

# FUNCTIONS ON GRAPHS AND SOME GENERALIZATIONS

A thesis submitted towards  
the degree of Doctor of Philosophy  
at the University of London

COLIN WILLIAM VOUT

Royal Holloway College

July 1978

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## ABSTRACT

The underlying theme of this thesis is the investigation of some functions defined on graphs. In one chapter results are obtained for a particular type of function. In another a known result on expressing graph functions multiplicatively is established by other methods which suggest certain generalizations of graphs; these then enable us to see how much the properties depend on graphs per se, and how much on the wider nature of the generalizations.

Chapter 1 introduces our basic terminology and notation, and contains the acknowledgements.

Chapter 2 establishes the multiplicative expansion of a graph function by two new methods.

Chapter 3 is simply a survey of some combinatorial structures and the definition of some new ones. The 'old' ones are introduced for the purpose of comparison with the new ones, which in turn afford useful generalizations of graphs which are utilised in later chapters.

Chapter 4 investigates interaction models on graphs that possess a certain additive property; this is then extended to hypergraphs and related to rank polynomials.

Chapter 5 pursues the notion of 'avitoids', defined in chapter 3. A rank function is defined on them and some of its properties studied.

Chapter 6 is concerned with the idea of 'molecules', also defined in chapter 3. A simple way to evaluate, in general circumstances, an important matrix that emerged in chapter 2 is presented.

Chapter 7 concludes the thesis with comments on connected and resultant items.

More detailed summaries are provided at the beginning of each chapter.

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## CHAPTER 1

### INTRODUCTION

Section 1.1 Acknowledgements

Section 1.2 Definitions

Section 1.3 Notation

This chapter acknowledges sources and states the conventions used throughout the thesis. In general the terminology is standard, but some notational innovations are used for the sake of brevity.

## 1.1 Acknowledgements

Chapter 2 is concerned with a known result of Tutte. In sections 1-3 a new proof is presented and any existing results are explicitly acknowledged there. Section 4 is derived from Whitney [27] except that I use graph types rather than grouping together graphs with the same rank and nullity. The observation that Whitney's theorem 7A is simply an inversion of a triangular matrix is mine, but the use of this to elucidate the theorem of Tutte is due to Biggs [5]. The development of my proof of Biggs's result leans heavily on the ideas of Whitney.

In chapter 3 the sections 1 & 2 are digests of existing concepts, but sections 3-5 are original. In chapter 4 acknowledgements are made as appropriate; chapters 5 & 6 are entirely original.

I would like to thank my research supervisor, Norman Biggs, for much guidance and advice while I was preparing this thesis.

## 1.2 Definitions

The usual graph theory terms and definitions will be utilised. A graph will comprise a set of vertices and a family of unordered pairs thereof, called edges. Thus the graphs are undirected, not necessarily simple, and may have isolated vertices. A subgraph will comprise the same set of vertices but a subfamily of edges. Graphs will be diagrammed in the usual way.

We shall use some standard terminology for hypergraphs and matroids. When we draw hypergraphs it is sometimes clearer to denote edges of size greater than 2 by oval regions containing the points (as in chapter 4), and sometimes to represent them by blacked-in regions touching the points (as elsewhere).

When we first define a term it will be underlined. Also, note that in general we shall use minimal to mean minimal by inclusion and smallest to mean smallest in size.

Basic terminology not defined in the text can be found in the following books, according to the topic: graphs, Wilson [28]; interaction models, Biggs [5]; hypergraphs, Berge [2]; and matroids, Welsh [26].

### 1.3 Notation

In general, graphs will be denoted by Greek capitals.  $V\Gamma$  and  $E\Gamma$  will respectively stand for the vertex-set and edge-set of the graph  $\Gamma$ ;  $\Gamma^*$  will be the dual of  $\Gamma$  (as appropriate),  $\Gamma'_e$  the graph with the edge  $e$  deleted, and  $\Gamma''_e$  that with  $e$  contracted.  $\Delta \leq \Gamma$  will mean  $V\Delta = V\Gamma$ ,  $E\Delta \subseteq E\Gamma$  and if in addition  $E\Delta \neq E\Gamma$  we may simply write  $\Delta < \Gamma$ ; if also  $\Delta$  is nonseparable we may write  $\Delta \leq \Gamma$  and  $\Delta < \Gamma$ , respectively. This notation will be carried through for avitoids as well.

The symbol  $\exists$  is shorthand for 'for some' (corresponding to  $\forall$  for 'for all') and is used as little as possible; that is, only in subscripts for summations or products where alternatives are unduly long. The symbol  $\square$  will be used to denote the end of a proof. We shall often use s.t. to stand for 'such that'.

When the edge referred to is obvious, we shall often write  $\Gamma'$  instead of  $\Gamma'_e$  and  $\Gamma''$  for  $\Gamma''_e$ . In chapter 2 we shall use  $\Delta \triangleleft \Gamma$  to mean that  $\Delta$  is a block of  $\Gamma$ ; and  $\Gamma^{\triangleleft}$  will denote the set of  $\Delta \triangleleft \Gamma$ , with  $\Gamma^{\leq}$  having a corresponding meaning.

Other notation is either standard or will be defined as it is introduced.



## CHAPTER 2

### THE MULTIPLICATIVE EXPANSION

Section 2.1 The subgraph expansion

Section 2.2 Nonseparable graphs

Section 2.3 A theorem of Tutte

Section 2.4 Some results of Whitney

Section 2.5 A theorem of Biggs

This chapter proves a result of Tutte in two new ways: the first is shorter but the second, deriving from a simplification of some ideas of Whitney and presenting the result in Biggs's form, has more applications.

## 2.1 The subgraph expansion

Many graph functions  $F(\Gamma)$  are defined in terms of subgraph expansions of the form  $F(\Gamma) = \sum_{\Delta \in \Gamma} f(\Delta)$ . In fact, any graph function may be expressed in this way, since once we know the values  $F$  takes we may define  $f(\Gamma) = \sum_{\Delta \in \Gamma} (-1)^{|E\Gamma| - |E\Delta|} F(\Delta)$  by Möbius inversion; however, the usefulness is when  $f$  is in some sense simpler than  $F$ .

For instance, an important example is the Whitney rank polynomial,  $R(\Gamma; x, y) = \sum_{\Delta \in \Gamma} x^{R\Delta} y^{C\Delta}$ , which includes the reduced chromatic function,  $n^{-|V\Gamma|} C(\Gamma; n)$ , when  $x = -1/n$ ,  $y = -1$ . Furthermore, the partition function of any interaction model is of the prescribed type, as may be seen by putting  $p = q = 1$  in lemma 2 of section 4.2.

## 2.2 Nonseparable graphs

A nonseparable graph is one without cut-vertices and having precisely one nontrivial connected component; this is equivalent to demanding that the graph be nonseparable in the usual sense when we ignore any isolated vertices. The importance of this notion for our purposes lies in the fact that many of the useful graph functions defined as in 2.1 have the property that  $f(\Delta) = \prod_{\Lambda} f(\Lambda)$  where the product is taken over the maximal nonseparable subgraphs of  $\Delta$ , often called its blocks. We shall call any function  $f$  with this property multiplicative.

A simple consequence of  $f$  being multiplicative is that  $F$  is too, as noted by Tutte [25].

LEMMA 1: If  $f(\Delta) = \prod_{\Lambda \triangleleft \Delta} f(\Lambda)$  and  $F(\Gamma) = \sum_{\Delta \in \Gamma} f(\Delta)$  then  $F(\Gamma) = \prod_{\Lambda \in \Gamma} F(\Lambda)$ .

