On the determination of weights for the high temperature star cluster expansion of the free energy of the Ising model in zero magnetic field

1974 J. Phys. A: Math. Nucl. Gen. 7 1589

(http://iopscience.iop.org/0301-0015/7/13/013)

J. Phys. A: Math., Nucl. Gen., Vol. 7, No. 13, 1974. Printed in Great Britain. © 1974

On the determination of weights for the high temperature star cluster expansion of the free energy of the Ising model in zero magnetic field

M F Sykes† and D L Hunter‡

†Wheatstone Physics Laboratory, King's College, London, UK

‡ Department of Physics, St Francis Xavier University, Antigonish, Nova Scotia, Canada

Received 3 September 1973, in final form 22 April 1974

Abstract. Some results relevant to the derivation of the high temperature series expansion for the zero-field free energy of the Ising model are collected from the literature. The general theory of the star cluster expansion is summarized and some methods for the derivation of the appropriate weights are given in outline.

1. Introduction

High temperature series expansions for the free energy of the Ising model in the absence of a magnetic field have been investigated by many authors (Rushbrooke and Eve 1962, Baker 1963, Hunter 1967, 1969; for a comprehensive review of early work see Domb 1960). Since the early studies of Domb (1949), Trefftz (1950), Wakefield (1951) and Potts (1951) there have been many improvements in techniques for the derivation of such expansions. In this article we collect together some useful results many of which find their origin deep in the literature. In § 2 we give a generalized configurational formulation which relates the free energy to a key configurational function; the direct configurational method was used by most early investigators. In § 3 we describe the formal cluster expansion for the free energy and demonstrate that it is a star cluster expansion. In § 4 we describe in outline some methods available for the determination of the weights and state and prove a powerful result due to Domb that enables the weights to be generated explicitly. In § 5 we prove a general substitution theorem for deriving the key configurational function of stars with at least one articulation set of order 2 from simpler stars. The configurational problem presented by the star cluster expansion is described in a companion paper (Sykes *et al* 1974). We use the basic definitions in graph theory of Sykes *et al* (1966, 1974) and Essam and Fisher (1970).

For any graph G we take the associated simple Ising model to be a set of spins located on the N vertices of G, one spin on each and every vertex, which interact in pairs delineated by the $\mathcal{N}$ edges of G. We denote by J the energy of interaction between pairs of spins and write $v = \tanh K$ with $K = J/kT$. We also associate with G the generalized Ising model in which the interactions between pairs of spins are all distinct. If the edges of the graph are labelled $1, 2, \ldots, i, \ldots$ we denote the energy corresponding to the ith edge by J_i and write $v_i = \tanh K_i$ with $K_i = J/kT$.

When G represents a small finite cluster of spins the partition function may be obtained explicitly by enumerating all the possible states. Since we are primarily concerned with identifying G with an infinite crystal lattice we have recourse to series developments.

2. Generalized configurational formulation and abridged notation

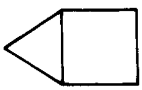
The starting point of the direct configurational method is the well known result that if $[\Lambda(G)]^N$ is the partition function of the Ising model associated with G we may write, in the absence of an applied magnetic field,

$$N \ln \Lambda = N \ln 2 + \mathcal{N} \ln(\cosh K) + L(v, G) \tag{2.1}$$

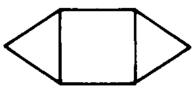
$$\exp L(v, G) = 1 + \sum_{1}^{\mathcal{N}} p(r) v^r = P(v) \tag{2.2}$$

where $p(r)$ denotes the number of independent choices of r edges of G such that the linear graph formed is one all of whose vertices are of even degree (no-field graph). In other words the quantity $p(r)$ is the total number of possible weak embeddings in G of all no-field graphs of r edges. This elegant result is apparently due to Van der Waerden (1941); a detailed modern treatment is given by Domb (1960, § 3.4.1). *The key configurational function* $P(v)$ is readily found by inspection for simple graphs.

As examples we illustrate two graphs and their corresponding key configurational functions:



$$P(v) = 1 + v^3 + v^4 + v^5 \tag{2.3}$$

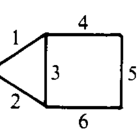


$$P(v) = 1 + 2v^3 + v^4 + 2v^5 + 2v^6. \tag{2.4}$$

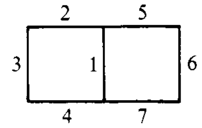
In the second the coefficient of v^6 corresponds to one embedding of a six-sided polygon and one embedding of a pair of (separated) triangles; there are no other no-field graphs with six edges embeddable in the graph.

