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THE n-COMPONENT CUBIC MODEL AND FLOWS: SUBGRAPH BREAK-COLLAPSE METHOD

by

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ABSTRACT

We generalise to the n-component cubic model the subgraph break-collapse method which we previously developed for the Potts model. The relations used are based on expressions which we recently derived for the $Z(\lambda)$ model in terms of mod-λ flows. Our recursive algorithm is similar, for $n = 2$, to the break-collapse method for the $Z(4)$ model proposed by Mariz and coworkers. It allows the exact calculation for the partition function and correlation functions for n-component cubic clusters with n as a variable, without the need to examine all of the spin configurations.

Key-words: Cubic model; Subgraph break-collapse method; Graph theory; Statistical mechanics.

1. INTRODUCTION

The n-component cubic model was introduced by Kim, Levy and Uffer (1975) in the description of phase transitions in cubic rare-earth compounds which have sixfold-degenerate ground states (and hence correspond to n = 3). Aharony (1977) generalised this model in order to include quadrupolar interactions, besides the dipolar ones. This extended cubic model, which we will henceforth call for simplicity the cubic model, is a discrete version of the continuous n-component spin model. Since its introduction, the cubic model has been studied by several methods (Kim and Levy 1975, Kim et al 1976, Hilhorst 1976, Domany and Riedel 1979, Nienhuis et al 1983, Badke et al 1985, Badke 1987, Tsallis et al 1988). It contains many interesting limiting cases (e.g., self-avoiding walks, spin 1/2 Ising model, the Ashkin-Teller model and the Potts model) and for n = 1 and n = 2 it becomes identical to the Ising and Z(4) models respectively. For a general value of n, the cubic model is a particular case of the Z(2n) model in which many values of the pair interaction energy become degenerate leading to only three which are distinct.

In a recent paper on the Z(λ) model (de Magalhães and Essam 1988a, "The Z(λ) Model and Flows"), herein referred to as ZF, we developed a recursive algorithm for the calculation of the exact partition function and pair correlation functions of Z(λ) clusters. These clusters were represented by graphs, the vertices and edges of which represented respectively the atoms and the pair interactions between them. This technique, the subgraph break-collapse method (SBCM), is an extension of the SBCM for the Potts model which we presented in paper III of the series of papers with the general title "Potts model and Flows" (de Magalhães and Essam 1988b, herein referred to as PF3). The SBCM for the Z(λ) model is based on a number of equations - the "graph reduction equations", the proofs of which were given in ZF through the use of mod-λ flows in graphs. One of these equations, the effective break-collapse equation, relates the partition function and correlation functions for a graph G with those for the "broken" graphs, "collapsed" graphs and graphs with "frozen edges". These graphs are obtained from G by respectively deleting, contracting and fixing the value of the flow in a chosen edge f. The other graph reduction equations allow the calculation of the above mentioned functions for articulated graphs and graphs in series or in parallel. The SBCM provides an efficient way of computing the partition function and the correlation functions by applying recursively the graph reduction equations, thereby avoiding the time-consuming summation over states.

An alternative method for calculating the above functions is the break-collapse method (BCM) of Mariz and coworkers (Mariz et al 1985, 1988, Tsallis 1988). The latter method differs from the SBCM in three main aspects: (i) it only replaces a subgraphs which is a combination of edges in series and/or in parallel by a single effective edge whereas the SBCM uses a more general subgraph replacement; (ii) its break-collapse equation contains graphs with "precollapsed" edges instead of "frozen" ones; (iii) with the exception of graphs with two vertices, the recursion terminates when all the edges of G are precollapsed rather than when just c(G) of them are frozen (here c(G) is the number of independent cycles in G). In ZF precollapsed edges were shown to correspond to edges on which the flow can take on several values (namely $0,\beta,\lambda-\beta$). Although therefore, for $\lambda > 4$, the BCM generates less graphs in each iteration than the SBCM, it was argued in ZF that for any λ the BCM is still less efficient than the SBCM. The reasons for this are twofold: (a) it needs more iterations; (b) for $\lambda>4$ the determination of the weight to be associated with a terminal graph (i.e. graphs with all edges precollapsed) is an enumeration problem whose computing time grows exponentially with the number of cycles in the graph. For $\lambda=4$ a simple formula for the weight of a terminal graph is available.

Here we specialise the above SBCM to the n-component cubic model taking advantage of the high degree of symmetry of its Hamiltonian. In particular, the effective break-collapse equation contains a sum of terms corresponding to the chosen edge f being frozen with values 0,2,4,..,2n-2. These terms can be naturally grouped together leading to a single term which corresponds to a graph for which the flow on f must be even. We call such an edge "even-frozen", and for n = 2 it becomes identical with the precollapsed edge introduced by Mariz et al (1985) in the Z(4) algorithm. Unlike the BCM for the $Z(\lambda)$ model, in our algorithm for the cubic model the weights of the terminal graphs with all edges even frozen are given by simple formulae *for any value of n*. Besides not having the inconvenience of the BCM mentioned in (b) above, our method allows the calculation of correlation functions for cubic clusters *for all values of n simultaneously* through a single application of the SBCM.

In section 2 we introduce the model and summarise previous results concerning the partition function (Biggs 1976,1977) and correlation functions (ZF) for the $Z(\lambda)$ model. In §3, we establish the relationship between the cubic model and the Z(2n) model. We also prove that the equivalent vector transmissivity (from which one can calculate the correlation functions) has only two different components. The graph reduction equations of the SBCM are given in section 4. In §5, we describe the SBCM algorithm and illustrate it by the example of the Wheatstone bridge graph. Finally our conclusions are presented in section 6.

2. MODEL AND REVIEW OF KNOWN RESULTS

In this section we define the model and summarise previous results obtained for the $Z(\lambda)$ model (Biggs 1976,1977 and ZF) which will be needed in the development of the subsequent sections.

2.1 The Cubic Model.

We consider the n-component cubic model for a graph G with vertex set V and edge set E. With each vertex i of V we associate an n-component vector which can point in one of the 2n directions (positive and negative) of the cartesian axes in an n-dimensional space, i.e.

$$S_i = (\pm1,0,0,\ldots,0) \text{ or } (0,\pm1,0,\ldots,0) \text{ or } \ldots (0,0,0,\ldots,\pm1). \quad (2.1)$$

The cubic model can be described by the following dimensionless Hamiltonian (Aharony 1977)

$$\beta H(G) = -\sum_{e\in E} [nK_e \mathbf{S}_i.\mathbf{S}_j + nL_e(\mathbf{S}_i.\mathbf{S}_j)^2] \quad (2.2)$$

where $\beta=1/k_BT$, and K_e and L_e are the respective dimensionless coupling constants associated with the dipolar and quadrupolar interactions between spins $\mathbf{S}_i$ and $\mathbf{S}_j$ located at the vertices i and j of the edge e. The sum in eq (2.2) is over all interacting spin pairs on G.

The Hamiltonian (2.2) may be written also in terms of an n-state Potts variable α_i ($\alpha_i = 0,1,\ldots,n-1$) and an Ising spin variable σ_i ($\sigma_i = \pm1$) as (Aharony 1977):

$$\beta H(G) = -\sum_{e\in E} [nK_e\sigma_i\sigma_j\delta(\alpha_i,\alpha_j) + nL_e\delta(\alpha_i,\alpha_j)] \quad (2.3)$$

which is a particular case of the (N_α,N_β) model (corresponding to $N_\beta=2$ and $K_{1,1} = K_{1,0}$) introduced by Domany and Riedel (1979).