Proof. Let the blocks of  $\Gamma$  be  $\Gamma_1, \Gamma_2, \dots, \Gamma_s$ ; there is then an obvious correspondence between subgraphs  $\Delta \in \Gamma$  and  $n$ -tuples  $\Delta_1, \Delta_2, \dots, \Delta_s$  with  $\Delta_i \in \Gamma_i$  for  $i=1, 2, \dots, s$ . Using this we obtain

$$F(\Gamma) = \sum_{\Delta \in \Gamma} f(\Delta) = \sum_{\substack{\Delta_i \in \Gamma_i \\ i=1, \dots, s}} f(\bigcup_{i=1}^s \Delta_i) = \sum_{\substack{\Delta_i \in \Gamma_i \\ i=1, \dots, s}} \prod_{i=1}^s f(\Delta_i) =$$

$$\prod_{i=1}^s \sum_{\Delta_i \in \Gamma_i} f(\Delta_i) = \prod_{i=1}^s F(\Gamma_i). \quad \blacksquare$$

COROLLARY 1: If  $F$  is multiplicative then so is  $f$ .

Proof.  $F$  being multiplicative implies that  $(-1)^{|E\Delta|} F(\Delta)$  is, which by the above lemma and the inversion formula of 2.1 implies that  $(-1)^{|E\Delta|} f(\Delta)$  is, which implies that  $f$  is.  $\blacksquare$

Whitney rank functions and partition functions are both multiplicative. Also, our small and capital letters correspond

to Tutte's [25] where he refers to lower and upper polynomials respectively.

Any graph function  $F(\Gamma)$  can be written as a multiplicative expression involving prescribed sorts of subgraph, by defining  $q(\Gamma) = F(\Gamma) / \prod_{\Delta} q(\Delta)$  where  $\Pi$  involves all the relevant proper subgraphs of  $\Gamma$ ; however, if  $\Gamma$  is not of the prescribed form we must ensure that the resulting  $q(\Gamma)$  equals 1. In the case we are dealing with, where the subgraphs we are concerned with are the nonseparable ones, this follows if the function is itself multiplicative. Also, we may encounter difficulties if some of the  $F(\Gamma)$  are 0, so it is clearer if we deal only with formal expressions for as long as possible, to defer the problems of convergence.

Accordingly, we shall be concerned with polynomials, rational polynomials and power series over the ring of integers, with a different variable  $f(\Lambda)$  for every nonseparable graph  $\Lambda$ . The graph functions  $F$  will be polynomials and any  $f$  will be a monomial, and in both cases all terms have unit coefficients; the function  $q(\Lambda)$  whose properties we investigate will be a rational polynomial which we can formally divide out to obtain a power series.

For example, if  $\Gamma$  were a graph with only one edge we might have  $f(\Gamma) = x$ ,  $F(\Gamma) = 1+x$  and  $q(\Gamma) = 1+x$ ; in this case the denominator of  $q$  is 1. Using the graph of a triangle for another example, if the value of  $f$  for that is  $t$ , and for the three edges is  $x$ ,  $y$  or  $z$ , then for that graph  $F = 1+x+y+z+xy+yz+zx+t$  and  $q = F/(1+x)(1+y)(1+z) = 1 + (t - xyz)/(1+x+y+z+xy+yz+zx+xyz)$ . Note that we take an indeterminate for each value of  $f$ , in contrast to Tutte's treatment which assigns polynomial values; but in

common with Tutte [25] we do not as yet introduce the notion of graph type (see section 2.4).

We shall introduce some notation to be used in the following sections of this chapter.  $\mathcal{H}$  will represent the set of all monomials, with unit coefficients, in the variables concerned, and a typical member will be  $X$ . To avoid lengthy repetition we define the function  $u: \mathcal{H} \rightarrow \{\text{graphs}\}$  by letting  $u(X)$  be the union of those nonseparable graphs whose indeterminates appear in  $X$ , and defining the sets  $K, L$  by:

$$K(\Gamma, \Lambda; X) = \left\{ z: \Gamma \rightarrow \mathcal{H} \mid \bigcup_{\substack{\Theta \subset \Gamma \\ \text{st. } z(\Theta) \neq 1}} \Theta = \Lambda, \prod_{\Theta \subset \Gamma} z(\Theta) = X \right\};$$

$$L(\Lambda; X) = \left\{ z: \Lambda \rightarrow \mathcal{H} \mid \bigcup_{\substack{\Theta \subset \Lambda \\ \text{st. } z(\Theta) \neq 1}} \Theta = \Lambda, \prod_{\Theta \subset \Lambda} z(\Theta) = X \right\}.$$

That is,  $K$  is the set of all functions from the set of nonseparable proper subgraphs of  $\Gamma$  to the set of monomials with unit coefficients, such that the product of the values is  $X$  and the union of those subgraphs not sent to 1 is  $\Lambda$ ; and  $L$  has as its domain the set of all nonseparable subgraphs of  $\Lambda$  instead.

### 2.3 A theorem of Tutte

We establish, by a different method, a theorem of Tutte on the coefficients of the power series  $q(\Lambda)$ . This is done by induction on the set of all graphs concerned, which we order firstly by increasing number of edges and then by increasing number of blocks, with the further ordering being arbitrary. The graphs concerned might be subgraphs of some suitably large graph; the reason for not dealing with all possible graphs is that we are differentiating between isomorphic graphs with different edge-sets, so there would be an infinite number of graphs of each isomorphism type (except for the null type).

We inductively define  $q(\Gamma) = F(\Gamma) / \prod_{\Lambda \leq \Gamma} q(\Lambda)$  as stated, and note that our requirements necessitate  $q(\Gamma) = f(\Gamma) = F(\Gamma) = 1$  if  $\Gamma$  is a null graph. We write  $q(\Gamma)$  as a power series  $\sum_{X \in \mathcal{H}} A_{X, \Gamma}$  where  $A$  is indexed firstly by elements of  $\mathcal{H}$  and secondly by nonseparable graphs. As stated in the previous section, we would obtain  $q(\Gamma) = 1$  for  $\Gamma$  separable, so the formula  $F(\Gamma) = \prod_{\Lambda \leq \Gamma} q(\Lambda)$  holds for all  $\Gamma$ . Consequently we investigate the function  $q$  for nonseparable graphs only.

**THEOREM 1:** For any graph  $\Gamma$ :  $\sum_{z \in L(\Gamma; X)} \prod_{\Lambda \leq \Gamma} A_{z(\Lambda), \Lambda} = 0$  if  $X \neq f(\Gamma)$ .

And if  $\Gamma$  is nonseparable:  $A_{1, \Gamma} = 1$ ;  $A_{f(\Gamma), \Gamma} = 1$ ;  $A_{X, \Gamma} = 0$  if  $u(X) \neq \Gamma$  but  $X \neq 1$ .

**Proof.** We have already remarked that we have a basis for induction, when  $\Gamma$  is a null graph. We shall now prove the two propositions in reverse order.

