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Finite cluster partition functions for the D-vector model

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Abstract. Systematic methods are developed for calculating the partition functions of star topologies in the D-vector model. A particularly simple technique (ladder transformation) is proposed for topologies containing a 2-cycle (ladder topologies), and these constitute numerically the majority of star topologies. The fewer non-ladder topologies need individual attention and three methods are suggested: (i) making a selected bond infinite, (ii) using direct averages, (iii) considering the behaviour as $D \to \infty$. By suitable renormalization of the interaction it is shown that as $D \to 0$ the self-avoiding walk model results (as has been demonstrated previously by other methods).

1. Introduction

A pioneering investigation of the classical Heisenberg model was published by Joyce in 1967. In it he calculated the eigenvalues and eigenfunctions of the integral equation which characterizes the one-dimensional chain, and used them to derive the partition functions of finite clusters of spins. He established the important result that the partition function of any finite cluster was determined basically by its *topology*, i.e. by the structure and position of vertices of degree three or more (for a general introduction to graph theoretical terminology see e.g. Domb 1974a). The insertion of vertices of degree two into the cluster could then be dealt with in an elementary manner. Joyce also showed that the partition function for a cluster with articulation points is equal to the product of the *star clusters* obtained by cutting the corresponding graph at all its articulation points. Thus the partition functions of all finite clusters are determined by the partition functions of star clusters with different topologies, and Joyce showed how these could be determined for topologies of cyclomatic number $c(G) \leq 4$.

The method used by Joyce was to expand the exponential factor in the integral representing the partition function in terms of the eigenfunctions and eigenvalues of the integral equation characterizing the one-dimensional chain. Because of the spherical symmetry of the Hamiltonian these eigenfunctions involve spherical harmonics, and the multiple integrals which arise with products of spherical harmonics for the various star topologies can be expressed in terms of the Wigner 3-j and 6-j symbols.

The star cluster partition functions derived by this method were used by Joyce and Bowers (1966) to calculate high temperature series expansions for the model for various crystal lattices. Independent calculations by alternative methods were undertaken by Stanley and Kaplan (1966) and Wood and Rushbrooke (1966) and the method

of Stanley and Kaplan was generalized by Stanley (1968b) to the case of interacting isotropic spins in D dimensions (the D-vector model, for a general review see Stanley 1974). However, despite the efforts of these groups of investigators, the number of terms of high temperature expansions available for the D-vector model (9 or 10) is appreciably less than for the Ising model (more than 15, see Domb 1974b, McKenzie 1975), and estimates of critical exponents are therefore far less reliable. For the Ising model the finite cluster method has been used very effectively for high temperature expansions, and substantial data on star lattice constants have been assembled. It would be advantageous if the data could be put to effective use for the D-vector model.

The theory described in the first two paragraphs above for the classical Heisenberg model generalizes immediately to the D-vector model. But its practical implementation for the calculation of star cluster partition functions would require formulae analogous to the 3-j and 6-j symbols for D-dimensional hyperspherical harmonics, and these are not readily available. Also, the method cannot be extended to topologies with $c(G)>4$ without a great increase in complication.

The present paper therefore formulates an alternative method of calculating star cluster partition functions by systematically building up graphs with cyclomatic number c from those with cyclomatic number $(c-1)$. The coefficients of the products of eigenfunctions in these partition functions are not expressed in closed form for all orders, as in Joyce's treatment, but are derived as rational functions of D. The principal aim of the investigation is to extend high temperature series expansions for various crystal lattices, but we think that the partition functions of the clusters and their dependence on D have an intrinsic interest of their own. Particular attention will be focused on the cases $D\to 0$ and $D\to\infty$ with a suitably renormalized interaction. In the former case the only surviving graphs are polygons (as first indicated by de Gennes 1972). In the latter case we shall obtain a limiting function which for an infinite lattice is identical with the spherical model; however, the two models are no longer equivalent for clusters of finite size.

Preliminary steps in the direction of the present approach were described in a previous publication (Domb 1972). We there differentiated between ladder and non-ladder topologies (see later § 3 for further details) and pointed out that the former can be dealt with simply and automatically by a suitable linear transformation. The latter need individual attention but are less numerous, and the derivation of twelve terms in the high temperature series expansion of the partition functions for the face-centred cubic (FCC) lattice requires only six non-ladder topologies. We shall derive an explicit form for the 'ladder transformation', and describe a number of different methods of dealing with non-ladder topologies which should be sufficient to cover cases of practical interest. We shall adopt the notation of Stanley in which D represents the spin dimension and d the space dimension (in our previous publication d was used for spin dimension).

2. Structure of partition functions of finite clusters

Following Joyce we consider star topologies with different interactions along the different bonds. Typical examples are the α and β topologies shown in figure 1.