2.2 Known Results for the $Z(\lambda)$ model.

In ZF, a $Z(\lambda)$ cluster is represented by a graph G with vertex set V, edge set E, number of vertices ν and number of edges ϵ. With each vertex i of V is associated a state variable n_i which can take on one of the λ integer values $0,1,\ldots,\lambda-1$. The dimensionless Hamiltonian is given by:

$$\beta H(G) = \sum_{e\in E} h_e(n_i-n_j) \quad (2.4)$$

where n_i-n_j is calculated mod-λ and the pair interaction energy is independent of the ordering of i and j so that

$$h_e(\lambda-\alpha) = h_e(\alpha). \qquad (2.5)$$

The components $t_e(\alpha)$ of the λ-dimensional vector transmissivity t_e (Alcaraz and Tsallis 1982) of the edge e are defined by:

$$t_e(\alpha) = \frac{1}{z_e} \sum_{\beta=0}^{\lambda-1} e^{2\pi i\alpha\beta/\lambda} e^{-h_e(\beta)} \qquad (\alpha = 0,1,\ldots,\lambda-1) \qquad (2.6a)$$

where

$$z_e = \sum_{\alpha=0}^{\lambda-1} e^{-h_e(\alpha)} \qquad (2.6b)$$

Of these λ-components only $\lambda = [\lambda/2]$ (where [ ] stands for the integer part) are independent since $t_e(0) = 1$ and $t_e(\lambda-\alpha) = t_e(\alpha)$.

The partition function Z(G) can be expressed (Biggs 1976, 1977) in terms of $t_e(\alpha)$ as:

$$Z(G) = \lambda^{\nu-\varepsilon} \left(\prod_{e\epsilon E} z_e \right) D(G). \qquad (2.7a)$$

Here D(G) is the generating function for flows given by:

$$D(G) = \sum_{\varphi\epsilon F(G)} \prod_{e\epsilon E} t_e(\varphi(e)) \qquad (2.7b)$$

where $\varphi(e)$ is the value of the mod-λ flow φ on the edge e, and F(G) is the set of all mod-λ flows on G. Given an arbitrary directing of the edges $e\epsilon E$, one can define a mod-λ flow (see, for example, Essam and Tsallis 1986) as a function defined on E which assigns to each edge e one of the integer values $0,1,\ldots,\lambda-1$ subject to a "conservation condition" at each vertex $i\epsilon V$, i.e., the sum of the inward flows minus the sum of the outward flows at i is zero mod λ.

Pair correlation functions can normally be written as the thermal average of some function $f(n_1-n_2)$ which depends only on the difference, mod λ, of state variables n_1 and n_2. Here 1 and 2 refer to arbitrarily chosen vertices (called roots of the graph), and the thermal average can be Fourier decomposed as (ZF):

$$<f(n_1-n_2)>_{thermal} = \frac{1}{\lambda} \sum_{\alpha=0}^{\lambda-1} f_{\lambda-\alpha}\, T_\alpha(1,2;G) \tag{2.8}$$

where

$$T_\alpha(1,2;G) \equiv <e^{-2\pi i(n_1-n_2)/\lambda}>_{thermal} = \frac{N_\alpha(1,2;G)}{D(G)} \tag{2.9a}$$

with

$$N_\alpha(1,2;G) = \sum_{\varphi\epsilon F_\alpha(G)} \prod_{e\epsilon E} t_e(\varphi(e)) \tag{2.9b}$$

In (2.9b) , $F_\alpha(G)$ is the set of all *rooted mod-*λ *α-flows*, i.e., of mod-λ flows subject to a fixed external flow α entering at root 1 and leaving at root 2. **N**(1,2;G) = $\{N_\alpha(1,2;G), \alpha=0,1,\ldots,\lambda-1\}$ is called the *flow-vector*, although strictly speaking each of its components is a generating function for internal flows having a fixed external flow α in at 1 and out at 2. Notice that $N_0(1,2:G)$ is exactly D(G) given by (2.7b).

The vector T(1,2;G) = $\{T_\alpha(1,2;G), \alpha=0,1,\ldots,\lambda-1\}$ is called the *equivalent vector transmissivity* between the roots 1 and 2 of G since it is equal to the vector transmissivity t_{eff} of a single *effective edge* between 1 and 2 having an equivalent Hamiltonian $h_{eq}(n_1-n_2)$ given by:

$$Tr' \left[\exp\left[-\sum_{e\epsilon E} h_e(n_i-n_j)\right]\right] = C \exp\left[-h_{eq}(n_1-n_2)\right] \tag{2.10}$$

where C is a constant and Tr' denotes the sum over all possible values of n_i for all vertices i different from the roots 1 and 2. The replacement of a cluster of atoms by a single effective edge connecting just two atoms with an effective interaction plays a fundamental role in real space renormalisation group calculations and also, as we will see later on, in the SBCM.

In the case of the Potts model we have that:

$$h_e(n_i-n_j) = \begin{cases} h_e(0) & \text{for } n_i = n_j \\ \lambda K_e + h_e(0) & \text{for } n_i \neq n_j \end{cases} \tag{2.11}$$

and, therefore, $t_e(\alpha) = t_e$ for any $\alpha \neq 0$, where t_e is the thermal transmissivity (eq (2.2) of PF3) used in many real space renormalisation group calculations (see, for example, Tsallis 1988). Eq. (2.9b) reduces, for the Potts model to:

$$N_1(1,2;G) = N_2(1,2:G) = \dots = N_{\lambda-1}(1,2:G) \equiv N(1,2;G) =$$

$$= \sum_{G' \subseteq G} F_{12}(\lambda,G') \prod_{e \in E'} t_e \tag{2.12a}$$

and

$$N_0(1,2;G) = D(G) = \sum_{G' \subseteq G} F((\lambda,G') \prod_{e \in E'} t_e \tag{2.12b}$$

where $F_{12}(\lambda,G')$ and $F(\lambda,G')$ are respectively the two-rooted and unrooted flow polynomials (see Essam and Tsallis 1986) of the partial graph G' of G. They correspond to the respective numbers of proper (i.e. $\varphi(e) \neq 0$ for all e) rooted mod-λ α-flows and unrooted flows.

3. THE TWO-COMPONENT EQUIVALENT VECTOR TRANSMISSIVITY

3.1 Relationship between the Cubic Model and the Z(2n) Model.

For n=1 and 2 the n-component cubic model is equal to the Ising and Z(4) models respectively. For general n, the cubic model is the particular case of the Z(2n) model in which the pair interaction energies $h_e(\alpha)$ ($\alpha = 0,1,\ldots,2n-1$) become highly degenerate, namely:

$$h_e(1) = h_e(2) = \ldots = h_e(n-1) = h_e(n+1) = \ldots = h_e(2n-1) \tag{3.1}$$

and where the energy differences are related to the dimensionless coupling constants K_e and L_e through:

$$h_e(n) - h_e(0) = 2nK_e \tag{3.2a}$$

and

$$h_e(1) - h_e(0) = n(K_e+L_e) \tag{3.2b}$$

Combining eqs (3.1) and (3.2) with the definition (2.6) of $t_e(\alpha)$ we arrive at only two components of the vector transmissivity which are different:

$$t_e(\alpha) = \frac{1 - e^{-2nK_e}}{1+2(n-1)e^{-n(K_e+L_e)}+ e^{-2nK_e}} = t_e(1) \qquad (\alpha = 1,3,\ldots,2n-1) \tag{3.3a}$$

and

$$t_e(\alpha) = \frac{1 - 2e^{-n(K_e+L_e)}+ e^{-2nK_e}}{1 + 2(n-1)e^{-n(K_e+L_e)}+ e^{-2nK_e}} = t_e(2) \qquad (\alpha = 2,4,\ldots,2n-2) \tag{3.3b}$$

The variables $t_e(1)$ and $t_e(2)$ are precisely the respective variables $\tilde{x}_\beta = \tilde{z}$ and $\tilde{x}_\alpha$ which appear in the model of Domany and Riedel (1979) specialised to the cubic Hamiltonian. The two-dimensional vector $(t_e(1),t_e(2))$ is the vector thermal transmissivity of Tsallis et al (1988) used in their renormalisation group calculation of the critical frontier of the ferromagnetic cubic model on the square lattice.