If  $\Gamma$  is nonseparable we seek to compare terms in  $\sum_{\Delta \in \Gamma} f(\Delta)$  and  $\prod_{\Lambda \leq \Gamma} q(\Lambda)$ . This latter may be written as  $\sum_{\Lambda \leq \Gamma} \sum_{X \in \mathcal{H}} A_{X, \Lambda} X$

$$= \sum_{z: \Gamma \rightarrow \mathcal{K}} \prod_{\Lambda \triangleleft \Gamma} A_{z(\Lambda), \Lambda} z(\Lambda) = \sum_{\substack{X \in \mathcal{K} \\ \Xi \triangleleft \Gamma}} X \sum_{z \in K(\Gamma, \Xi; X)} \prod_{\Theta \triangleleft \Gamma} A_{z(\Theta), \Theta}$$

Now, every nonzero term in this has  $u(X) = \Xi$  because  $\Xi = \bigcup_{\substack{\Theta \triangleleft \Gamma \\ \text{st } z(\Theta) \neq 1}} \Theta$

$$= \bigcup_{\substack{\Theta \triangleleft \Gamma \\ \text{st } u(z(\Theta)) = \Theta}} \Theta = u\left(\prod_{\Theta \triangleleft \Gamma} z(\Theta)\right) = u(X). \text{ If we omit the terms for}$$

which  $\Xi = \Gamma$  the sum of the remaining terms then equals

$$\sum_{\substack{X \in \mathcal{K} \\ \Xi \triangleleft \Gamma}} X \sum_{z \in L(\Xi; X)} \prod_{\Theta \triangleleft \Xi} A_{z(\Theta), \Theta}. \text{ When and only when } X = f(\Xi) \text{ the only}$$

term is that for which  $z: \Theta \rightarrow f(\Theta)$  if  $\Theta \triangleleft \Xi$  and  $z: \Theta \rightarrow 1$  otherwise, which has numerical value 1 and corresponds to the term  $f(\Xi)$  in  $\sum_{\Delta \in \Gamma} f(\Delta)$ . When  $X \neq f(\Xi)$  the sum is zero by the inductive hypothesis.

Therefore the expressions  $\sum_{\Delta \in \Gamma} f(\Delta)$  and  $\prod_{\Lambda \triangleleft \Gamma} q(\Lambda)$  agree in all terms except those for which  $u(X) = \Gamma$ .  $\sum_{\Delta \in \Gamma} f(\Delta)$  has only one such term, namely  $f(\Gamma)$ , and this cannot occur in  $\prod_{\Lambda \triangleleft \Gamma} q(\Lambda)$  since  $\Gamma$  is nonseparable and so the relevant terms which do arise cannot involve the indeterminate  $f(\Gamma)$ . Consequently on formal division we obtain  $A_{1, \Gamma} = 1$ ,  $A_{f(\Gamma), \Gamma} = 1$ , and  $A_{X, \Gamma} = 0$  if  $u(X) \neq \Gamma$ ,  $X \neq 1$  because there are no terms with  $u(X) \neq \Gamma$  and  $X \neq 1$  in either expression.

For the first part of the inductive hypothesis which we assert holds even for separable  $\Gamma$ , we consider the product  $\prod_{\Lambda \triangleleft \Gamma} q(\Lambda)$  (for we have now determined  $q(\Gamma)$  if  $\Gamma$  is nonseparable). This is  $\sum_{\substack{X \in \mathcal{K} \\ \Xi \triangleleft \Gamma}} X \sum_{z \in L(\Xi; X)} \prod_{\Theta \triangleleft \Xi} A_{z(\Theta), \Theta}$ , which will equal the polynomial  $\sum_{\Delta \in \Gamma} f(\Delta)$

which now accounts for all the terms with  $X = f(\Xi)$ . Hence, comparing coefficients and using the inductive hypothesis we establish  $\sum_{z \in L(\Gamma; X)} \prod_{\Theta \triangleleft \Gamma} A_{z(\Theta), \Theta} = 0$  if  $X \neq f(\Gamma)$ , as required.  $\blacksquare$

In Tutte's papers [22], [25] where the important part of this theorem is proved, he uses a proof involving information

about the structure of the graphs; in fact, he constructs the function  $q$  as the basis of his method. The difference between his two proofs of the theorem is that [25]'s is a generalized and modified version of [22]'s. In establishing the above theorem we have not explicitly used structural information; we could in principle write a computer programme to determine the coefficients  $A_{X,r}$  based upon the proof. This makes this treatment more amenable to providing estimates of the coefficients; however, we shall see later that another approach is even more helpful in these respects.



## 2.4 Some results of Whitney

An alternative approach to the result of Tutte is presented in this and the following section. It uses some ideas of Whitney [27]; first we present a slight adaptation of his theorem 7A, with a simple proof.

In this exposition we consider the type of a graph; that is, the family of isomorphism classes of its non-null blocks. For example, forests with the same number of edges have the same type; as another example, all three graphs shown in the accompanying

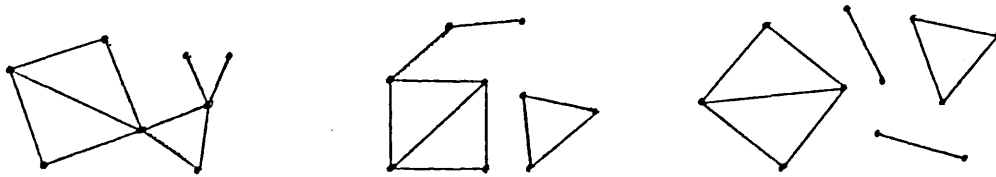
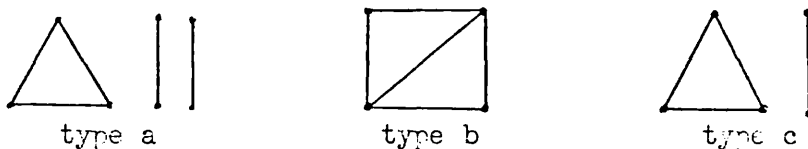


diagram have the same type. The type of a graph is completely determined by the numbers of blocks isomorphic to each nonseparable graph.

We now define three infinite matrices  $N$ ,  $B$  and  $M$ , indexed by graph types denoted by small letters  $a$ ,  $b$ ,  $c$  etcetera. They are defined as follows:  $M_{c,b}$  is the number of subgraphs of type  $c$  of a graph of type  $b$ ;  $N_{a,b}$  is the number of ways of embedding the blocks of a graph of type  $a$  in a graph of type  $b$ ; and  $B_{a,c}$  is the number of ways of embedding the blocks of a graph of type  $a$  in a graph of type  $c$  such that their union is that latter graph. For instance, with the three graphs shown here we find that the



values are  $M_{c,b} = 4$ ,  $B_{a,c} = 7$  and  $N_{a,b} = 50$ . It is obvious that these entries are well-defined, since it does not matter what graph we choose to represent a given graph type.

THEOREM 1:  $N = BM$ . Also,  $B^{-1}$  is well-defined and  $M = B^{-1}N$ .

Proof. The first part of the statement is immediate from the definitions when we sum  $B_{a,c}M_{c,b}$  over all relevant  $c$  (that is, those for which the term is nonzero). Further, if we order graph types in a similar way to the ordering of graphs in 2.3 it is clear that  $B$  is lower triangular while  $M$  is upper triangular, and so the sum of the nonzero terms in  $\sum_a B_{a,c}^{-1}M_{c,b}$  is finite for any values of  $c$  and  $b$ , and so the second part is established. This is another simple application of inversion.  $\blacksquare$

The terms of the matrix  $N$  are easy to calculate, using the following result. If  $p$  is the type of a nonseparable graph then we shall denote by  $a_p$  the number of blocks of type  $p$  in a graph of type  $a$ .

THEOREM 2:  $N_{a,b} = \prod_p \left( \sum_q b_q M_{p,q} \right)^{a_p}$ .

Proof. Again, this is immediate from the definitions, when we consider the number of ways of embedding each block in turn.  $\blacksquare$

Theorems 1 and 2 together imply Whitney's theorem 7A, that all the entries in the  $M$  matrix are determined once we know all the entries  $M_{p,q}$  with  $p$  and  $q$  being nonseparable types; moreover, that there is a polynomial expression for an entry  $M_{c,b}$  in the unknowns  $N_{p,b}$  with coefficients independent of  $b$ ,

namely  $M_{c,b} = \sum_a B_{c,a}^{-1} \prod_p M_{p,b}^{a_p}$ .