The eigenvalues of the D-vector model in one dimension are (Stanley 1969)

$$\lambda_r = 2^{\frac{1}{2}D-1}\Gamma(\tfrac{1}{2}D)K^{-\frac{1}{2}D+1}I_{\frac{1}{2}D-1+r}(K) \qquad (r=0,1,2,\ldots) \tag{1}$$

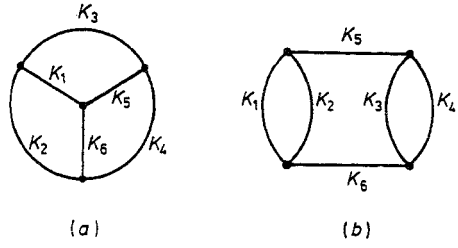

Figure 1. (*a*) α topology; (*b*) β topology. Each bond has a different interaction.

where $K = J/kT$, and $I_\nu(K)$ is the Bessel function of order ν. The degeneracies are

$$1, D, \frac{(D+2)(D-1)}{2!}, \frac{(D+4)D(D-1)}{3!},$$
$$\ldots \frac{(D+2r-2)(D+r-3)(D+r-4)\ldots(D-1)}{r!}, \ldots. \tag{2}$$

Hence the partition function for a polygon with n bonds is given by (Bowers 1969, Liu and Joseph 1971)

$$Z(p_n, K) = \lambda_0^n + D\lambda_1^n + \frac{(D+2)(D-1)}{2!}\lambda_2^n + \ldots \frac{(D+2r-2)(D+r-3)\ldots(D-1)}{r!}\lambda_r^n + \ldots. \tag{3}$$

For a linear chain with n bonds the partition function has the simpler form

$$Z(c_{n+1}; K) = \lambda_0^n. \tag{4}$$

Following the approach of Joyce (1967) the following general results can readily be established for the D-vector model. The partition function of a general topology G with r links is of the form

$$Z(G; K_1, K_2, \ldots K_r) = \sum_{a.b\ldots h} C(a, b, \ldots h)_G \lambda_a(K_1)\lambda_b(K_2)\ldots\lambda_h(K_r) \tag{5}$$

the sum being taken over all integral $a, b, \ldots h$ including zero. The $C(a, b, \ldots h)_G$ are functions of D and our main task in this paper is to show how to calculate them.

If any vertex of order two is inserted in a given bond (say the rth) and the interaction K_r is replaced by K_r', K_r'' (figure 2), the only change in equation (5) is to replace $\lambda_h(K_r)$ by $\lambda_h(K_r')\lambda_h(K_r'')$. Generalizing this result, if t vertices of order 2 are inserted and the interaction is unchanged $\lambda_h(K_r)$ is replaced by $\lambda_h^{t+1}(K_r)$. For example, the partition function of a polygon having n_1 bonds with interaction K' and n_2 bonds with interaction K'' is given by equation (3) with the general term λ_r^n replaced by $\lambda_r(K')^{n_1}\lambda_r(K'')^{n_2}$.

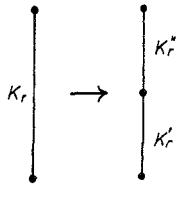

Figure 2. Insertion of a 2-degree vertex.

The argument given by Joyce regarding the partition functions of articulated clusters also generalizes to the D-vector model, i.e. they are the products of the partition functions of the constituent stars. Hence, if we can calculate the $C(a, b, \ldots h)_G$ for all star topologies we can easily write down the partition function of any finite cluster.

3. Ladder transformation

We shall now consider the transformation indicated in figure 3 in which a section of a topology has its interaction changed from K to K^*, which is then replaced by two branches with interactions K' and K''. For the change from K to K^*, any term $\lambda_t(K)$ in

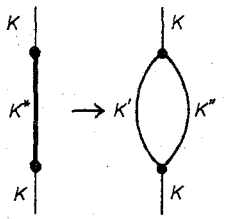

Figure 3. Ladder transformation.

the partition function is replaced by $\lambda_t(K)\lambda_t(K^*)$. We now substitute $K'+K''$ for K^*, and require a relation between $\lambda_t(K'+K'')$ and $\lambda_r(K')$, $\lambda_s(K'')$. From the general theory of Bessel functions (Watson 1966) it is easy to show that there is a linear relation of the form

$$\lambda_t(K'+K'') = \sum d_{rs}^{(t)} \lambda_r(K')\lambda_s(K''). \tag{6}$$

We shall use the standard difference relations for Bessel functions to calculate the $d_{rs}^{(t)}$.

We write for convenience

$$\lambda_t = 2^\nu \Gamma(\nu+1) K^{-\nu} I_{\nu+t}(K) \qquad (\nu = \tfrac{1}{2}D - 1;\ t = 0, 1, 2, \ldots). \tag{7}$$

Differentiating, and using the difference formulae

$$I'_\theta = \tfrac{1}{2}(I_{\theta-1} + I_{\theta+1}) \qquad \theta I_\theta / K = \tfrac{1}{2}(I_{\theta-1} + I_{\theta+1}) \tag{8}$$

we find after a little manipulation,

$$\lambda'_t = \tfrac{1}{2}\left(\frac{t}{\nu+t}\lambda_{t-1} + \frac{2\nu+t}{\nu+t}\lambda_{t+1}\right). \tag{9}$$

We now apply this formula to (6). Differentiating the left-hand side we obtain

$$\frac{\mathrm{d}\lambda_t(K'+K'')}{\mathrm{d}K'} = \tfrac{1}{2}\left(\frac{t}{\nu+t}\lambda_{t-1}(K'+K'') + \frac{2\nu+t}{\nu+t}\lambda_{t+1}(K'+K'')\right)$$

$$= \frac{t}{2(\nu+t)} \sum_{r,s=0}^{\infty} d_{rs}^{(t-1)} \lambda_r(K')\lambda_s(K'') + \frac{2\nu+t}{2(\nu+t)} \sum_{r,s=0}^{\infty} d_{rs}^{(t+1)} \lambda_r(K')\lambda_s(K''). \tag{10}$$