3.2 The Two-component vector equivalent transmissivity

In this section we prove that, similarly to eqs (3.3), only two of the 2n-1 components of the flow vector of the Z(2n) model with $\alpha \neq 0$ are distinct in the case of the cubic model:

$$N_1(1,2;G) = N_3(1,2;G) = \ldots = N_{2n-1}(1,2;G) \tag{3.4a}$$

and

$$N_2(1,2;G) = N_4(1,2;G) = \ldots = N_{2n-2}(1,2;G) \tag{3.4b}$$

where $N_\alpha(1,2;G)$ is defined in (2.9b) with

$$t_e(\varphi(e)) = t_e(1) \qquad \text{for odd } \varphi(e) \tag{3.5a}$$

and

$$t_e(\varphi(e)) = t_e(2) \qquad \text{for even } \varphi(e) \tag{3.5b}$$

The equalities (3.4) are related to the fact that, for the Potts model, $N_\alpha(1,2;G)$ for $\alpha \neq 0$ is independent of the external flow α (see eq 2.12a).

We first recall that, as shown in the appendix of ZF, one can generate the rooted mod-λ α-flows starting from the unrooted mod-λ flows. For this, one must choose a spanning tree τ on G which then determines a unique path θ which connects the roots 1 and 2. One can then construct a rooted mod-λ α-flow by adding, to each of the $\lambda^{c(G)}$ unrooted mod-λ flows, a flow Φ_α having value α on the path θ from 1 to 2 and zero on all other edges. For example, for the graph G of Fig. 1a and the spanning tree τ of Fig. 1b, one can generate from the unrooted mod-6 flows shown in the first column of Fig. 2, the corresponding rooted mod-6 1-flows and rooted mod-6 3-flows drawn in the 2nd and 3rd column respectively. These were obtained from the unrooted mod-6 flows by adding the flow Φ_δ shown in Fig (1d) with $\delta = 1$ and $\delta = 3$ respectively.

We begin the proof by noting that similarly to the above procedure, one can generate the rooted mod-2n $(\alpha+2)$-flows contributing to $N_\alpha(1,2;G)$ by adding, to each of the rooted mod-2n α-flows which are generated by $N_\alpha(1,2;G)$, a flow Φ_2 having value 2 on the unique path θ from 1 to 2 and zero on all other edges. This provides a bijective mapping between the flows of $N_\alpha(1,2;G)$ and those of $N_{\alpha+2}(1,2;G)$. Notice that for λ even (which is the case we are considering here with $\lambda = 2n$), this procedure cannot change the value of the flow on any edge from odd to even.

Now let us consider an n-component cubic cluster in which, for notational simplicity, we shall assume that $t_e = t$ for all edges e. By the above construction the powers of t(1) (which are, in the cubic model, associated with the odd flows according to eq (3.5a)) must be the same for any rooted mod-2n α-flow and its corresponding rooted mod-2n $(\alpha+2)$-flow. Also when $t(1) = t(2) = t$ we must regain the Potts model formulae. It follows that, since any term $[t(1)]^k[t(2)]^\ell$ $(k,\ell = 0,1,\ldots,\epsilon)$ which appears in $N_\alpha(1,2;G)$ for the cubic model becomes $t^{k+\ell}$ in N(1,2;G) for the Potts model, the power of t(2) for corresponding flows may be different but if and only if the power of t is different for the Potts model. Considering that for $\alpha>0$: (i) N(1,2;G) is independent of the external flow for the Potts model, (ii) the addition of the flow Φ_2 does not change the number of edges with odd values of flow, we conclude that the changes in the power of t for different mod-2n flows with a fixed number k of edges on which their values are odd compensate in such a way as to maintain the same sum. This induces a compensation in the powers of t(2) for the cubic model in such a way that the term

$$[t(1)]^k \sum_{\ell=0}^{\epsilon-k} a_\ell [t(2)]^\ell$$

is the same for both $N_\alpha(1,2;G)$ and $N_{\alpha+2}(1,2;G)$. In the last two examples of Fig. 2 we show the compensation between the terms $[t(1)]^2$ and $[t(1)]^2[t(2)]^2$ which occur in $N_1(1,2;G)$ and $N_3(1,2;G)$ for the 3-component cubic model on the graph G of Fig. 1a.

In general, as this compensation happens for any power k ($k = 0,1,\ldots,\varepsilon$) of t(1), then it follows that $N_\alpha(1,2;G) = N_{\alpha+2}(1,2;G)$ leading thus to eqs. (3.4).

The combination of equations (3.4) and (2.9a) shows that the equivalent vector transmissivity has only two distinct components.

4. GRAPH REDUCTION EQUATIONS OF THE SBCM

The main purpose of the SBCM is to calculate the flow vector for a graph G (and hence the partition function and pair correlation functions) in terms of those for "smaller" graphs. Three methods of reducing the size of a graph are used in the SBCM:

(i) splitting into pieces at articulation vertices;

(ii) replacement of subgraphs attached at only two vertices by effective edges;

(iii) removal of (effective) edges through the use of the effective break-collapse equation.

The graph reduction equations for the n-component cubic model associated with the above mentioned procedures will now be derived from those for the Z(2n) model.

4.1 Splitting of Articulated Graphs.

Suppose that a two-rooted graph G is composed of two subgraphs G_1 and G_2 which intersect only at the articulation point i (see Fig. 3). Two cases can arise, namely: (a) both roots 1 and 2 belong to one of the subgraphs, say G_1 (Fig. 3a); (b) the root 1 belongs to, say, G_1 and 2 is in G_2 (Fig. 3b). In case (b) if $i \neq 1$ or 2 then G_1 and G_2 are said to be in series.

(a) Both roots in G_1

Eq. 3.2 of ZF gives:

$$N_\alpha(1,2;G) = N_\alpha(1,2;G_1)\, D(G_2) \qquad (\alpha = 0,1,2) \qquad \textbf{(4.1)}$$

(b) G_1 and G_2 are in series:

It follows from (3.3) of ZF that

$$N_\alpha(1,2;G) = N_\alpha(1,i;G_1)\, N_\alpha(i,2;G_2) \qquad (\alpha = 0,1,2) \tag{4.2}$$

which, for two ordinary edges ($G_1 = e_1$ and $G_2 = e_2$) recovers Tsallis et al's result (1988).

4.2 Parallel Combination of Graphs.

Now let us consider a two-rooted graph G which is the union of two sugraphs G_1 and G_2 which intersect only at roots 1 and 2 (see Fig. 3c). In this case, G_1 and G_2 are said to be in parallel. Using eqs. (3.4) of ZF and eqs. (3.4) we find:

$$D(G) = D(G_1)D(G_2) + nN_1(1,2;G_1)N_1(1,2;G_2) + (n-1)N_2(1,2;G_1)N_2(1,2;G_2) \tag{4.3a}$$

$$N_1(1,2;G) = D(G_1)N_1(1,2;G_2) + D(G_2)N_1(1,2;G_1) + (n-1)[N_2(1,2;G_1)N_1(1,2;G_2) + N_1(1,2;G_1)N_2(1,2;G_2)] \tag{4.3b}$$

and

$$N_2(1,2;G) = D(G_1)N_2(1,2;G_2) + D(G_2)N_2(1,2;G_1) + nN_1(1,2;G_1)N_1(1,2;G_2) + (n-2)N_2(1,2;G_1)N_2(1,2;G_2). \tag{4.3c}$$

Eqs. (4.3) particularised for two ordinary edges e_1 and e_2 in parallel give

$$t_p(1) = \frac{N_1(1,2;G)}{D(G)} = \frac{t_1(1)+t_2(1)+ (n-1)[t_1(2)t_2(1)+t_1(1)t_2(2)]}{1 + nt_1(1)t_2(1)+ (n-1)\ t_1(2)t_2(2)} \tag{4.4a}$$

and

$$t_p(2) = \frac{N_2(1,2;G)}{D(G)} = \frac{t_1(2)+t_2(2)+ nt_1(1)t_2(1)+(n-2)t_1(2)t_2(2)}{1 + nt_1(1)t_2(1)+ (n-1)\ t_1(2)t_2(2)} \tag{4.4b}$$

which agrees with Tsallis et al's parallel algorithm (1988).