Theorem 1 is also proved by Biggs [5], where the notation differs slightly; his  $B$  is the same, but his  $c_g$  is a column of our  $M$  (for the equivalent of which he uses  $N$ ) and his  $UJc_g$  a

row of our  $N$ . In Whitney's paper  $m$  corresponds to our  $M$ , and  $N$  to our  $N$  or  $M$  since he only applies it to nonseparable types; in both cases the column subscript (which we have called  $b$ ) is implicit. Further, he uses different subscripts for these two quantities, although the notion of 'type' does appear in the paper; this and the form of his proof obscure the straightforward nature of the result.

As a corollary to theorem 2 we note that if  $p$  and  $q$  are types of nonseparable graphs then  $N_{p,q} = M_{p,q}$ . Other relations involving the entries in  $N$ ,  $B$  and  $M$  are possible but we shall only need the following, which is Whitney's 12A; the remaining results in this section are also due to him, occurring in chapters III and IV of his paper.

In the following two lemmas we require the concept of addition of graph types; we define the sum of two types to be the type of a graph that is the union of two (vertex-)disjoint graphs of the appropriate types. Consequently the number of blocks of a given type in the sum is just the sum of the two respective numbers for the summands. With this addition, and remembering that we have a suitable zero type (the type of a null graph) the set of types forms a semigroup.

LEMMA 1:  $M_{c,b+d} = \sum_{x+y=c} M_{x,b} M_{y,d}$ .

Proof. From the definition of  $M$ , the left-hand side equals the number of subgraphs of type  $c$  of a graph of type  $b+d$ . However, any block of a subgraph of type  $c$  must be entirely contained in a graph of type  $b$ , or of type  $d$ ; hence the required number equals the sum over all suitable  $x$  and  $y$  of the product of the number of subgraphs of type  $x$  of a graph of type  $b$  and

that of type  $y$  of one of type  $d$ , which is the right-hand side.  $\blacksquare$

We now derive a matrix  $W$  from  $M$ , but to do this we need some more definitions. Let  $\phi$  be a function defined on graph types such that  $\phi(a) = \prod_p \phi(p)^{a_p}$ , with a different variable for each nonseparable graph type  $p$ ; this is similar to the multiplicative function  $f$  of section 2.2. Then write  $M_b[\phi]$  for the power series  $\sum_a M_{a,b} \phi(a)$ , and similarly let  $W_b[\phi] = \sum_a W_{a,b} \phi(a)$ .  $W$  is then defined by the formal relation  $W_b[\phi] = \log(M_b[\phi])$ . Note that if  $a$  is the null graph type then  $\phi(a) = 1$  from the definition of  $\phi$  and the usual meaning of an empty product; consequently the constant term in  $M_b[\phi]$  is  $M_{a,b} = 1$ , and so we may use the formal expansion for  $\log$  as an infinite sum of powers, namely  $\log(1+Y) = Y - \frac{1}{2}Y^2 + \frac{1}{3}Y^3 - \dots$ . This gives only a finite sum for the coefficient of any particular  $\phi(a)$ , and since also the definition is independent of the function  $\phi$ , we see that  $W_{a,b}$  is well-defined.

LEMMA 2:  $W_{c,b+d} = W_{c,b} + W_{c,d}$ .

Proof. From lemma 1 we see that  $M_{b+d}[\phi] = M_b[\phi] M_d[\phi]$ . Therefore  $W_{b+d}[\phi] = \log(M_{b+d}[\phi]) = \log(M_b[\phi] M_d[\phi]) = \log(M_b[\phi]) + \log(M_d[\phi]) = W_b[\phi] + W_d[\phi]$ , and the result is immediate on comparing coefficients of  $\phi(c)$ .  $\blacksquare$

Now, we know that  $M_{c,b} = \sum_a B_{c,a}^{-1} \prod_p N_{p,b}^{a_p}$ , a polynomial in the unknowns  $N_{p,b}$ ; it follows that  $W_{c,b}$  is also a polynomial in them, since we have just remarked (prior to lemma 2) that any entry in  $W$  is a finite sum of products of the  $M_{c,b}$ .

LEMMA 3:  $W_{c,b}$  is equal to a polynomial in the  $N_{p,b}$  that is homogeneous of degree 1.

Proof. By lemma 2,  $W_{c,nb} = nW_{c,b}$  where  $nb$  is the sum of  $n$  types  $b$ ; and  $N_{n,nb} = nN_{p,b}$ . So any nonlinear terms in a polynomial for  $W_{c,b}$  must cancel for all sets of numbers  $N_{p,b}$  corresponding to graph types  $b$ . Therefore  $W_{c,b}$  will take the same values if we ignore any nonlinear terms.  $\blacksquare$

In fact we could establish, as Whitney does in theorems 5A etcetera, that this implies that  $W_{c,b}$  is precisely such a polynomial (instead of simply taking equal values) since the  $N_{p,b}$  are independent variables; however, this lemma is enough for our purposes. The following theorem is now straightforward.

THEOREM 1:  $W_{c,b}$  is equal to the linear terms of  $M_{c,b}$  when it is expressed as a polynomial in the  $N_{p,b}$ .

Proof. From the definition of  $W_{c,b}$  we know that it is a polynomial in the  $M_{e,d}$ , the only linear term being  $M_{c,b}$  itself; hence, since all nonlinear terms cancel,  $W_{c,b}$  is actually equal to the linear terms of  $M_{c,b}$ .  $\blacksquare$

## 2.5 A theorem of Biggs

This section concludes the chapter with a treatment of the result expounded by Biggs [5] for interaction models. Here we continue with formal expressions in variables corresponding to nonseparable graphs.

THEOREM 1: If  $\Phi(b) = \sum_c M_{c,b} \phi(c)$  is a multiplicative function

then there is an expression for  $\Phi(b)$  as a product of formal power series, namely  $\Phi(b) = \prod_p \psi(p)^{M_{p,b}}$  where  $\psi(p) = \exp(\sum_c B_{c,p}^{-1} \phi(c))$ .

$$\begin{aligned} \text{Proof. } \Phi(b) &= \sum_c M_{c,b} \phi(c) = \exp\left(\sum_c W_{c,b} \phi(c)\right) = \\ & \exp\left(\sum_c \phi(c) \sum_p B_{c,p}^{-1} N_{p,b}\right) = \exp\left(\sum_p N_{p,b} \sum_c \phi(c) B_{c,p}^{-1}\right) = \\ & \prod_p \left(\exp\left(\sum_c B_{c,p}^{-1} \phi(c)\right)\right)^{N_{p,b}} = \prod_p \psi(p)^{M_{p,b}}. \quad \blacksquare \end{aligned}$$

## CHAPTER 3

### STRUCTURES OTHER THAN GRAPHS

- Section 3.1 Clusterings, clutters and chain-groups
- Section 3.2 Hypergraphs
- Section 3.3 Paragraphs
- Section 3.4 Avitoids
- Section 3.5 Molecules

In this chapter we study a few generalizations of graphs. The first two sections summarize existing structures, and the last three introduce new ones. Paragraphs are mentioned for their use in generalizing oriented graphs. Avitoids provide a general setting for the machinery of chapter 2, and will be used again to investigate duality in chapter 5. Molecules too provide a general setting for chapter 2 but will prove useful in investigating the process of evaluating certain parameters in chapter 6.

### 3.1 Clusterings, clutters and chain-groups

These structures will be explained here for the purpose of comparison with those of later sections.