But differentiating the right-hand side we obtain

$$\frac{d\lambda_t(K'+K'')}{dK'} = \sum_{r,s=0}^{\infty} d_{rs}^{(t)} \lambda_r'(K')\lambda_s(K'')$$

$$= \tfrac{1}{2} \sum_{r=1,s=0}^{\infty} \frac{r}{\nu+r} \lambda_{r-1}(K')\lambda_s(K'') + \tfrac{1}{2} \sum_{r,s=0}^{\infty} \frac{2\nu+r}{\nu+r} \lambda_{r+1}(K')\lambda_s(K''). \tag{11}$$

Equating coefficients of $\lambda_r(K')\lambda_s(K'')$ in equations (10) and (11), and converting back to D we find that

$$\frac{D+t-2}{D+2t-2} d_{r,s}^{(t+1)} = \frac{r+1}{D+2r} d_{r+1,s}^{(t)} + \frac{D+r-3}{D+2r-4} d_{r-1,s}^{(t)} - \frac{t}{D+2t-2} d_{r,s}^{(t-1)}. \tag{12}$$

Relation (12) enables us to calculate $d_{rs}^{(t+1)}$ from $d_{rs}^{(t)}$ and $d_{rs}^{(t-1)}$. We start with $t=0$ for which the coefficients can most easily be obtained by applying the transformation to a point pair (figure 4). We know the resulting partition functions from equation (3), and we deduce that

$$\lambda_0(K'+K'') = \sum d_{rr}^{(0)} \lambda_r(K')\lambda_r(K''), \tag{13}$$

$$d_{rr}^{(0)} = \frac{(D+2r-2)(D+r-3)!}{(D-2)!r!}. \tag{14}$$

All $d_{rs}^{(0)}$ with $r \neq s$ are zero.

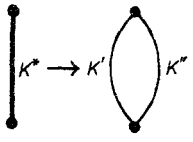

Figure 4. Ladder transformation applied to a point pair, yielding a polygon.

Putting $t=0$ in equation (12) the last term on the right-hand side does not enter, and we find that

$$d_{r,r-1}^{(1)} = d_{r-1,r}^{(1)} = \frac{(D+r-3)!}{(D-2)!(r-1)!} \tag{15}$$

all other $d_{rs}^{(1)}$ being zero.

When we put $t=1$, there are two different types of non-zero term:

$$d_{r,r-2}^{(2)} = d_{r-2,r}^{(2)} = \frac{D(D+r-3)!}{(D+2r-4)(D-1)!(r-2)!}, \tag{16}$$

$$d_{rr}^{(2)} = \frac{2(D+r-3)!}{(D+2r)(D+2r-4)(D-1)!(r-1)!} \times [D^3+3D^2(r-2)+2D(r^2-6r+6)-(2r-2)(2r-4)]. \tag{17}$$

It will be seen that the second is now considerably more complicated.

We could proceed to derive general formulae for higher order t, but because of the increase in complication it is better to calculate these numerically for individual r, s. However, we note the following general property: if $r \geqslant s \geqslant t$ the only non-zero terms

are those for which $r+s+t$ is even and $t \geqslant r-s$. This is a general form of the triangle condition for the 3-j symbols which are relevant in the $D=3$ case (Joyce 1967).

When $D=2$ the difference relation (12) gives trouble when $r=1$. However, this is a particularly simple case which we can deal with exactly in an elementary manner; since

$$\lambda_t = I_t(K), \tag{18}$$

we can use standard formulae for Bessel functions (Watson 1966)

$$I_n(K'+K'') = \sum_{p=-\infty}^{\infty} I_p(K')I_{n-p}(K'') \qquad (I_{-n}(x) = I_n(x)). \tag{19}$$

We thus find that the only non-zero values of $d_{rs}^{(t)}$ are given by

$$d_{rs}^{(t)} = 1 \qquad r \neq s, \qquad |r-s| = t; \qquad d_{rr}^{(0)} = 2. \tag{20}$$

It should be noted that formulae (15), (16) and (17) are correct when $D=2$.

We now show how the ladder transformation can be used to derive the $C(a, b, \ldots h)$ for a number of topologies. The term *ladder topology* will be used to describe any topology which can be derived from a topology with lower cyclomatic number by means of a ladder transformation. From the list of topologies with $c \leqslant 4$ reproduced in figure 5 (from Essam and Sykes 1966) we note that $\theta, \beta, \gamma, \delta, D, E, H, I, K, L, M, N, O, P$ and Q are ladder topologies derivable from a polygon p; for all of these topologies the $C(a, b, \ldots h)$ can be calculated in terms of the $d_{rs}^{(t)}$. The *non-ladder topologies* are α, A, B and F; C, G and J are ladder topologies derivable from α.

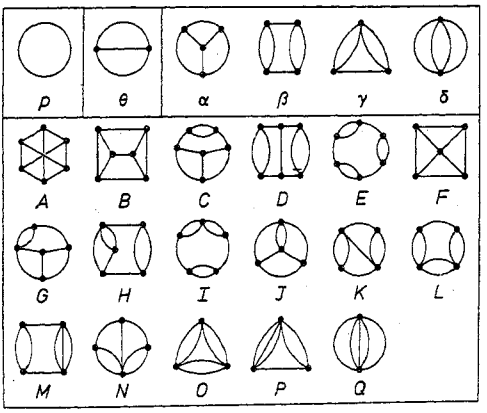

Figure 5. Topologies with cyclomatic number $c \leqslant 4$ (after Essam and Sykes 1966).