Eqs. (4.3) can be written in a factorised form similar to the series equation as (ZF)

$$\tilde{N}_\beta(1,2;G) = \tilde{N}_\beta(1,2;G_1)\ \tilde{N}_\beta(1,2;G_2) \tag{4.5}$$

where the discrete Fourier transforms $\tilde{N}_\beta$ are:

$$\tilde{D}(G) = D(G) + nN_1(1,2;G) + (n-1)N_2(1,2;G) \tag{4.6a}$$

$$\tilde{N}_n(1,2;G) = D(G) - nN_1(1,2;G) + (n-1)N_2(1,2;G) \tag{4.6b}$$

and

$$\tilde{N}_\alpha(1,2;G) = D(G) - N_2(1,2;G) \qquad (\forall\ \alpha\neq 0 \text{ or } n) \tag{4.6c}$$

When G is a single ordinary edge e connecting 1 and 2, then $\tilde{N}_\beta\ /\tilde{N}_0$ is equal to the dual variable $[t(\beta)]^D$ of $t(\beta)$ defined for the $Z(\lambda)$ model in Alcaraz and Tsallis's paper (1982). The dual vector transmissivity for the n-component cubic model is, therefore, given by:

$$[t_e(n)]^D = \tilde{N}_n/\tilde{D} = \frac{1-nt_e(1)+(n-1)t_e(2)}{1+nt_e(1)+(n-1)t_e(2)} = e^{-2nK_e} \tag{4.7a}$$

and for $\alpha\neq 0$ or n

$$[t_e(\alpha)]^D = \tilde{N}_\alpha/\tilde{D} = \frac{1-t_e(2)}{1+nt_e(1)+(n-1)t_e(2)} = e^{-n(K_e+L_e)} \tag{4.7b}$$

which are respectively the variables x_β and x_α used in the model of Domany and Riedel (1979) specialised to the cubic Hamiltonian. Combining eqs. (4.5) and (4.7) we get the following alternative equation for two ordinary edges in parallel:

$$[t_p(\beta)]^D = [t_1(\beta)]^D \, [t_2(\beta)]^D \qquad (\forall\beta) \tag{4.8}$$

4.3 Replacement of a Subgraph by an Effective Edge

Let us consider a two-rooted graph G which is the union of two subgraphs H and L which intersect at only two vertices, i and j. Furthermore both roots 1 and 2 belong to H (see Fig 4) with the possibility that i and/or j are rooted. When both i and j are rooted then L and H are in parallel and we recover the results of §4.2.

In ZF it was proved, through the use of flows, that one can replace the subgraph L by a single effective edge e_L having an effective flow vector equal to the flow vector of L. This result can be stated for the cubic model as:

$$N_\alpha(1,2;H\cup L) = N_\alpha(1,2;H\cup e_L) \tag{4.9a}$$

with

$$N_\alpha(i,j;e_L) = N_\alpha(i,j;L) \qquad (\alpha = 0,1,2). \tag{4.9b}$$

$N_\alpha(i,j;e_L)$ can be calculated through the SBCM or by performing the partial trace over the internal vertices of L as mentioned in §2.2. Eq (4.9a) may be repeatedly applied as long as there are further subgraphs which satisfy the above conditions on L. Also the subgraphs replaced may themselves contain effective edges.

The replacement of a subgraph by an effective edge is an essential step in the SBCM. The subgraphs to be replaced are considered to be of three types: (i) two (effective) edges in series, (ii) two (effective) edges in parallel, (iii) subgraphs which are not combinations of series and/or parallel (effective) edges. The latter replacement will be called, as in ZF, a non-reducible subgraph replacement. The search for suitable subgraphs is performed in this order.

4.4 The Effective Break-Collapse Equation

When no more subgraph replacements can be made, then one must apply the effective break–collapse equation. Combining eq. (3.16) of ZF with eqs. (3.4) we get the following effective break–collapse equation for the cubic model:

$$N_\alpha(1,2;G) = [D_{eff} - N_{2eff}]\, N_\alpha(1,2;G_f{}^\delta) + N_{1eff}N_\alpha(1,2;G_f{}^\gamma) +$$
$$+ (N_{2eff} - N_{1eff})\, N_\alpha{}^{ev}\,(1,2;f;G) \qquad (\alpha = 0,1,2) \qquad (4.10a)$$

where

$$N_\alpha{}^{ev}(1,2;f;G) = N_{\alpha 0}(1,2;f;G) + N_{\alpha 2}(1,2;f;G) + N_{\alpha 4}(1,2;f;G) + \ldots$$
$$+ N_{\alpha 2n-2}(1,2;f;G) \qquad (4.10b)$$

In (4.10a), $G_f{}^\delta$ and $G_f{}^\gamma$ are respectively the deleted and contracted graphs obtained from G by deleting a chosen (effective) edge f and contracting it (i.e. identifying the endpoints of f in $G_f{}^\delta$). D_{eff}, N_{1eff} and N_{2eff} are the components of the flow vector of the (effective) edge f. $N_{\alpha\beta}(1,2;f;G)$ is the generating function for rooted mod–2n α–flows having a fixed flow β in the edge f. Such an edge will be called, as in ZF, a *frozen edge*.

The components of the flow vectors for the deleted and contracted graphs are related to $N_{\alpha\beta}$ through (ZF):

$$N_\alpha(1,2;G_f^\delta) = N_{\alpha 0}(1,2;f;G) \qquad (4.11)$$

and

$$N_\alpha(1,2;G_f^\gamma) = \sum_{\beta=0}^{2n-1} N_{\alpha\beta}(1,2;f;G). \qquad (4.12)$$

In other words, to delete an edge f is equivalent to having a frozen edge f having a zero flow on it, and to contract f is equivalent to summing over all possible flows for this edge.

Now using the relationship between N_α and $N_{\alpha\beta}$ (see eq. 3.10 of ZF) with $t_f(\beta)=N_{\beta eff}$ particularised for the cubic model, namely

$$N_\alpha(1,2;G) = D_{eff}N_{\alpha 0}(1,2;f;G) + N_{1eff}[N_{\alpha 1}(1,2;f;G) + N_{\alpha 3}(1,2;f;G) + \dots + N_{\alpha 2n-1}(1,2;f;G)] + N_{2eff}[N_{\alpha 2}(1,2;f;G) + N_{\alpha 4}(1,2;f;G) + \dots + N_{\alpha 2n-2}(1,2;f;G)] \quad (4.13)$$

and comparing it with eq. (4.10b), it follows that

$$N_\alpha^{ev}(1,2;f;G) = N_\alpha(1,2;G) \Big|_{\substack{N_{1eff} = 0 \\ D_{eff} = N_{2eff} = 1}} \quad (4.14)$$

The right hand side of eq. (4.14) is similar to the flow vector $N_\alpha^{bc}(1,2;G)$ for the Z(4) model defined for the graph G with a chosen edge, f, "precollapsed" (Mariz et al 1985). However, for the Z(4) model, $N_\alpha^{bc}(1,2;G)$ is the generating function for rooted mod-4 α-flows having value 0 or 2 on the edge f (see ZF), while here $N_\alpha^{ev}(1,2;f;G)$ is the generating function for rooted mod-2n α-flows having value 0,2,4,...,2n-2 on f. In this condition f will be called an *even frozen edge.*

If f is an ordinary edge then eq. (4.10a) recovers a conjectured result (Tsallis, private communication).