Regular clusterings were introduced by Tutte [25] in order to generalize the structures for which his 'theorem of the vanishing coefficients' ([22] and see our chapter 2) applies, and were employed in the problem of vertex-reconstruction.

A regular clustering on a set  $Q$  is a set of non-null subsets thereof called clusters, such that every minimal non-null separator of any subset is a cluster, where a separator  $S$  of a subset  $M$  is such that any cluster contained in  $M$  is contained in either  $S$  or  $M \setminus S$ . An alternative definition has been given by Manvel, who demands that every one-element subset of  $Q$  be a cluster and also that the union of two intersecting clusters be a cluster.

Clutters and their blockers were defined by Edmonds and Fulkerson [10], and further results on them have been obtained by Seymour [18,19] who also defined the operations of deletion and contraction.

A clutter on a set  $E$  is a set  $L$  of subsets thereof such that none includes another; the blocker of a clutter is the set of minimal subsets of  $E$  having nonempty intersection with every element of  $L$ . The deletion of a set  $D$  from a clutter leaves those elements of  $L$  that do not intersect  $D$ , and the contraction of a set  $C$  results in the set of minimal sets  $A \setminus C$  for elements  $A$  of  $L$ .

Note that the blocker, deletion and contraction of a clutter are themselves clutters, that deletion and contraction are



commutative, that the blocker of a blocker is the original clutter, and that the blocker of a deletion is the corresponding contraction of a blocker. If we associate a suitable clutter with a matroid or graph then the blocker or deletion/contraction (respectively) of the clutter will correspond to the dual of the matroid or the deletion/contraction of the graph [18].

Chain-groups are due to Tutte [21] and can provide a halfway stage between graphs and matroids [23].

A chain-group on a finite set  $E$  over an integral domain  $R$  is a set  $N$  of mappings from  $E$  to  $R$  that is closed under the (obvious) operations of addition and multiplication by an element of  $R$ . If  $R$  were a field this would just be a vector space, but in most applications  $R$  is the ring of integers. The dual chain-group is the set of mappings that are orthogonal to every element of the original chain-group; that is, the set  $\{h: E \rightarrow R \mid \sum_{x \in E} h(x)g(x) = 0 \forall g \in N\}$ . The support of an element of  $N$  is the set of elements of  $E$  whose images are not zero; and a dendroid is a minimal subset of  $E$  that meets the support of every nonzero element of  $N$ .

We can associate a chain-group with a given graph by letting  $E$  be the edge-set and taking as  $N$  the set of those mappings that represent linear combinations of circuits of that graph when oriented [21]. Then a dendroid will represent the complement of a spanning forest of the graph; it is in fact the same notion as an element of a blocker for a clutter.

### 3.2 Hypergraphs

Hypergraphs are the generalization of graphs that is appropriate in many instances. The fact that they possess vertices means that we can build interaction models on them (see chapter 4). However, it is not possible to define circuits on them in a way that satisfies the matroid axioms. In this section we briefly discuss hypergraphs and shall later see how they also lead into paragraphs (section 3) and prove useful when dealing with avitoids (section 4).

A hypergraph  $\Gamma$  is a finite set  $V^\Gamma$  of vertices and a finite family  $E^\Gamma$  of nonempty subsets of  $V$ , called edges. Deletion of an edge is effected by removing it from the family  $E^\Gamma$  and contraction of the edge  $e$  by identifying all the vertices it contains to form a new one, deleting the edge  $e$  and, in any other edge containing any of the coalesced vertices, removing those vertices and replacing them with the new one.

Note that this does not quite accord with the usual definitions for graphs; there it is usual to call a loop an edge with two identical end-points, but here it is more natural to let a loop be an edge of size 1. Our definition of a hypergraph does allow multiple edges, but we shall call a hypergraph elementary if no edge contains another; this precludes multiple edges and means that any vertex in a loop occurs in no other edge.

### 3.3 Paragraphs

The definition given by Biggs [4] for an interaction model that allows him to form an equivalent flow model involves orienting the edges. If we wish to extend this to hypergraphs it is appropriate to define a structure based on the same notion as that for a chain-group.

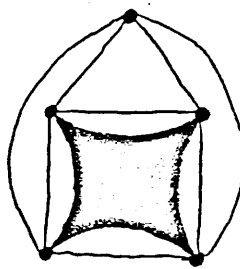
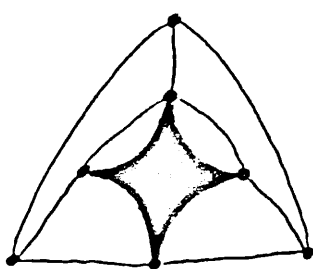
A paragraph consists of finite sets  $V$  of vertices and  $E$  of edges, together with an incidence matrix  $A$ , indexed by vertices and edges, with entries being rational, such that  $\sum_{v \in V} A_{v,e} = 0 \quad \forall e \in E$ . We can easily associate a paragraph with a given hypergraph by putting  $A_{v,e} = 0$  if  $v$  is not included in the edge  $e$ , and giving nonzero values that sum to zero for the other entries corresponding to the edge  $e$ . For graphs this is achieved by assigning the values  $+1$  and  $-1$  to the two nonzero entries for each edge, which is what is meant by 'orienting the edges'. Note that we cannot deal with loops, though, because we have no way of associating them with a particular vertex.

It is helpful to use  $0$ ,  $+1$  and  $-1$  as entries in  $A$  as much as possible, but other values may be better suited to given cases we wish to investigate. It may even be useful to allow entries in fields other than the rational in some circumstances.

The appropriate definition of a dual is as follows: a paragraph with vertex-set  $C$ , incidence matrix  $B$  but the same edge-set  $E$  is a dual if  $\sum_{e \in E} A_{v,e} B_{c,e} = 0 \quad \forall c \in C, v \in V$  and the ranks of the matrices  $A$  and  $B$  sum to  $|E|$ . We also usually require the ranks of each to be 1 less than the number of its rows. The operation of deletion is effected by removing the column corresponding to the specified edge  $e$  from the matrix; and

contraction involves choosing a vertex  $v$  incident with  $e$ , then adding suitable multiples of the respective row to other rows having a nonzero entry in the  $e$  column in order to make that entry zero, and then deleting the  $e$  column and the  $v$  row. This then ensures that deletion and contraction are dual operations, and that we still have paragraphs left after performing them.

We shall not pursue this topic further, but merely remark that this has applications in electrical network theory. Bloch, in [6], showed how it is possible to form networks having the characteristics of the duals of non-planar graph networks, by using 'ideal transformers'. These, in effect, simply provide elements representing hyperedges in the dual, as may be seen by considering their behaviour. Below we show paragraph duals of  $K_5$  and  $K_{3,3}$  respectively; as we have drawn them the opposite vertices of the edges of size 4 have the same value (+1 or -1), but which pair, and which end of any other edge, has the value +1 depends on the orientation of the original graph.



## 3.4 Avitoids

We shall find it helpful to deal with something having slightly more structure than a regular clustering; what we propose satisfies all but one of the matroid axioms. This then allows us to consider duals and the operations of deletion and contraction, although the concept of rank must be amended, and loses some of its power.

An avitoid is a finite set  $E$  and a set of nonempty subsets thereof, called circuits, such that none includes another. A subset of  $E$  is dependent if it possesses a circuit as a subset, and independent otherwise; a base is a maximal (by inclusion) independent set. A subset  $S$  of  $E$  is separable if there exist at least two disjoint nonempty sets whose union is  $S$  such that every circuit contained in  $S$  is contained in one of the sets; a cluster is a nonseparable set. We shall also define a loop as a circuit with just one element.