We first consider the θ topology, which can be derived from the polygon (figure 6). We find that

$$C(r, s, t)_\theta = d_{rr}^{(0)} d_{rs}^{(t)}. \tag{21}$$

Since $C(r, s, t)_\theta$ is symmetric in (r, s, t) the triangle condition can be extended to any pair of (r, s, t). Numerical examples of this condition for small (r, s, t) are

$$C(4, 1, 1)_\theta = C(5, 2, 1)_\theta = C(6, 2, 2)_\theta = 0.$$

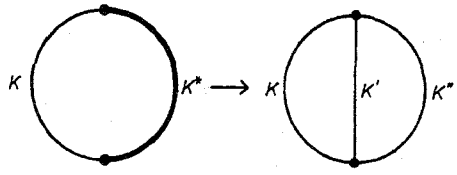

Figure 6. θ topology derived by ladder transformation from polygon.

Some typical values are

$$C(2,1,1)_\theta = D(D-1)$$
$$C(3,2,1)_\theta = D^2(D-1)/2 \tag{22}$$
$$C(2,2,2)_\theta = (D+2)^2(D-2)(D-1)/(D+4).$$

The E topology can be handled in the same way (figure 7), and we find that the non-zero coefficients are

$$C(r,s,t,r',s',t,r'',s'',t)_E = d^0_{tt} d^{(t)}_{rs} d^{(r)}_{r's'} d^{(t)}_{r''s''}. \tag{23}$$

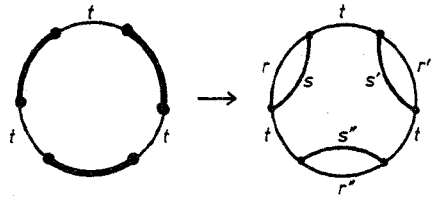

Figure 7. E topology derived by 3 ladder transformations from polygon.

For the δ topology we find from figure 8 that

$$C(r,s,r',s')_\delta = \sum_t C(t)_p d^{(t)}_{rs} d^{(t)}_{r's'}. \tag{24}$$

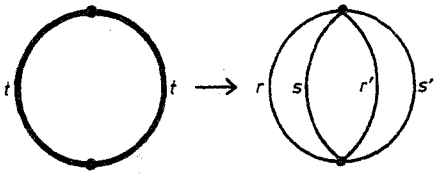

Figure 8. δ topology derived by 2 ladder transformations from polygon.

If there is no value for t for which the triangle conditions on (r, s, t) and (r', s', t) can be satisfied simultaneously then $C(r, s, r', s')_\delta$ is zero. For example

$$C(5,1,1,1)_\delta = C(6,2,1,1)_\delta = 0. \tag{25}$$

The Q topology involves two vertices of degree 5. It can most easily be derived by a ladder transformation on the δ topology, and we find that

$$C(r,s,r',s',r'')_Q = \sum_{t'} C(r,s,r',t')_\delta d_{s't''} = \sum_{t,t'} (C_t)_p d^{(t)}_{rs} d^{(t)}_{r't'} d^{(t)}_{s't''}.$$

The coefficient is zero if no t, t' can be found such that

$$(rst) \quad (tr't') \quad (t's'r'') \tag{26}$$

all satisfy the triangle conditions. The generalization to vertices of higher degree is straightforward.

4. Vertex functions

Following the general argument given in Joyce (1967), the coefficients $C(l_1, l_2, \ldots l_r)_G$ can be written as sums of certain *vertex functions* over the graph. From equation (3.5) of Joyce's paper we deduce that for $D = 3$,

$$C(l_1, l_2, \ldots l_r)_G = \sum_{\{m_i\}} \prod_{\substack{\{\text{all vertices}\} \\ v \text{ in } G}} \int_\Omega \prod_{\substack{\{\text{all } \delta \text{ at} \\ \text{vertex } v\}}} Y_{l_\delta m_\delta}(\theta, \phi)\, \mathrm{d}\Omega. \tag{27}$$

Here the $Y_{l_\delta m_\delta}(\theta, \phi)$ are spherical harmonics, and the pairs of $Y_{l_\delta m_\delta}(\theta, \phi)$ with the same subscripts (corresponding to the two ends of a particular bond) must be complex conjugates. Hence, Joyce was able to evaluate the $C(l_1, l_2, \ldots l_r)_G$ for all the topologies with $c \leqslant 4$ (figure 5) in terms of the Wigner 3-j, 6-j and 9-j symbols. As typical examples we quote the formulae for the θ topology

$$C(l_1, l_2, l_3)_\theta = (2l_1+1)(2l_2+1)(2l_3+1)\begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix}^2, \tag{28}$$

and for the α topology (figure 1)

$$\begin{aligned} C(l_1, l_2, l_3, l_4, l_5, l_6)_\alpha &= \Big(\prod_{i=1}^{6} (2l_i+1)\Big)(-1)^{l_4+l_5+l_6}\begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & l_5 & l_6 \\ 0 & 0 & 0 \end{pmatrix} \\ &\quad \times \begin{pmatrix} l_4 & l_2 & l_6 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_4 & l_5 & l_3 \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} l_1 & l_2 & l_3 \\ l_4 & l_5 & l_6 \end{Bmatrix}. \end{aligned} \tag{29}$$

These closed form formulae valid for all l_i are extremely useful as a general check on more general formulae for specific l_i which we shall derive for general D.