The configurational formulation (2.1–2) is easily extended to the generalized Ising model associated with G. The key function $P(v)$ is replaced by a polynomial in the variables v_i; it is the sum of all products, of any number of factors, for which the corresponding edges form a no-field graph. It follows from this restriction that if a set of edges a, b, c correspond to a bridge of G, then the variables $v_a, v_b, v_c, \ldots$ will always occur together. It is less cumbersome to label the *bridges* by letters $r, s, t, \ldots$ and write r for the product of variables corresponding to the bridge r and so on. We describe this as an *abridged notation*. A detailed treatment, with many examples, is given by Domb (1970, § 3). It is evident that the abridged form of the function P is immediately applicable to any homeomorph of G.

As examples we illustrate the key configurational functions for two theta graphs with labelled edges:

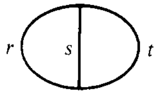


$$P = 1 + v_1 v_2 v_3 + v_3 v_4 v_5 v_6 + v_1 v_2 v_4 v_5 v_6 \tag{2.5}$$



$$P = 1+v_1v_2v_3v_4+v_1v_5v_6v_7+v_2v_3v_4v_5v_6v_7 \quad (2.6)$$

and these results can be summarized by labelling the bridges of the theta graph topology r, s, t and writing in abridged notation:



$$P = 1+rs+rt+st. \quad (2.7)$$

3. The star cluster expansion

As an alternative to the direct configurational method the function $L(v, G)$ may be written as a cluster expansion

$$L(v, G) = \sum_g w(v, g)(g; G) \quad (3.1)$$

where g is any graph, $(g; G)$ denotes the number of weak embeddings of g in G (weak lattice constant) and the w are functions of v called the weak weight functions; they are independent of G. Our notation follows Sykes *et al* (1966, § 5), where a detailed theoretical treatment is given. The whole subject of cluster expansions has been treated exhaustively in the literature (Kubo 1962, Strieb *et al* 1963, Abe 1964). In the absence of an applied magnetic field the summation in (3.1) may be restricted to multiply connected graphs. In the present context we follow the usual practice of calling these star graphs; this latter term as usually defined includes the bond but no confusion should arise; the weight of the bond is to be taken as zero. The fact that (3.1) is a *star cluster expansion* is implicit in the Mayer development (Uhlenbeck and Ford (1962); other relevant papers are those of Yvon (1945), Rushbrooke and Scoins (1955, 1962), Domb and Hiley (1962) and particularly Domb (1960, § 5.2.10) and references there cited).

A direct demonstration of the star-graph restriction can be given. Any articulated graph G, formed from two graphs G_1 and G_2 with a point in common (the articulation point) has a key configurational function P that may be written as a product

$$P = P_1 P_2 \quad (3.2)$$

of the key functions of G_1 and G_2 (Hunter 1967). For suppose g is any no-field subgraph of G. Then if g is neither wholly in G_1 nor wholly in G_2 it must be the sum graph of two no-field sub-graphs, g_1 wholly in G_1, and g_2 wholly in G_2; for if either was not no-field this could only be because the vertex at the articulation point was odd, and odd vertices must occur in pairs. The product (3.2) therefore enumerates all the possible embeddings that contribute to P. From (3.2) and (2.2) it follows that

$$L(G) = L(G_1)+L(G_2). \quad (3.3)$$

But (3.3) is the necessary and sufficient condition for the cluster expansion of L to be a star cluster expansion. A proof of this quite general result is given by Essam and Sykes (1966, equation (3.13) *et seq*).

Explicitly if the number of weak embeddings per site of the graphs , , , ,  are denoted by $p_3, p_4, p_5, p_{5a}, p_6$ respectively, then for any graph the expansion starts:

$$\frac{1}{N}L(v, G) = p_3v^3+p_4v^4+p_5v^5+(p_6-p_{5a}-\tfrac{1}{2}p_3)v^6+\ldots. \tag{3.4}$$

The coefficient of p_3 on the right-hand side corresponds to the weak weight function for the triangle. Its expansion starts:

$$w(v, p_3) = v^3-\tfrac{1}{2}v^6\ldots. \tag{3.5}$$

For the graph given as an example in (2.4) $p_3 = \frac{1}{3}$, $p_4 = \frac{1}{6}$, $p_5 = \frac{1}{3}$, $p_{5a} = 0$, $p_6 = \frac{1}{6}$ and it may be verified by exponentiation that (3.4) is in agreement with (2.4).