Not every regular clustering can be considered as an avitoid. For instance, if we only have  $\{a\}$ ,  $\{b\}$ ,  $\{c\}$ ,  $\{a,b\}$  and  $\{a,b,c\}$  as clusters then these are the only candidates for circuits; but  $\{a,b\}$  and  $\{a,b,c\}$  cannot both be circuits and if either is not it follows that it must be separable. However, the converse is true.

**THEOREM 1:** The clusters of an avitoid define a regular clustering.

**Proof.** If we are given an avitoid then let us consider a minimal non-null separator  $A$  of any of its subsets. This means that for every proper non-null subset  $B$  of  $A$  there is a cluster  $C$  that meets both  $B$  and  $A \setminus B$ ; but from our definition of a cluster we know that there must now be a circuit that meets both  $C \cap B$  and  $C \setminus B$  (or else  $C$  would be separable), so it also meets both  $B$  and

$A \setminus B$ . Therefore  $A$  is a cluster by our definition, and so we do have a regular clustering. ■

We can see that the set of avitoids giving rise to the same regular clustering are those that have the same circuits of size greater than 1.

As an example of an avitoid let  $E$  be  $\{a,b,c\}$  with circuits  $\{a,b\}$  and  $\{a,c\}$ . For this the independent sets are  $\emptyset$ ,  $\{a\}$ ,  $\{b\}$ ,  $\{c\}$  and  $\{b,c\}$ , the bases are  $\{a\}$  and  $\{b,c\}$ , and the clusters happen to be just the dependent sets, namely  $\{a,b\}$ ,  $\{a,c\}$  and  $\{a,b,c\}$ , plus the trivial ones  $\{a\}$ ,  $\{b\}$  and  $\{c\}$ .

As in the case of a matroid, we may uniquely define an avitoid in terms of its bases or dependent or independent sets. The defining requirement for bases is that there be at least one and that none includes another; for independent sets, there must be at least one and every subset of one is itself independent; and for dependent sets, they must be nonempty and every superset of one must also be dependent. Consequently the null set must be independent, can be a base but cannot be a circuit; and there may be no circuits or dependent sets, but there must be some bases and independent sets. Once we have determined the bases we can define a set as independent if it is included in a base and dependent otherwise, and a circuit will then be a minimal dependent set.

The dual of an avitoid comprises the same set  $E$  together with a set of bases that are the complements of the bases of the original. The result of deleting an element  $e \in E$  is the deletion avitoid which consists of a set  $E \setminus \{e\}$  and as independent sets those that were originally independent and did not contain  $e$ . The result of contracting an element  $e \in E$  is the contraction avitoid which

is obtained by dualizing, deleting  $e$ , and dualizing back again. These definitions make it evident that the order in which we delete several elements is immaterial, and similarly for contracting; however, the operations of deletion and contraction do not commute. The dual of a dual is obviously the original avitoid.

We shall use the notations  $\Gamma^*$ ,  $\Gamma'_A$ ,  $\Gamma''_A$  to stand for the avitoids resulting from taking the dual, deleting the edges in the set  $A$ , and contracting the edges in the set  $A$ , respectively, of the avitoid  $\Gamma$ . Since  $\Gamma''_e = \Gamma^{*'}_e$ , we find that, as in the case of graphs,  $\Gamma'^*_A = \Gamma''_A$ ; we shall make use of this sort of interchange in section 5.3.

Note that these definitions, in following through those of a matroid, do not correspond to those for a clutter. The operation of deletion carries through, but the blocker does not equal the dual, nor does contraction correspond. If we define the elements of a clutter as the circuits of an avitoid, then the elements of the blocker will be the bases of the dual avitoid, and vice versa. Also, an empty set can be the set of circuits of an avitoid or the set of elements of a clutter but not the set of bases of an avitoid, whereas the set comprising the empty set can be either of the last two but not the first. Lastly, as we have remarked, contraction and deletion commute in a clutter [18] but not in an avitoid.

Using the example introduced earlier in this section we observe that it is self-dual. When we delete  $b$  and then contract  $c$  we are left with a single element set  $\{a\}$  that is a circuit; and when we contract  $c$  and then delete  $b$  the same set remains but it is not a circuit.

### 3.5 Molecules

We shall introduce the notion of a molecule to generalize the idea of a graph type in chapter 2. In investigating functions on graphs we may wish to distinguish between subgraphs that have the same type; for instance, horizontal and vertical edges in a square lattice. This treatment is couched in the widest possible terms in order to include set-theoretic structures such as aperiodic structures, and to investigate how far the results for such things depend upon their structure.

Suppose that we have a finite set  $A$  and a matrix  $N$  with non-negative integral entries indexed by pairs of its elements; and also that a positive integer-valued function  $w$  is defined on  $A$ . Then we call the elements of  $A$  atoms and  $w$  the weight function if  $N_{a,a} = 1 \forall a \in A$  and  $w(a) \geq w(b) \Rightarrow N_{a,b} = 0$  unless  $a=b$ . A molecule is then defined as a finite collection of atoms, or equivalently a vector with non-negative integral entries indexed by elements of  $A$ . We then extend  $w$  and  $N$  to deal with molecules by  $w(m) = \sum_{a \in A} m_a w(a)$

$$\text{and } N_{m,n} = \prod_{a \in A} \left( \sum_{b \in A} n_b N_{a,b} \right)^{m_a}.$$

Two other notions will prove useful. The set of particles is  $P = \{p \in A \mid N_{a,p} = 0 \forall a \in A \text{ st. } a \neq p\}$ , and the atomic number is a function  $v$  defined on molecules by  $v(m) = \sum_{p \in P} N_{p,m}$ . Thus the atomic number of a particle equals 1, and we note the following result.

LEMMA 1:  $v(m) = \sum_{a \in A} m_a v(a).$

Proof.  $v(m) = \sum_{p \in P} N_{p,m} = \sum_{p \in P} \sum_{a \in A} m_a N_{p,a} = \sum_{a \in A} m_a \left( \sum_{p \in P} N_{p,a} \right)$   
 $= \sum_{a \in A} m_a v(a). \quad \blacksquare$



If we have a total ordering on the atoms consistent with non-decreasing weight we can extend this to one on molecules as follows. We take as our alphabetical order the given ordering of atoms, and write each molecule as a 'word' with its constituent atoms as its 'letters' in reverse alphabetical order with appropriate repetitions; then we order the molecules firstly by increasing weight and secondly by reverse lexicographical order, except that between atoms of the same weight we preserve the forwards lexicographical order. We shall denote this ordering by  $\prec$ .

It is worth mentioning that although this may seem unduly complicated, it is in fact a fairly straightforward way to specify the ordering completely; this is certainly true if we wish to use a computer (although then it is convenient to ignore the 'exception' which was only introduced to make the new ordering a genuine extension). Also, our new ordering does not agree with that on graph types in section 2.4 but they are both derived from the same partial ordering that is dictated by the nature of the mathematics.

For avitoids and regular clusterings in general the atoms will represent clusters. The purpose of the weight function is to determine the ordering of the molecules, and the most sensible choice is usually the atomic number, especially if there is only one particle. Employing more than one particle is necessary when we wish to differentiate between the basic elements; most importantly, if we are investigating hypergraphs we wish to distinguish elements representing edges of different sizes (say, for the purpose of evaluating the weak chromatic polynomial).

The important point about structures that are representable by molecules is in effect the unique factorizability of those

that are separable. As we remarked in section 2.2, we can assign suitable values to the  $q$ -function to make the product of them for nonseparable graphs equal the desired value, but we must ensure that the values for separable graphs are what we want without multiplying by a 'correction factor'. This is why regular clusterings are suitable objects when we extend this idea to molecules; we can factorize a separable set into clusters in a unique way. However, it is sufficient that we be able to factorize uniquely into cluster-types, so that it is possible that structures more general still than regular clusterings may be represented by molecules.