A feature of equation (27) is that, at any vertex of degree 3, the vertex function is zero unless $(l_1 l_2 l_3)$ satisfy the triangle condition which is expressed for general positive l_1, l_2, l_3 in the form

$$l_1 + l_2 - l_3 \geqslant 0, \qquad l_2 + l_3 - l_1 \geqslant 0, \qquad l_3 + l_1 - l_2 \geqslant 0. \tag{30}$$

This condition is identical with the one we derived in the previous section for the θ topology in the D-vector model; if it is not satisfied the integral of the product of any three spherical harmonics,

$$\int Y_{l_1 m_1}(\theta, \phi) Y_{l_2 m_2}(\theta, \phi) Y_{l_3 m_3}(\theta, \phi)\, \mathrm{d}\Omega, \tag{31}$$

is zero.

For a vertex of degree 4 one can show similarly that the integral of the product of four spherical harmonics is zero unless there exists an l for which $(l_1\, l_2\, l)$ and $(l\, l_3\, l_4)$ satisfy the triangle condition (30). This is identical with the condition we derived in the

previous section for the δ topology in the D-vector model. For a vertex of degree 5 a relation analogous to equation (25) must be satisfied.

Equation (27) generalizes immediately to the D-vector model, the spherical harmonics being replaced by hyperspherical harmonics (Gegenbauer polynomials, see Erdélyi 1953). The above relations for non-zero coefficients obtained when $D=3$ are identical with those derived in the previous section for vertices of ladder topologies for general D; we thus have a strong indication that they are satisfied for vertices of all topologies in the D-vector model, i.e. that relations analogous to equation (31) are valid for hyperspherical harmonics. This result can be established quite generally, and we shall assume it to be the case in the remainder of this paper.

We shall now deal specifically with $D=2$ since there are a number of simplifying features. The circular harmonics are the functions $\exp(\pm \mathrm{i}m\phi)$, and for a vertex of degree 3 a non-zero term can only be obtained if one of the relations in equation (30) is an equality. Likewise, at a vertex of degree 4 it must be possible to find a combination of positive and negative signs for which

$$l_1 \pm l_2 \pm l_3 \pm l_4 \tag{32}$$

reduces to zero; the generalization to higher order vertices is straightforward. Because of the complex conjugate condition a function $\exp(+\mathrm{i}m\phi)$ at one end of a bond must be matched by $\exp(-\mathrm{i}m\phi)$ at the other end of the bond. Hence, the evaluation of $C(l_1, l_2 \ldots l_r)_G$ when $D=2$ is an elementary combinatorial problem and is analogous to the determination of horizontal weights in the X–Y model (Betts 1974). As typical examples we find for the α topology,

$$C(2,2;2,2;2,2)_\alpha = 0, \qquad C(3,1;2,2;1,1)_\alpha = 2. \tag{33}$$

A diagrammatic illustration of the last result is shown in figure 9.

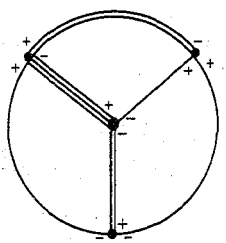

Figure 9. Configuration calculation of $C(3,1;2,2;1,1)_\alpha$ for $D=2$.

5. Non-ladder topologies

We build up topologies successively by increasing the cyclomatic number c. For a non-ladder topology with this cyclomatic number, any coefficient $C(l_1, l_2, \ldots l_r)_G$ with any of the l_i zero corresponds to a coefficient in a topology of cyclomatic number less than c and can be assumed known. Our task is to calculate the coefficients when none of the l_i are zero. We shall propose three different methods.

5.1. Coalesce two vertices by allowing a chosen bond to become infinite

We obtain a topology with the same c, but which has fewer vertices, and is therefore

either a ladder topology or 'closer' to one. Examples are shown in figure 10. Let G^* be the topology derived from G by coalescing the two vertices on bond 1.

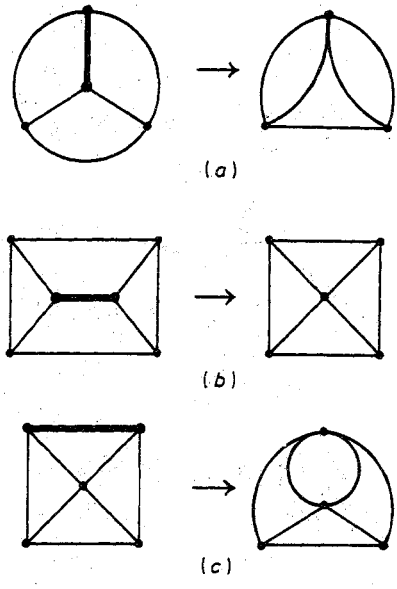

Figure 10. Making a bond infinite to coalesce two vertices. (*a*) $\alpha \rightarrow \gamma$; (*b*) $B \rightarrow F$; (*c*) $F \rightarrow J$.