4. Determination of the weak weight functions for the star cluster expansion

A series development can now be obtained by grouping the formal summation (3.1) in powers of v:

$$L(v, G) = \sum_g\sum_r [w_r(g)(g; G)]v^r. \tag{4.1}$$

The coefficients are determined by the successive weights $w_r(g)$ which are the coefficients in the expansions of the weak weight functions:

$$w(v, g) = \sum_r w_r(g)v^r. \tag{4.2}$$

We call the numbers $w_r(g)$ the L-weights, or simply the weights, of g. The weight functions are defined by (3.1) and by successive application of this equation *in turn* to each graph in a suitably ordered graph dictionary they may be calculated explicitly and the L-weights derived. The necessary manipulations may be performed directly or recursively (Sykes *et al* 1966, equations (5.22) and (5.23)). The method consists essentially in subtracting off the contributions of all the sub-graphs of g (*method of sub-graph subtraction*). A variety of procedures can be used; it is not necessary to restrict the sub-graphs considered to stars since the total effect of other sub-graphs is zero. Thus, for example, if G is a star and we denote the function L for the graph formed by deleting s bridges from G by L_s then, by a straightforward application of the principle of inclusion and exclusion (Riordan 1958 chap 3, Ryser 1963, chap 2),

$$w(G) = L(G)-\sum L_1(G)+\sum L_2(G)-\ldots+(-1)^s\sum L_s(G)+\ldots \tag{4.3}$$

the summations being taken over all distinct choices of bridges.

In practice it is usually more convenient to avoid sub-graph subtraction altogether and exploit a powerful technique introduced by Domb (1970, § 3). Suppose a star G has bridges $r, s, t, \ldots$ and we write the key configurational function for the generalized model in abridged form:

$$\exp L(G) = P(r, s, t, \ldots). \tag{4.4}$$

Then to follow the method of sub-graph subtraction we would first expand the function L formally as

$$L(G) = \ln P = \sum A_{\alpha\beta\gamma\ldots}r^\alpha s^\beta t^\gamma\ldots \tag{4.5}$$

and subtract off the corresponding expansions for all the sub-graphs of G. *The result is equivalent to deleting from the right-hand side of* (4.5) *all those products which do not involve all the variables* $r, s, t, \ldots$. We denote the expansion after deletion of the incomplete products by $\ln {}^*P$. The modified expansion $\ln {}^*P$ is the expansion of the weight generating function of G and we can write (3.1) as

$$L(G) = \sum_{g} (g; G) \ln {}^*P(g). \tag{4.6}$$

This equation summarizes the *complete-term method.*

To prove the result we suppose it true for stars of cyclomatic number l or less. Then for any star of cyclomatic number $l+1$:

$$L(G) = \sum_{g \neq G} (g; G) \ln {}^*P(g) + w(G). \tag{4.7}$$

If we set any interaction equal to zero the left-hand side corresponds to a graph with cyclomatic number l whose L function must be correctly given by the first term on the right-hand side. Thus $w(G)$ vanishes identically for each interaction in turn and thus can only contain complete terms. This suffices to establish the result and (4.6) follows by induction.

To give a specific example we find from (2.7) that for any theta graph

$$\ln P = \sum rs - \tfrac{1}{2}\sum r^2s^2 - \sum r^2st + \tfrac{1}{3}\sum r^3s^3 + 2\sum r^3s^2t + 2\sum r^2s^2t^2 + \ldots \tag{4.8}$$

and on deleting the incomplete terms

$$\ln {}^*P = -\sum r^2st + 2\sum r^3s^2t + 2\sum r^2s^2t^2 + \ldots. \tag{4.9}$$

To particularize to the theta graph p_{5a} we replace r by v, s and t by v^2 and collect up the terms to obtain

$$\ln {}^*P = -v^6 - 2v^7 + \ldots. \tag{4.10}$$

The coefficient of v^6 in (4.10) now corresponds to the coefficient of $p_{5a}v^6$ in (3.4).

5. General substitution theorem

If a star has an articulation set of order two the calculation of its key configurational function can be simplified by a general substitution which we now prove. Suppose G has an articulation set of order two at the vertices R and S. Then by definition deletion of R and S, together with all their incident edges, leaves a graph with at least two connected components. Denote the vertex set of one of these by V' and that of all the others by V''. Denote by G' the section graph of G with the vertex set $V'+R+S$ together with a new bridge a', joining R to S, and by G'' that with vertex set $V''+R+S$ together with a new bridge a'', joining R to S. (We illustrate these graphs schematically in figure 1.)