## CHAPTER 4

### THE ADDITIVE PROPERTY FOR INTERACTION MODELS

- Section 4.1 The interaction model
- Section 4.2 The additive property for graphs
- Section 4.3 The extension to hypergraphs
- Section 4.4 The rank polynomial for hypergraphs

In this chapter we investigate the consequences of assuming that the partition function of an interaction model satisfies a certain linear relation. It is found that this necessitates the interaction being of a particularly simple form; and this is also sufficient. This is firstly done for graphs, and then generalized to hypergraphs; and finally the result is related to a sort of rank polynomial.

#### 4.1 The interaction model

It is a well-known fact that the chromatic polynomial of a graph is a linear combination of that function for the two graphs obtained by deleting or contracting any one edge that is not a loop; in fact, it is simply their difference. This additive property also arises in physical models, as demonstrated by Essam [11]; he also shows the relation of such functions to the rank polynomial. Tutte [20, 24] examined graph functions that satisfy this linear relation with unit coefficients, and extended the problem to include the case where the relation need not be satisfied if the edge concerned is an isthmus.

This chapter deals with the additive property quite generally, for functions that result from interaction models on graphs. We do not consider the aforementioned extension, though, because the corresponding generalization of lemma 3 in the next section does not hold; this is because an edge may be an isthmus of a subgraph  $\Delta$  of  $\Gamma$  while not being one of  $\Gamma$  itself.

Our definition of an interaction model will be less specific than that used by Biggs [4]. For a graph  $\Gamma$  and a finite set  $A$ , an interaction function is a function  $x: A \times A \rightarrow \mathbb{C}$ ; then from any function  $\omega: V\Gamma \rightarrow A$  we may derive the composition  $x*\omega: E\Gamma \rightarrow \mathbb{C}$ , given by  $(x*\omega)(e) = x(\omega(v_1), \omega(v_2))$  where  $v_1, v_2$  are the vertices incident with  $e$ . If  $e$  is a loop then  $v_1 = v_2$ ; if not, then it is in fact irrelevant which vertex is identified as  $v_1$ , but we shall assume that some choice is consistently made. Then the partition function associated with this model is defined as  $Z(\Gamma; x) = \sum_{\omega: V\Gamma \rightarrow A} \prod_{e \in E\Gamma} x*\omega(e)$ .

## 4.2 The additive property for graphs

We start this section with a few simple lemmas concerned with interaction models. Lemma 1 is a result we shall refer to repeatedly in this and the next section, and lemmas 2 and 3 are straightforward adaptations of common techniques for our purposes.

LEMMA 1: If  $\sum_{i=1}^n s_i^r = tz^{r-1} \forall r$  with  $n, r \in \mathbb{Z}^+$  and  $s_i, t, z \in \mathbb{C}$  then

$s_i = 0$  or  $z$  for any  $i$ , and  $t = z^{|\{1 \leq i \leq n \mid s_i = z\}|}$  if  $z \neq 0$ .

Proof. If the right-hand side equals zero then clearly  $s_i = 0 \forall i$ , and either  $z$  or  $t$  is zero so the statement is true. Otherwise we may divide by  $z^r$  to obtain  $\sum_{i=1}^n (s_i/z)^r = t \forall r$ , and this implies that all the summands are 0 or 1, which gives the result.  $\blacksquare$

LEMMA 2: If  $x, y$  are interaction functions defined for a set  $A$  and related by  $x(a, b) = py(a, b) + q \forall a, b \in A$  for some  $p, q \in \mathbb{C}$  with  $q \neq 0$ , then their partition functions are related by  $Z(\Gamma; x) = q^{|\mathbb{E}\Gamma|} \sum_{\Delta \subseteq \Gamma} (p/q)^{|\mathbb{E}\Delta|} Z(\Delta; y)$ .

Proof. By definition,  $Z(\Gamma; x) = \sum_{\omega: V\Gamma \rightarrow A} \prod_{e \in \mathbb{E}\Gamma} x^*\omega(e)$ , and by hypothesis this equals  $\sum_{\omega: V\Gamma \rightarrow A} \prod_{e \in \mathbb{E}\Gamma} (p(y^*\omega)(e) + q) = \sum_{\omega: V\Gamma \rightarrow A} \sum_{\Delta \subseteq \Gamma} q^{|\mathbb{E}\Gamma| - |\mathbb{E}\Delta|} p^{|\mathbb{E}\Delta|} \prod_{e \in \mathbb{E}\Delta} y^*\omega(e)$  which rearranges to  $\sum_{\Delta \subseteq \Gamma} q^{|\mathbb{E}\Gamma|} (p/q)^{|\mathbb{E}\Delta|} \sum_{\omega: V\Delta \rightarrow A} \prod_{e \in \mathbb{E}\Delta} y^*\omega(e) = q^{|\mathbb{E}\Gamma|} \sum_{\Delta \subseteq \Gamma} (p/q)^{|\mathbb{E}\Delta|} Z(\Delta; y)$ .  $\blacksquare$

LEMMA 3: If  $Z(\Delta; y) = dZ(\Delta'_e; y) + cZ(\Delta''_e; y)$  for all graphs  $\Delta$  and all edges  $e$  thereof that are not loops, and if  $x$  and  $y$  are related as in lemma 2, then for all graphs  $\Gamma$  and all edges  $e$  thereof that are not loops,  $Z(\Gamma; x) = (dp + q)Z(\Gamma'_e; x) + cpZ(\Gamma''_e; x)$ .

Proof. If  $q=0$  then clearly  $Z(\Gamma;x) = p^{|\mathbb{E}\Gamma|} Z(\Gamma;y)$  and so the result is immediate. Otherwise, from lemma 2,  $Z(\Gamma;x) = q^{|\mathbb{E}\Gamma|} \sum_{\Delta \in \Gamma} (p/q)^{|\mathbb{E}\Delta|} Z(\Delta;y) = q^{|\mathbb{E}\Gamma|} \left\{ \sum_{\substack{\Delta \in \Gamma \\ \text{st} \in \mathbb{E}\Delta}} (p/q)^{|\mathbb{E}\Delta|} (dZ(\Delta'_e;y) + cZ(\Delta''_e;y)) + \sum_{\substack{\Delta \in \Gamma \\ \text{st} \notin \mathbb{E}\Delta}} (p/q)^{|\mathbb{E}\Delta|} Z(\Delta;y) \right\}$ . Using an obvious correspondence, this then equals  $q^{|\mathbb{E}\Gamma'|} \left\{ \sum_{\Delta \in \Gamma'} (p/q)^{|\mathbb{E}\Delta|+1} dZ(\Delta;y) + \sum_{\Delta \in \Gamma''} (p/q)^{|\mathbb{E}\Delta|+1} cZ(\Delta;y) + \sum_{\Delta \in \Gamma'} (p/q)^{|\mathbb{E}\Delta|} Z(\Delta;y) \right\} = (dp+q)q^{|\mathbb{E}\Gamma'|} \sum_{\Delta \in \Gamma'} (p/q)^{|\mathbb{E}\Delta|} Z(\Delta;y) + (cp)q^{|\mathbb{E}\Gamma''|} \sum_{\Delta \in \Gamma''} (p/q)^{|\mathbb{E}\Delta|} Z(\Delta;y) = (dp+q)Z(\Gamma';x) + cpZ(\Gamma'';x)$  by

lemma 2 again.  $\blacksquare$

If  $A = A_1 \cup A_2 \cup \dots \cup A_n$  is a partition of the set  $A$  into equal-sized subsets and the interaction function has the property that one value is taken when both arguments lie in the same subset and another value (which may however be equal to the first) when they do not, then we shall say that the model is weakly resonant. The transformation in the statement of lemma 2 clearly preserves weak resonance.

