose elements are unity.

All the terms in (3.12) except for C_{ij} can be calculated from the matrix A after imposing the zero-field limit. It can be seen that

$$a_{ii} = -\tfrac{1}{2}R, \qquad a_{ij} = -(1/2R)F^{(ij)}/F^{(0)}, \tag{3.13}$$

where $F^{(ij)} = \Sigma_{l\geqslant 1}\, d_l^{(ij)}\, v^l$. The term $d_l^{(ij)}$ denotes the number of subgraphs of G with l edges and odd vertices i and j. To calculate C_{jk}, one has to differentiate the elements of C before imposing the zero-field limit. It can be shown that the elements of C_{jk} can be expressed in terms of subgraphs of G with 0, 2 and 4 odd vertices. Having calculated $\partial^3 \ln Z/\partial\rho^3$, one can write, for the cluster G,

$$\partial^3 \ln Z/\partial\rho^3 = (1/N) \sum_{G'} (G'; G)\, W_{G'}(v), \tag{3.14}$$

where the sum is over all star subgraphs G' of G, including G itself. $(G'; G)$ is the number of distinct embeddings of G' on G. Knowing the weights of all the star subgraphs of G, one can calculate $W_G(v)$ by using (3.14).

By considering all star graphs with up to n edges that can be embedded on a given lattice, and using (1.2), we obtain $\chi_0^{(2)}/\chi_0^4$ to order v^n. We have thus derived series expansions for the HSC, HBCC and HFCC lattices to order 16, 11 and 9 respectively. The coefficients for the HSC lattice are in agreement with Gaunt *et al* (1979). Those for the HBCC and HFCC lattices are new. Results of analysis of the series and a study of hyperscaling in four dimensions (on all three lattices) form the subject of an accompanying paper (McKenzie and Gaunt 1980).

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