As $K_1 \rightarrow \infty$ we find from the asymptotic formulae for Bessel functions that

$$\lambda_t(K_1)/\lambda_0(K_1) \rightarrow 1 \tag{34}$$

for all t. We then obtain the relation

$$C(l_2, l_3, \ldots, l_r)_{G^*} = \sum_{l_1=0}^{\infty} C(l_1, l_2, \ldots, l_r)_G. \tag{35}$$

Our aim is to choose l_1 so that as few as possible of the terms on the right-hand side are non-zero because of violation of the triangle conditions (30). We illustrate by examples from the α topology

$$\begin{aligned} C(2;1,1;1,1)_\gamma &= C(0,2;1,1;1,1)_\alpha + C(2,2;1,1;1,1)_\alpha + C(4,2;1,1;1,1)_\alpha \\ &= C(2,1,1)_\theta + C(2,2;1,1;1,1)_\alpha \end{aligned} \tag{36}$$

since the final term is zero. From this we deduce that

$$C(2,2;1,1;1,1)_\alpha = D(D-1)(D-2)/(D+2). \tag{37}$$

In an analogous manner we derive the following relations:

$$\begin{aligned} C(2,1;2,1;2,1)_\alpha &= D(D-1)(D-2) \\ C(3,1;2,2;1,1)_\alpha &= D^3(D-1)/(D+2) \\ C(3,2;2,1;1,2)_\alpha &= D^2(D-1)(D-2)/(D+4). \end{aligned} \tag{38}$$

The values can be checked for $D=3$ from equation (29).

This method is very simple and direct, but it may provide only a relation between unknown coefficients. For example, for the coefficient $C(2,2;2,2;2,2)_\alpha$ we find

$$C(2;2,2;2,2)_\gamma = C(0,2;2,2;2,2)_\alpha + C(2,2;2,2;2,2)_\alpha + C(4,2;2,2;2,2)_\alpha. \quad (39)$$

From this we deduce that

$$\begin{aligned} &C(2,2;2,2;2,2)_\alpha + C(4,2;2,2;2,2)_\alpha \\ &\quad = C(2,2,2)_\theta + C(2;2,2;2,2)_\gamma \\ &\quad = \frac{(D+2)^2(D-2)(D-1)}{(D+4)^2}(2D^2-D-12). \end{aligned} \quad (40)$$

To evaluate the coefficients separately we must resort to an alternative method.

5.2. *Direct averaging*

We use i, j to label the vertices of any topology G, $\langle ij\rangle$ denoting the bonds of G, and we denote by σ_α the component of a D-dimensional spin, α going from 1 to D. The high temperature expansion of the partition function is then

$$\begin{aligned} Z(G) &= \left\langle \exp \sum_{\alpha\langle ij\rangle} K_{ij}\sigma_{\alpha i}\sigma_{\alpha j} \right\rangle = \left\langle \prod_{\langle ij\rangle} \exp K_{ij} \sum_\alpha \sigma_{\alpha i}\sigma_{\alpha j} \right\rangle \\ &= \left\langle \prod_{\langle ij\rangle} \left[1 + K_{ij} \sum_\alpha \sigma_{\alpha i}\sigma_{\alpha j} + \tfrac{1}{2!}K_{ij}^2 \left(\sum_\alpha \sigma_{\alpha i}\sigma_{\alpha j} \right)^2 + \ldots + \tfrac{1}{r!}K_{ij}^r \left(\sum_\alpha \sigma_{\alpha i}\sigma_{\alpha j} \right)^r + \ldots \right] \right\rangle. \end{aligned} \quad (41)$$

We can pick out a term corresponding to any configuration, say $K_1^a K_2^b \ldots K_r^h$ and calculate its average. We can then evaluate the same term from

$$Z(G) = \sum C(a, b, \ldots h)_G \lambda_a(K_1)\lambda_b(K_2)\ldots\lambda_h(K_r) \quad (42)$$

and hence determine $C(a, b, \ldots h)_G$, assuming that lower order coefficients are known. The calculation of the average is somewhat complicated, but it is often unnecessary to complete it, since by merely considering its form we can gain enough information to evaluate $C(a, b, \ldots h)_G$.

We first note that the term we require is given by the average of a product

$$\frac{(\sigma_{\alpha i}\sigma_{\alpha j})^a}{a!} \frac{(\sigma_{\beta j}\sigma_{\beta k})^b}{b!} \cdots \frac{(\sigma_{\gamma m}\sigma_{\gamma p})^h}{h!}. \quad (43)$$

This can be visualized graphically as a bonding of G in which each bond can have one of D colours. For each colouring we average all the vertex configurations and multiply them together, and then we sum over all possible colourings. We can conveniently divide the averages into those corresponding to one colour (which can be chosen in D ways), corresponding to 2 colours (which can be chosen in $D(D-1)/2!$ ways), etc.

There are a number of simplifying features as follows:

(i) Any vertex having an odd number of bonds of a given colour has zero average.

(ii) A 4-vertex has an average of the form $A/D(D+2)$, a 6-vertex has an average of form $A/D(D+2)(D+4)$ and so on, *no matter what is the colouring of the vertex.* Only the value of A is affected by the colouring of the vertex.