In the SBCM, eq. (4.10a) is applied recursively so that the flow vector of G may be equal to that with several even frozen edges. In this case, $N\alpha^{ev}$ satisfies an effective break-collapse equation similar to eq (4.10a). The latter equation is applied as many times as needed to arrive at either graphs with just two vertices, or graphs with *all* edges even frozen. For such graphs (which we will denote by G_{ev}) $N_\alpha(1,2;G_{ev})$ is the number of rooted mod-2n α-flows with the constraint that the flow on all edges must be even frozen. Such flows will be called, as in ZF, *even rooted mod-2n α-flows.* Following along the same lines as in the proof of eqs (4.2) of ZF, one can easily show that *

$$N_1(1;2;G_{ev}) = 0 \quad (4.15a)$$

$$N_2(1,2;G_{ev}) = n^{c(G_{ev})}\gamma_{12}(G_{ev}) \quad (4.15b)$$

$$D(G_{ev}) = n^{c(G_{ev})} \quad (4.15c)$$

where $c(G_{ev})$ is the number of independent cycles in G_{ev}; $\gamma_{12}(G_{ev})$ is 1 if the roots are connected and zero otherwise.

It is worthwhile stressing that, unlike the effective break-collapse equation for the $Z(\lambda)$ model, eq. (4.10a) allows the calculation of the flow vector as a function of n rather than for a specified value of n. In the case of the $Z(\lambda)$ model the application of the break-collapse equation generates, besides the broken and collapsed graphs, a further $\lambda-3$ graphs, while in the cubic model it generates *only one further graph independently of the value of n*.

4.5 Particular Cases

Now let us show that our graph reduction equations reproduce correctly the expected results in different particular cases of the cubic model.

(a) n = 1 (Ising Model)

For n = 1, the vector transmissivity has only one component given by (eq. 3.3a):

$$t_e(1) = \tanh K_e \tag{4.16}$$

which is the thermal transmissivity t_e defined for the Ising model with coupling constant K_e. Our respective graph reduction equations (4.1), (4.2), (4.3a) and (4.3b) reduce, for n = 1, to eqs. (4.17a), (4.17b), (4.14b) and (4.14a) of PF3 particularised for a two-rooted Ising cluster. From eqs. (4.10b) and (4.11) it follows that for α=0,1:

$$N_\alpha^{ev}(1,2:f;G)\Big|_{n=1} = N_\alpha(1,2;G_f^\delta)\Big|_{n=1} \tag{4.17}$$

which combined with eq. (4.10a) leads to the effective break-collapse equation (see eqs. 4.13 of PF3) for the Ising model.

(b) $n = 2$ (symmetric Ashkin-Teller model)

Aharony (1977) showed that, for $n = 2$, the Hamiltonian of the cubic model (eq. 2.3) can be written in terms of two coupled Ising variables in the same form as that of the symmetric Ashkin and Teller (1943) model. The Hamiltonian of the latter model is identical to that for the Z(4) model described in eq. (1) of Mariz et al (1985) with coupling constants $K_1 = K$ and $K_2 = L/2$.

The components $t_e(1)$ and $t_e(2)$ of the vector transmissivity (eq. 3.3) become, for $n=2$, identical to the respective transmissivities t_1 and t_2 defined in eqs. (2a) and (2b) of Mariz et al (1985), where $K_1 = K$ and $K_2 = L/2$. One can easily see that our SBCM graph reduction equations reduce, for $n = 2$, to those derived in ZF for the Z(4) model, as it should be.

(c) $K_e = L_e$ (2n-state Potts model)

The case $K_e = L_e$ corresponds to a 2n-state Potts model with coupling constant $2nK_e$ (see Aharony 1977). In this case, eqs. (3.3) become:

$$t_e(1) = t_e(2) = \frac{1-e^{-2nK_e}}{1+(2n-1)e^{-2nK_e}} \tag{4.18}$$

which is the termal transmissivity (see eq. (1) of Tsallis and Levy 1981) of a 2n-state Potts model. Using the fact that, for the Potts model (see eq. 2.12a)

$$N_1(1,2;G) = N_2(1,2;G) = N(1,2;G) \tag{4.19}$$

one can easily show that our graph reduction equations reproduce the expected results (see PF3).

(d) $K_e = 0$ (n-state Potts model)

Setting $K_e = 0$ in eq. (2.3) leads to the Hamiltonian of an n-state Potts model with coupling constant nL_e. In this case eqs. (3.3) become:

$$t_e(1) = 0 \tag{4.20a}$$

$$t_e(2) = \frac{1 - e^{-nL_e}}{1 + (n-1)\, e^{-nL_e}} = t_e \tag{4.20b}$$

where t_e is the thermal transmissivity of an n-state Potts model. From eq. (4.20a) and (3.5a) we conclude that $N_\alpha(1,2;G)$ becomes, in the considered case, the generating function for *even* rooted mod-2n α-flows. From conservation of mod-2n flows it follows then, similarly to eq. (4.15a), that:

$$N_1(1,2;G) = 0. \tag{4.21}$$

Furthermore, for $\alpha = 2\beta$, there is a bijective correspondence between the even rooted mod-2n α-flows and the unrestricted rooted mod-n β-flows, obtained by replacing edges with flow 2ℓ by edges with flow ℓ ($\ell = 0,1,\ldots,n-1$). Consequently, in this case:

$$N_2(1,2;G) = N(1,2;G) \tag{4.22}$$

where $N(1,2;G)$ is the generating function for the rooted mod-n flows in the n-state Potts model.

Combining relations (4.21), (4.22) and (4.12), one can easily prove that, for $K_e = 0$, all our graph reduction equations for $D(G)$ and $N_2(1,2;G)$ reduce to those obtained for the Potts model (PF3).

5. SBCM FOR THE n-COMPONENT CUBIC MODEL

In this section we describe the modifications of the SBCM algorithm for the Potts model (PF3) necessary for treating the cubic model. We also illustrate the SBCM for the n-component cubic model using the Wheatstone bridge cluster.

5.1 The SBCM Algorithm.

The SBCM algorithm for the Potts model described in PF3 contains a recursive procedure T which executes the operations of splitting into pieces, replacement of (effective) edges in series or in parallel by a single effective edge, and the operation of non-reducible subgraph replacement as long as possible. It then applies the effective break-collapse equation. The use of this equation as well as the non-reducible subgraph replacement require calls to T, thus the algorithm is recursive. The terminal condition for the procedure arises when a graph with only two vertices is arrived at, in which case the equivalent transmissivity is calculated by the parallel reduction equation. The SBCM algorithm for the cubic model differs from that for the Potts model in the following respects:

(i) Instead of associating to each edge e = [i,j] the numerator N_e and denominator D_e of the effective thermal transmissivity of e, we associate the components $N_0(i,j;e)$, $N_1(i,j;e)$ and $N_2(i,j;e)$ of the effective flow vector of the edge e.

(ii) The effective break-collapse equation must be replaced by eq. (4.10a) which demands the calculation of $N_\alpha^{ev}(1,2;f;G)$. This may be accomplished by replacing step (IId4) of the algorithm by a loop with a further call to T for the graph G with an even frozen edge f. The series and parallel reduction equations work without modification provided we set $t_f(0) = t_f(2) = 1$ and $t_f(1) = 0$.

(iii) In the selection of the (effective) edge to be deleted and contracted (step (IId1) of the algorithm), this must now not be an even frozen edge.

(iv) A further terminal step must be added before the terminal condition mentioned in (IIe) of PF3. This refers to a graph with more than two vertices, the edges of which are all even frozen. In this case, there is no need for further applications of the effective break–collapse equation since the flow vector of the current graph is given by eqs. (4.15).

5.2 An Illustration of the SBCM

Now let us illustrate the SBCM by calculating the equivalent vector transmissivity of the Wheatstone bridge graph G of Fig. 5. We consider only the case when all edges have the same vector transmissivity t.