The embeddings that contribute to the key configurational function P' of G' are of two kinds: those that use the bridge a' and those that do not. We group these separately by writing

$$P' = 1 + \phi' + a'\psi' \tag{5.1}$$

where ϕ' and ψ' are independent of a'. The function ϕ' contains all no-field sub-graphs

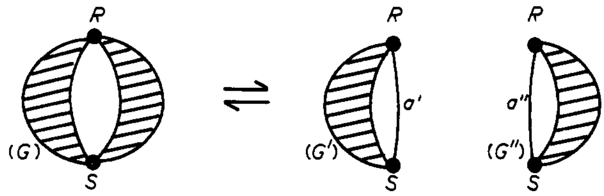


Figure 1. Schematic representation of the graphs whose key configurational functions are related by the general substitution theory of § 5. The vertices R and S of the articulation set are not restricted to nodes. The shaded portions represent any graph connecting R and S.

of G' that do not contain a'; the function ψ' contains all the sub-graphs of G' that contain R and S and have every vertex of even degree except R and S. We write likewise for G''

$$P'' = 1+\phi''+a''\psi'' \tag{5.2}$$

where the functions ϕ'' and ψ'' will correspond to sets of sub-graphs restricted as before. The embeddings which contribute to the key function for G divide into two mutually disjoint classes.

(i) Those that are the sum graph of two no-field embeddings (which may include the null-graph), one wholly in G', the other wholly in G''.

(ii) Those that are the sum graph of two magnetic embeddings, one wholly in G', the other wholly in G'', each having R and S as their odd (magnetic) vertices.

Now the first class must correspond identically to the product $(1+\phi')(1+\phi'')$ and the second to the product $\psi'\psi''$. Thus we may write

$$P = (1+\phi')(1+\phi'')+\psi'\psi'' \tag{5.3}$$

and the corresponding weight generating function is, by the complete term method,

$$\ln^*[(1+\phi')(1+\phi'')+\psi'\psi''] = \ln^*\left[1+\phi'+\left(\frac{\psi''}{1+\phi''}\right)\psi'\right]. \tag{5.4}$$

The equality follows because without the asterisks the right-hand side only differs from the left by $\ln(1+\phi'')$ and this cannot contribute any complete terms. But the weight generating function of G' is

$$\ln^*(1+\phi'+a'\psi') \tag{5.5}$$

and the joining of the two graphs G' and G'' at R and S, with deletion of a' and a'' is seen to be equivalent to the substitution

$$a' = \psi''/(1+\phi''). \tag{5.6}$$

This contains the results given by Domb (1972, theorems I and II and substitution (23)) but is more general. We have proved the substitution (5.6) for a graph; the argument will apply to any homeomorph of G and therefore is applicable, *mutatis mutandis*, to graph topologies.

By successive applications of the result of this section, and the methods of previous sections, the L weights of a large number of graphs have been determined (Hunter 1967); some general properties of L weights are summarized by Sykes *et al* (1974, § 2).

Acknowledgments

This research has been supported (in part) by a grant from the Science Research Council and (in part) by the National Research Council of Canada.

References

Abe R 1964 *Prog. Theor. Phys.* **31** 412–23
Baker G A 1963 *Phys. Rev.* **129** 99–102
Domb C 1949 *Proc. R. Soc.* A **199** 199–221
—— 1960 *Phil. Mag. Suppl.* **9** 149–361
—— 1970 *J. Phys.* C: *Solid St. Phys.* **3** 256–84
—— 1972 *J. Phys.* C: *Solid St. Phys.* **5** 1417–28
Domb C and Hiley B J 1962 *Proc. R. Soc.* A **268** 506–26
Essam J W and Fisher M E 1970 *Rev. Mod. Phys.* **42** 271–88
Essam J W and Sykes M F 1966 *J. Math. Phys.* **7** 1573–81
Hunter D L 1967 *PhD Thesis* University of London
—— 1969 *J. Phys.* C: *Solid St. Phys.* **2** 941–7
Kubo R 1962 *J. Phys. Soc. Japan* **17** 1100–20
Potts R B 1951 *DPhil Thesis* University of Oxford
Riordan J 1958 *An Introduction to Combinatorial Analysis* (New York: Wiley)
Rushbrooke G S and Eve J 1962 *J. Math. Phys.* **3** 185–9
Rushbrooke G S and Scoins H I 1955 *Proc. R. Soc.* A **230** 74–90
—— 1962 *J. Math. Phys.* **3** 176–84
Ryser H J 1963 *Combinatorial Mathematics* (New York: Wiley)
Strieb B, Callen H B and Horwitz G 1963 *Phys. Rev.* **130** 1798–808
Sykes M F, Essam J W, Heap B R and Hiley B J 1966 *J. Math. Phys.* 7 1557–72
Sykes M F, McKenzie D S and Heap B R 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** 1576–88
Trefftz E 1950 *Z. Phys.* **127** 371–80
Uhlenbeck G E and Ford G W 1962 *Studies in Statistical Mechanics* eds J de Boer and G E Uhlenbeck (Amsterdam: North-Holland)
Van der Waerden 1941 *Z. Phys.* **118** 473–88
Wakefield A J 1951 *Proc. Camb. Phil. Soc.* **47** 419–35
Yvon J 1945 *Cah. Phys.* no 28