Let us illustrate by considering the term $K_1^2K_2^2K_3^2K_4^2K_5^2K_6^2$ for the α topology. Each vertex is of order 6. Hence the general form of average is

$$\left(\frac{1}{D(D+2)(D+4)}\right)^4[a_0D+a_1D(D-1)+\ldots+a_5D(D-1)\ldots(D-5)]. \tag{44}$$

When we wish to examine the coefficients in equation (42) which contribute to this term we note first that

$$\begin{aligned}
\lambda_0(K)&=1+\frac{K^2}{2D}+\frac{K^4}{2\times4D(D+2)}\\
\lambda_1(K)&=\frac{K}{D}+\frac{K^3}{2D(D+2)}\\
\lambda_2(K)&=\frac{K^2}{D(D+2)}+\frac{K^4}{2D(D+2)(D+4)}\\
\lambda_s(K)&=\frac{K^s}{D(D+2)\ldots D(2s-2)}\left(1+\frac{K^2}{2(D+2s)}+\ldots\right).
\end{aligned} \tag{45}$$

Hence we find that the value of the term is

$$\begin{aligned}
&C(2,2;2,2;2,2)_\alpha/D^6(D+2)^6+4C(2)_p/(2D)^3D^3(D+2)^3+3C(2)_p/(2D)^2D^4(D+2)^4\\
&\quad+6C(2,2,2)_\theta/(2D)D^5+1/(2D)^6.
\end{aligned} \tag{46}$$

Equating equations (44) and (46) and cleaning up we find that

$$\begin{aligned}
&C(2,2;2,2;2,2)_\alpha+\tfrac{1}{4}(D-1)(D+2)^4+\tfrac{3}{8}(D-1)(D+2)^3\\
&\quad+3(D+2)^2(D-2)(D-1)/(D+4)+\tfrac{1}{64}(D+2)^6\\
&=\frac{D^3(D+2)^2}{(D+4)^4}[a_0+a_1(D-1)+a_2(D-1)(D-2)+\ldots].
\end{aligned} \tag{47}$$

We note that the right-hand side in equation (47) begins with D^3; hence the first three powers on the left-hand side must be zero, and if the expansion of $C(2,2;2,2;2,2)_\alpha$ (which we note by x for convenience) in powers of D starts with $A_0+A_1D+A_2D^2$, we calculate that

$$A_0=-6, \qquad A_1=11/2, \qquad A_2=13/4. \tag{48}$$

We can proceed likewise with $C(4,2;2,2;2,2)_\alpha$ (denoted by y) to determine the first terms in its expansion.

When $D=3$ we find, using Joyce's formula, that

$$x=-2\times3\times5^3\times7^{-3}, \qquad y=2^3\times3^2\times5^2\times7^{-3}. \tag{49}$$

The form of equation (49) suggests assuming the general form

$$x=\frac{(D+2)^2(D-2)(D-1)}{(D+4)^3}(B_0+B_1D+B_2D^2+B_3D^3). \tag{50}$$

From equation (48) we find that $B_0 = -48$, $B_1 = -16$, $B_2 = 6$, and using equation (40) we then find

$$x = (D+2)^3(D-2)(D-1)(D^2+4D-24)/(D+4)^3$$
$$y = D^2(D+2)^2(D+1)(D-1)(D-2)/(D+4)^3. \tag{51}$$

As a check we note that both x and y are zero when $D = 1$ or 2. Further checks can be obtained by calculating individual coefficients a_i in equation (44), some of which are quite easy to obtain. A final check is provided by the third method which we now describe.

5.3. *Limiting form of coefficients as $D \to \infty$*

Stanley (1968a) has shown that if the interaction is renormalized, i.e. the original interaction J replaced by λJ^* where λ is of order D, and $\ln Z$ is then divided by λ, a finite limiting solution is obtained which we shall call the infinite D limit. For an assembly of N spins *in the thermodynamic limit* $N \to \infty$, this limit is identical with the spherical model solution. For finite clusters this is not the case; nevertheless, the existence of an infinite D limit for finite clusters has important implications which we shall now discuss.

Firstly, we investigate the eigenvalues in the infinite spin limit. Stanley showed that

$$\lim_{\lambda\to\infty} \frac{1}{\lambda} \ln \lambda_0^* = -1 + (1+K^{*2})^{\frac{1}{2}} - \ln \tfrac{1}{2}[1+(1+K^{*2})^{\frac{1}{2}}]. \tag{52}$$

Renormalizing the sth eigenvalue

$$\lambda_s^* = 2^\nu \Gamma(\nu+1)(\lambda K^*)^{-\nu} I_{\nu+s}(\lambda K^*), \qquad (\nu = \tfrac{1}{2}D - 1) \tag{53}$$

we easily find (e.g. by taking $\lambda = \nu$) that in the limit $\nu \to \infty$,

$$\lambda_1^*/\lambda_0^* \to w = K^*[1+(1+K^{*2})^{\frac{1}{2}}] \tag{54}$$

$$\frac{\lambda_2^*}{\lambda_0^*} \to w^2, \qquad \frac{\lambda_3^*}{\lambda_0^*} \to w^3, \qquad \ldots \qquad \frac{\lambda_s^*}{\lambda_0^*} \to w^s. \tag{55}$$

Using Stanley's result, if we form $\ln Z(G)$ for any topology, remove the λ_0^* terms and obtain a series in w, then from equations (54) and (55) all terms of order D^2, $D^3, \ldots$ must disappear. This gives us useful information about the form of the higher coefficients once we know the lower order coefficients, and in any case can serve as a useful check on any evaluations.