Since G has 5 edges, then it is necessary to apply the effective break–collapse equation (eq. 4.10a) 5 times arriving thus at the graph G_{ev} of Fig. 5 whose edges are all even frozen. Fig. 5 shows the "tree" of graphs generated in the SBCM where the edges to be deleted and contracted were chosen in the following sequence e_5, e_2, e_1, e_3 and e_4. For the sake of simplicity, the further graphs resulting from the replacement of edges (which can be even frozen or not) in series and/or parallel by effective edges are not included in Fig. 5. The branching into two graphs refers to the splitting of articulated graphs, while the one into 3 graphs results from the application of the effective break–collapse equation. The effective flow vectors for the terminal graphs shown in Fig. 5 are the following:

$$N_\alpha(1,2;G_{11}) = n \qquad (\alpha = 0,2) \tag{5.1a}$$

$$N_1(1,2;G_{11}) = 0 \tag{5.1b}$$

$$N_\alpha(1,2;G_{12}) = N_\alpha(1,2;G_{ev}) = n^2 \qquad (\alpha = 0,2) \tag{5.2a}$$

$$N_1(1,2;G_{12}) = N_1(1,2;G_{ev}) = 0 \tag{5.2b}$$

$$N_\alpha(1,2;G_{10}) = 1 + (n-1)t(2) \qquad (\alpha = 0,2) \tag{5.3a}$$

$$N_1(1,2;G_{10}) = 0 \tag{5.3b}$$

$$N_\alpha(1,2;G_9) = n + n(n-1)t(2) \qquad (\alpha = 0,2) \tag{5.4a}$$

$$N_1(1,2;G_9) = n^2 t(1) \tag{5.4b}$$

$$N_\alpha(1,2;G_8) = 1 + (n-1)t(2) \qquad (\alpha = 0,2) \tag{5.5a}$$

$$N_1(1,2;G_8) = nt(1) \tag{5.5b}$$

$$N_\alpha(1,2;G_7) = 1 + 2(n-1)t(2) + (n-1)^2[t(2)]^2 \quad (\alpha = 0,2) \tag{5.6a}$$

$$N_1(1,2;G_7) = n^2[t(1)]^2 \tag{5.6b}$$

$$N_0(1,2;G_6) = 1 + (n-1)[t(2)]^2 \tag{5.7a}$$

$$N_1(1,2;G_6) = t(1) + (n-1)t(1)t(2) \tag{5.7b}$$

$$N_2(1,2;G_6) = 2t(2) + (n-2)[t(2)]^2 \tag{5.7c}$$

$$N_0(1,2;G_5) = 1+(n-1)t(2) + (n-1)[t(2)]^2 + (n-1)^2[t(2)]^3 + n^2[t(1)]^3 \tag{5.8a}$$

$$N_1(1,2;G_5) = t(1)+2(n-1)t(1)t(2)+n[t(1)]^2+n(n-1)[t(1)]^2 t(2)+ +(n-1)^2 t(1)[t(2)]^2 \tag{5.8b}$$

$$N_2(1,2;G_5) = 2t(2)+(3n-4)[t(2)]^2+(n-1)(n-2)[t(2)]^3+n^2[t(1)]^3 \tag{5.8c}$$

$$N_0(1,2;G_4) = 1 + n[t(1)]^2 + (n-1)[t(2)]^2 \tag{5.9a}$$

$$N_1(1,2;G_4) = 2t(1) + 2(n-1)t(1)t(2) \tag{5.9b}$$

$$N_2(1,2;G_4) = 2t(2) + n[t(1)]^2 + (n-2)[t(2)]^2 \tag{5.9c}$$

Combining the above expressions together with the appropriate graph reduction equations of section 4, we get that:

$$N_0(1,2;G_1) = 1 + n[t(1)]^4 + (n-1)[t(2)]^4 \qquad (5.10a)$$

$$N_1(1,2;G_1) = 2\{[t(1)]^2 + (n-1)[t(1)]^2[t(2)]^2\} \qquad (5.10b)$$

$$N_2(1,2;G_1) = 2[t(2)]^2 + n[t(1)]^4 + (n-2)[t(2)]^4 \qquad (5.10c)$$

$$N_0(1,2;G_2) = \{1+n[t(1)]^2 + (n-1)[t(2)]^2\}^2 \qquad (5.11a)$$

$$N_1(1,2;G_2) = 4[t(1)]^2\{1+(n-1)\ t(2)\}^2 \qquad (5.11b)$$

$$N_2(1,2;G_2) = \{2t(2) + n[t(1)]^2 + (n-2)[t(2)]^2\}^2 \qquad (5.11c)$$

$$N_0^{ev}(1,2;e_5;G_3) = 1 + 2(n-1)[t(2)]^2 + n^2[t(1)]^4 + (n-1)^2[t(2)]^4 \qquad (5.12a)$$

$$N_1^{ev}(1,2;e_5;G_3) = 2[t(1)]^2+4(n-1)[t(1)]^2t(2)+2(n-1)^2[t(1)]^2[t(2)]^2 \qquad (5.12b)$$

$$N_2^{ev}(1,2;e_5;G_3) = 4[t(2)]^2+4(n-2)[t(2)]^3+n^2[t(1)]^4+(n-2)^2[t(2)]^4 \qquad (5.12c)$$

Combining eqs. (5.10)-(5.12) with the effective break-collapse equation for $f = e_5$, namely (see eq. 4.10a) :

$$N_\alpha(1,2;G) = [1-t(2)]N_\alpha(1,2;G_1) + t(1)N_\alpha(1,2;G_2) + [t(2) - t(1)]N_\alpha^{ev}(1,2;e_5;G_3) \qquad (5.13)$$

we finally arrive at the flow vector of G:

$$N_0(1,2;G) = 1 + 2n[t(1)]^3 + 2(n-1)[t(2)]^3 + n[t(1)]^4 + (n-1)[t(2)]^4 + (n-1)(n-2)[t(2)]^5 + 2n(n-1)[t(1)]^3[t(2)]^2 + n(n-1)\ [t(1)]^4t(2) \qquad (5.14a)$$

$$N_1(1,2;G) = 2[t(1)]^2 + 2[t(1)]^3 + 6(n-1)[t(1)]^2[t(2)]^2 + 2(n-1)(n-2)[t(1)]^2[t(2)]^3 + 4(n-1)[t(1)]^3t(2) + 2(n-1)^2[t(1)]^3[t(2)]^2 \qquad (5.14b)$$

$$N_2(1,2;G) = 2[t(2)]^2 + 2[t(2)]^3 + n[t(1)]^4 + 5(n-2)\ [t(2)]^4 + 4n[t(1)]^3t(2) + 2n(n-2)[t(1)]^3[t(2)]^2 + n(n-1)[t(1)]^4[t(2)] + (n-2)(n-3)[t(2)]^5 \qquad (5.14c)$$

Combining eqs. (5.14) with the definitions of t(1) and t(2) (eqs 3.3), one obtains an equivalent vector transmissivity which has effective coupling constants K_{eff} and L_{eff} equal to the respective renormalised coupling constants K' and NL' of Tsallis et al's paper (1988).

Notice that eqs. (5.14) recover, for all the particular cases considered in §4.5, the expected results (see PF3 and Mariz et al 1985).

CONCLUSIONS

We have generalised to the n-component cubic model the subgraph break-collapse method (SBCM) of the Potts model which we presented elsewhere. While in the latter model the equivalent transmissivity was a scalar, it becomes a two-dimensional vector for all values of n in the cubic model. The effective break-collapse equation involves also, besides the broken and collapsed graphs which appear in the Potts model, a graph on which the value of the flow is even. We have called the latter an even frozen edge.

Our graph reduction equations were derived from those we developed recently for the Z(λ) model. However, the SBCM algorithm for the cubic model differs from that for the Z(2n) in the following aspects: (i) it contains graphs with even frozen edges instead of frozen edges having fixed flows; (ii) its effective break-collapse equation generates only 3 flow vectors for all values of n instead of (2n-1); (iii) it gives the equivalent vector transmissivity as a function of n rather than for a fixed value of n; (iv) it requires more iterations since the terminal condition refers to graphs with all edges even frozen rather than a number of frozen edges equal to the number of independent cycles.

An even frozen edge is equal, for n = 2, to the precollapsed edge which appears in the break-collapse method (BCM) for the Z(4) model (Mariz et al 1985). In this case, our algorithm becomes similar to the BCM but with the important difference that we include non-reducible subgraph replacements.

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FIGURE CAPTIONS

FIGURE 1 A graph G whose edges are given arbitrary directing, indicated by the arrows. The roots 1 and 2 are represented by small circles and unrooted vertices by full dots. An arbitrary spanning tree τ of G and its corresponding path θ between the roots are shown in (b) and (c) respectively. By adding the flow Φ_δ (d) to unrooted flows one generates rooted δ-flows.

FIGURE 2 Examples of unrooted mod-6 flows (1st column) and its corresponding rooted 1-flows (2nd column) and rooted 3-flows (3rd column) on the graph G of Fig. 1a. These rooted flows were obtained from the unrooted ones by adding the flow Φ_δ of Fig. 1d for $\delta = 1$ and 3 respectively. A missing edge indicates that the value of the flow on it is zero. α represents the external flow in at the root 1 and out at the root 2. To each edge with a non-zero even (odd) value of flow is associated a transmissivity t(2)(t(1)). Below each α-flow the corresponding term contributing to the generating function $N_\alpha(1,2;G)$ is given.

FIGURE 3 Pictorial representations of two graphs G_1 and G_2 which share an articulation vertex i ((a) and (b)) or which are in parallel (c). In (b) the graphs G_1 and G_2 are in series.

FIGURE 4 Pictorial representation of a two-reducible graph G = HUL with the roots 1 and 2 in H. Each subgraph is represented by a half-moon shape.

FIGURE 5 A schematic representation of the SBCM calculation of N(1,2;G) for the Wheatstone Bridge graph. The further steps are not shown for graphs which are combinations of series and/or parallel edges. The splitting of an articulated graph is indicated by the sign X between the two subgraphs. The crossed line represents an even frozen edge whose vector transmissivity is given by t(0) = t(2) = 1 and t(1) = 0. The vector transmissivity associated to any other edge is **t**.

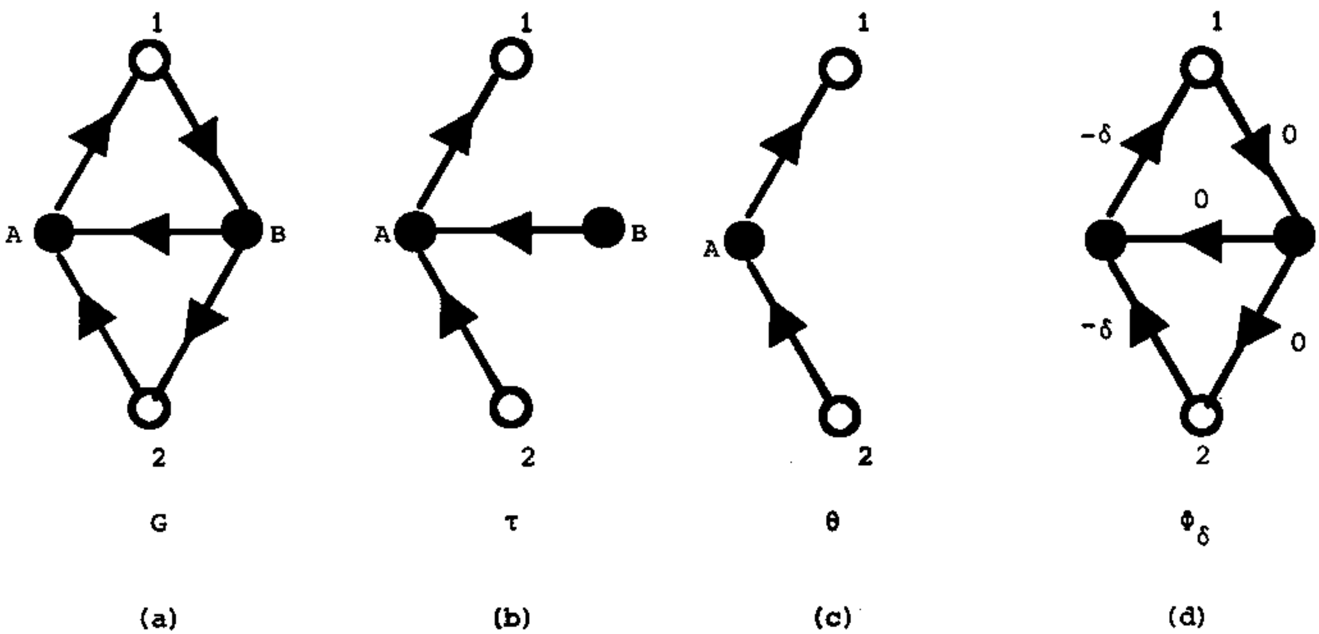

FIG. 1

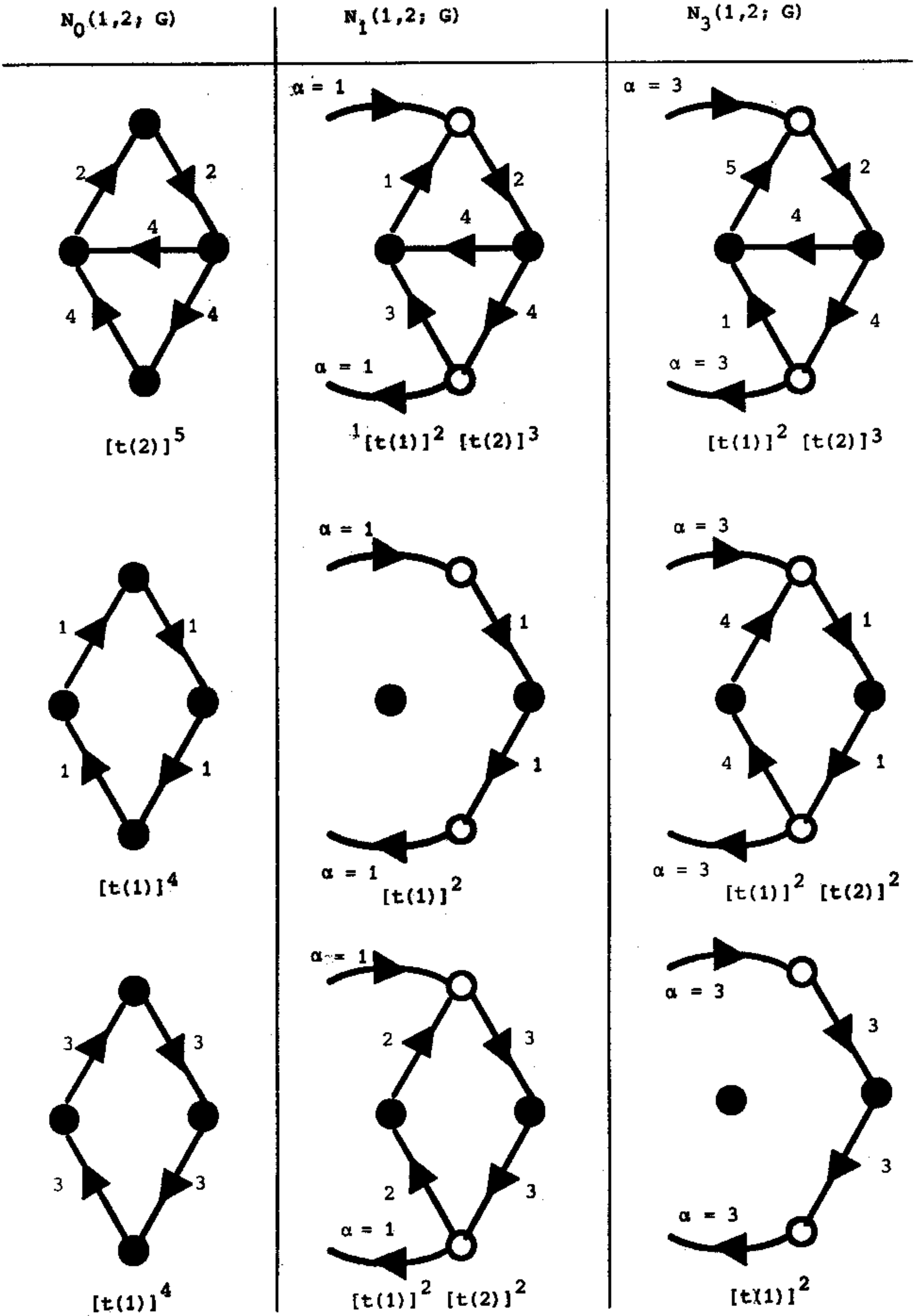
N0(1,2; G)
N1(1,2; G)
N3(1,2; G)
α = 1
α = 3
[t(2)]5
1[t(1)]2 [t(2)]3
[t(1)]2 [t(2)]3
[t(1)]4
[t(1)]2
[t(1)]2 [t(2)]2
[t(1)]4
[t(1)]2 [t(2)]2
[t(1)]2