5.4. *Examples*

5.4.1. *Simple polygon*

$$\ln Z(p) - \ln \lambda_0^* = \ln[1 + Dw + \tfrac{1}{2!}(D+2)(D-1)w^2 + \tfrac{1}{3!}(D+4)D(D-1)w^3 + \ldots] \tag{56}$$

$$= Dw + \tfrac{1}{2!}(D+2)(D-1)w^2 - \tfrac{1}{2}D^2w^2 + [\tfrac{1}{3!}(D+4)D(D-1) - \tfrac{1}{2!}D(D+2)(D-1) + \tfrac{1}{3}D^3]w^3$$

$$= Dw + \tfrac{1}{2!}(D-2)w^2 + \tfrac{1}{3}Dw^3 \ldots . \tag{57}$$

5.4.2. θ graph. We can check individual coefficients in the expansion of $\ln Z(\theta) - \Sigma \ln \lambda_0^*$, e.g. the coefficient of $w^2w'w''$ is given by

$$C(2,1,1)_\theta - C(1,1,0)_\theta C(1,0,1)_\theta = D(D-1) - D^2 = -D. \tag{58}$$

The coefficient of $w^2w'^2w''^2$ is given by

$$\begin{aligned} &C(2,2,2)_\theta + 2C(1,0,1)_\theta C(0,1,1)_\theta C(1,1,0)_\theta - C(1,0,1)_\theta C(1,2,1)_\theta \\ &\quad - C(1,1,0)_\theta C(1,1,2)_\theta - C(0,1,1)_\theta C(2,1,1)_\theta \\ &\quad = D^3\left[\left(1+\frac{2}{D}\right)^2\left(1-\frac{2}{D}\right)\left(1-\frac{1}{D}\right)\left(1+\frac{4}{D}\right)^{-1} + 2 - 3\left(1-\frac{1}{D}\right)\right] \end{aligned} \tag{59}$$

and the coefficients up to the $1/D$ term in the square bracket vanish.

5.4.3. $C(2,2;2,2;2,2)_\alpha$ coefficients. As a more severe test we try the $C(2,2;2,2;2,2)_\alpha$ coefficients. The general procedure for obtaining terms in $\ln Z(\alpha)$ is to decompose into all possible cycles as in the Ising model, and enumerate the terms corresponding to each set of cycles. We find for the coefficient of $w_1^2w_2^2w_3^2w_4^2w_5^2w_6^2$

$$\begin{aligned} &C(2,2;2,2;2,2)_\alpha - 6[C(1)_p]^4 + 12[C(1)_p^2 C(2,1,1)_\theta] - 3[C(2,1,1)_\theta]^2 \\ &\quad - 4[C(2,1;2,1;2,1)_\alpha C(1)_p] + 2[C(1)_p]^3 - 3[C(2,2;1,1;1,1)_\alpha C(1)_p]. \end{aligned} \tag{60}$$

The first group of 4 terms corresponds to combinations of triangles and the last two to combinations of quadrilaterals. On substituting in equation (60) we find that the coefficients of D^4, D^3 and D^2 vanish, which is often a powerful check.

From this analysis it is clear that for any bonding the C coefficient for large D is of order D^σ where σ is the maximum number of cycles in the bonding. To ensure cancellation in any particular term the corresponding configuration must be decomposable into cycles (a double bond does not count as a cycle). We noted this property empirically in a previous paper (Domb 1972) and have now been able to establish that the vertex conditions in the previous section and decomposability into cycles are mathematically equivalent (Domb 1976). This result provides a generalization of the classic problem of the Königsberg bridges solved by Euler.

Of the three methods listed above only the second gives a definite answer in all cases. For many configurations the first method gives a simple and immediate answer, and in the few cases of failure the second and third methods can be invoked without involving calculations of too great complexity. We hope in this way to be able to tackle non-ladder configurations required for 16 terms of the high temperature expansion of the partition function.

6. Limiting behaviour as $D \to 0$

To complete the picture of the D-vector model from the finite cluster point of view we examine the behaviour of the model as $D \to 0$. It was first indicated by de Gennes (1972) that the self-avoiding walk model (see, e.g. Domb 1970) would then result; an alternative proof has been given by Bowers and McKerrell (1973).

We first renormalize the interaction so that $D \to 0$, $J \to 0$ but J/D remains finite and equal to J^*. We then find with reference to equation (45) that

$$\lambda_0(K) \to 1, \qquad \lambda_1(K) \to K^*, \qquad \lambda_r(K) \to 0 \qquad (r \geq 2). \tag{61}$$

Hence the only surviving terms in the finite cluster expansion are those with single bonds. But we can now readily show that the coefficients of all but the simple polygon tend to zero as $D \to 0$. To do this we make use of the method of direct averages described in the previous section. Consider any topology G with p points and l lines. Using relations analogous to equation (44), and equation (45), we find that

$$C(1, 1, 1, \ldots 1)_G = D^{l-p}\phi(D) \tag{62}$$

where $\phi(D)$ is a rational function which remains finite as $D \to 0$. We thus see that for any topology whose cyclomatic number c is greater than 1 the coefficient $C(1, 1, 1, \ldots 1)_G$ tends to zero as $D \to 0$.

For the susceptibility expansion which involves a single broken bond (Domb 1972) the only surviving term is the simple chain. We are thus led very simply and naturally to the self-avoiding walk model.

7. Conclusions

The major aim of this investigation was to formulate systematic methods of calculating finite cluster partition functions needed for the generation of series expansions for the D-vector model. For the majority of topologies (ladder topologies) this can be done in a simple automatic manner, and a suitable computer program has been devised by D L Hunter and P S English at St Francis Xavier University, Nova Scotia, Canada. The non-ladder topologies are much fewer in number, but require individual handling. Three methods have been proposed for calculation in these cases, with the aid of which it is hoped that the calculations can be performed without undue labour.

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