FIG. 2

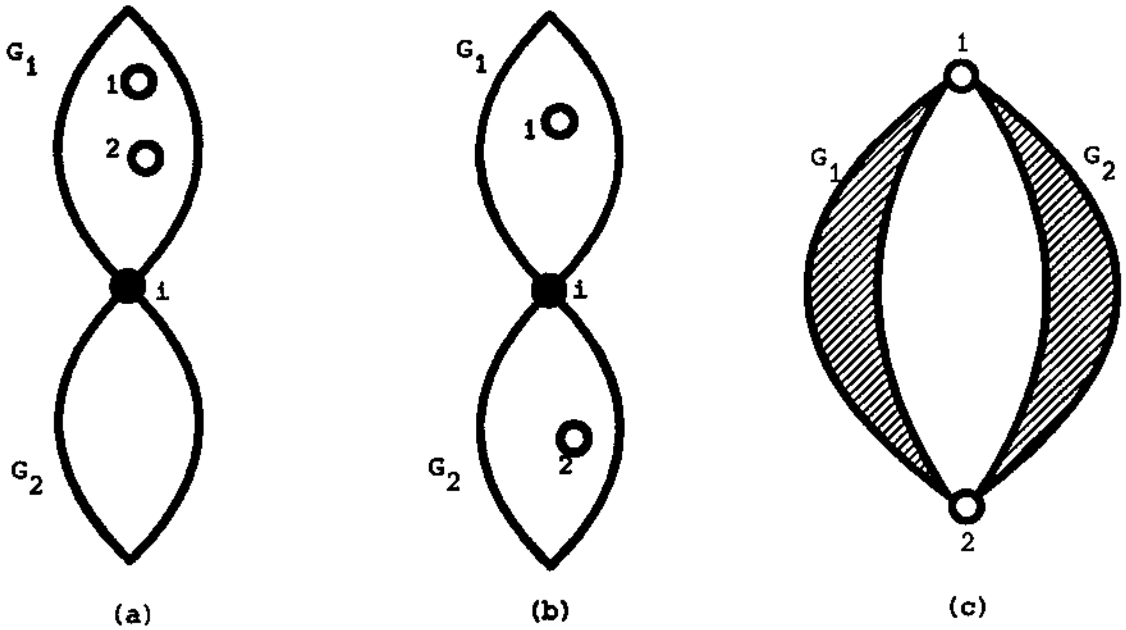

FIG. 3

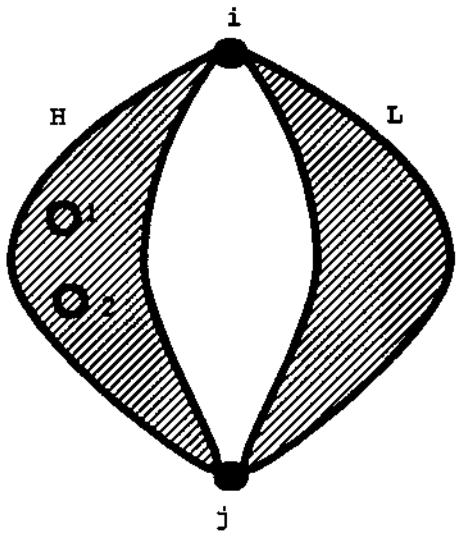

FIG. 4

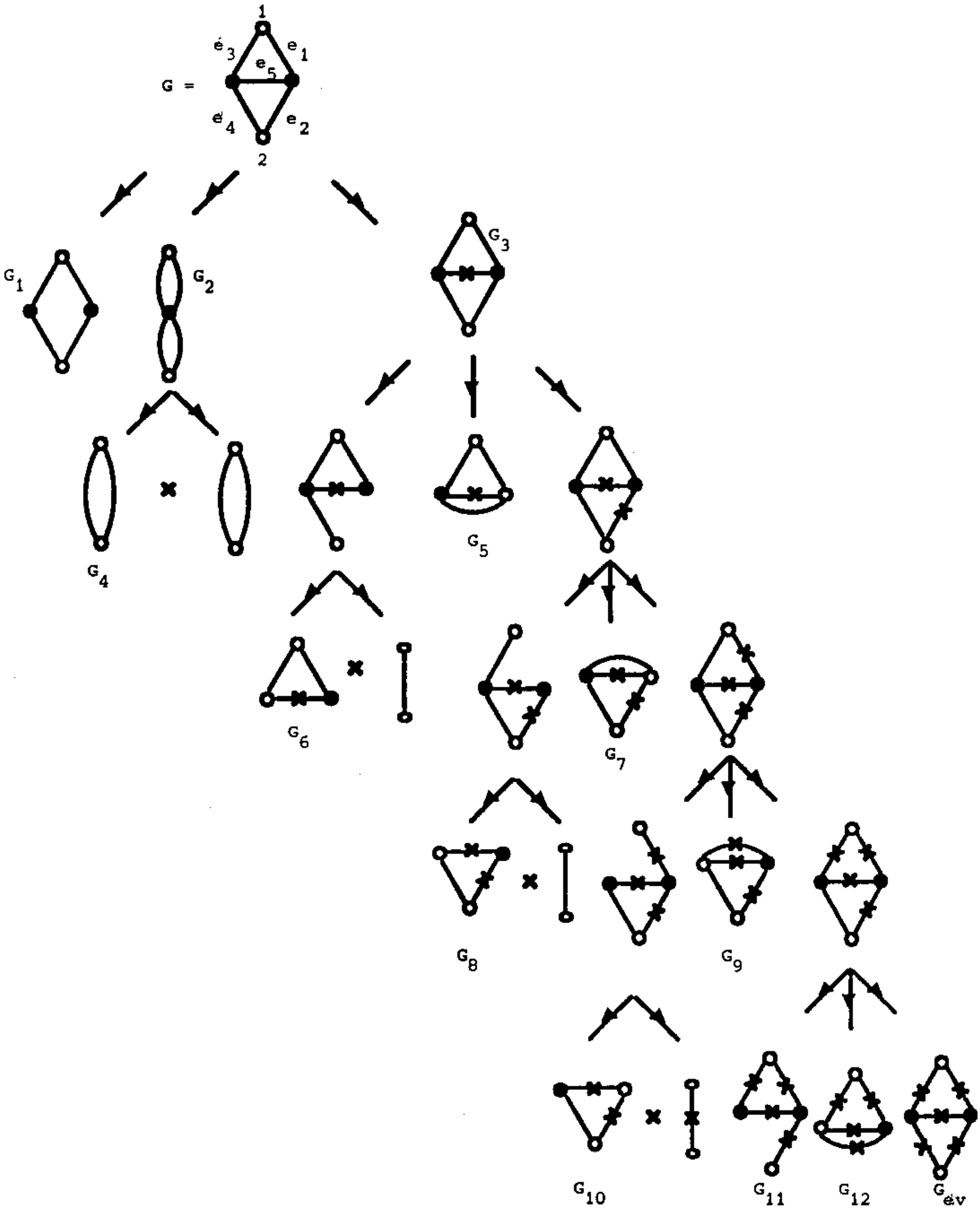

FIG. 5

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