**THEOREM 1:** If  $Z(\Delta;y) = dZ(\Delta'_e;y) + cZ(\Delta''_e;y)$  for all graphs  $\Delta$  and all edges  $e$  thereof that are not loops, then the interaction model is weakly resonant; moreover the two values referred to above are  $d+c/k$  when both arguments are in the same subset and  $d$  when they are not, where  $k$  is the common size of the subsets; and conversely.

Proof. Given the hypothesis, let us first examine the case where  $c=0$ . For this, consider the graph consisting of two vertices and  $r$  edges between them, for each of which the same vertex is designated  $v_1$ . Applying the hypothesis tells us that  $\sum_{a,b \in A} y(a,b)^r = d \sum_{a,b \in A} y(a,b)^{r-1}$ , which inductively gives  $\sum_{a,b \in A} y(a,b)^r = d^r |A|^2$ .

This then implies by lemma 1 that  $y(a,b) = d \quad \forall a,b \in A$  which is weakly resonant and is included in the formula of the proposition for the special case  $c=0$ , when of course any partition of  $A$  into equal-sized subsets is suitable.

Alternatively, if  $c \neq 0$  then we may put  $p=1/c$ ,  $q=-d/c$  in the transformation of lemma 2, and consider the interaction function  $x(a,b) = (y(a,b) - d)/c$  instead. This will satisfy, by lemma 3,  $Z(\Delta;x) = Z(\Delta'';x)$ ; and applying this to the graph described above gives  $\sum_{a,b \in A} x(a,b)^r = \sum_{a \in A} x(a,a)^{r-1}$ . This already tells us by lemma 1 that  $x$  takes only two values, one of them being 0. Further, if the other value is  $m$ , then  $|\{a,b \in A | x(a,b) = m\}| = (1/m) |\{a \in A | x(a,a) = m\}|$ ; but when  $r=1$  we obtain  $|\{a,b \in A | x(a,b) = m\}| \cdot m = |A|$ , because the context requires  $x(a,a)^0 = 1$  even if  $x(a,a)$  equals 0. Hence  $x(a,a) = m \quad \forall a \in A$ , and there are in all  $|A|/m$  pairs  $a,b \in A$  with  $x(a,b) = m$ .

Now we turn our attention to the circuit graph with  $r$  vertices and edges, for which we shall choose the  $v_1$ 's and  $v_2$ 's such that each vertex is  $v_1$  for one of its incident edges and  $v_2$  for the other. The recurrence relation we have now generated for  $Z(\Delta;x)$  implies that the partition functions for all these graphs are the same, because contracting an edge reduces the circuit graph with  $r$  vertices to that with  $r-1$ . So, inductively and writing  $C_r$  for the circuit graph as described above,  $Z(C_r;x) = Z(C_1;x) = m|A|$ . Also, we know that  $m|A| = Z(C_2;x) = \sum_{a,b \in A} x(a,b)x(b,a)$ , which has at most  $|A|/m$  nonzero terms (one for each  $x(a,b) \neq 0$ ) each equal to  $m^2$ . Therefore it has precisely that many nonzero terms and we know that  $x(a,b) = m \Rightarrow x(b,a) = m$ .

However, we may evaluate the partition functions for circuit graphs in another way, known as the transfer matrix method (as

for instance used by Biggs [5]). If we form the complex-valued matrix  $T$  indexed by elements of  $A$  and defined by  $T_{a,b} = x(a,b)$ , then  $Z(C_r; x) = \text{trace}(T^r)$ ; but since the trace of the  $r$ th power of a matrix is simply the sum of the  $r$ th powers of its eigenvalues, this implies that  $\sum \lambda^r = m|A| \forall r \in \mathbb{Z}^+$ , where the summation is over all the eigenvalues (with appropriate repetitions). This requires, by lemma 1, that all the eigenvalues be 0 or 1; now, though, we may use the Perron-Frobenius theorem (as stated by Lancaster [16]), which tells us that the eigenvalue of greatest absolute value of a real nonnegative irreducible matrix has unit multiplicity. This is applicable because the matrix  $T$  is known to be real and nonnegative since its only entries are 0 and  $m$ , the quotient of two positive integers; and the symmetry of the function  $x$  implies that the matrix is symmetric, so if  $T$  is not irreducible we may re-order the rows and columns (correspondingly) so that there are zeros everywhere except for (maximal by inclusion) irreducible blocks of 0's and  $m$ 's along the diagonal. The eigenvalues of the whole matrix are then of course the eigenvalues of these blocks; and the Perron-Frobenius theorem informs us that each block has one eigenvalue of 1 and the rest are all 0. However, this means that each block is equal to  $X^{-1} \text{diag}(1, 0, \dots, 0) X$  for some matrix  $X$ , and the  $(i,j)$ th entry of this is simply  $(X)_{i,1} (X^{-1})_{1,j}$ ; and since none of the diagonal elements is zero, none of the other elements can be. Therefore every block consists entirely of  $m$ 's; and if there are  $t$  blocks of sizes  $k_i \times k_i$  for  $i=1, \dots, t$  then

$$|A|/m = |\{a, b \in A \mid x(a,b) = m\}| = \sum_{i=1}^t k_i^2 \geq |A|^2/t \text{ (since } \sum k_i = |A|)$$

$= |A|/m$  because the trace of  $T$  equals the sum of the traces of its blocks, and so  $|A|/m = t \cdot 1$ . Hence we have equality throughout and this requires that  $k_i = |A|/t$  for  $i=1, \dots, t$ .

So we have established that there is a partition of  $A$  into



sets of size  $k$ , with  $x(a,b) = m = 1/k$  when  $a$  and  $b$  are in the same subset, and  $x(a,b) = 0$  when they are not. Transforming back to the  $y$  function we find that the values are  $d + c/k$  and  $d$  respectively, as claimed in the statement of the theorem.

Conversely, suppose that we are given an interaction function of such a type. If  $c = 0$  then  $y(a,b) = d \quad \forall a, b \in A$  and so  $Z(\Delta; y) = |A|^{|V\Delta|} d^{|E\Delta|} = dZ(\Delta'; y)$ . If  $c \neq 0$  then make the transformation as before to get  $x(a,b) = 1/k$  or  $0$  as appropriate. Then the only nonzero terms in the sum for  $Z(\Gamma; x)$  are those for which  $\omega$  assigns values in the same subset of  $A$  to vertices in the same component of  $\Gamma$ ; and any nonzero term will necessarily be equal to  $(1/k)^{|E\Gamma|}$ . Hence  $Z(\Gamma; x) = |A|^{K\Gamma} k^{-|V\Gamma| - K\Gamma} (1/k)^{|E\Gamma|} = |A|^{K\Gamma} k^{-C\Gamma} = Z(\Gamma''; x)$ , where  $K\Gamma$  and  $C\Gamma$  are the number of components and cycle number respectively of  $\Gamma$ . Therefore transforming back again will yield  $Z(\Delta; y) = dZ(\Delta'; y) + cZ(\Delta''; y)$ .  $\blacksquare$

The fact that it is irrelevant which vertex we identify as  $v_1$  or  $v_2$  for a given edge  $e$  is immediate for models with the additive property because this choice makes no difference to the derived graphs  $\Gamma'_e$  and  $\Gamma''_e$ ; however, this observation is not enough to prove that the function must be symmetric. Interaction models are usually defined with the requirement that the interaction function be symmetric, in any case, because this is an obvious property of any physical system they model.

Resonance as defined by Biggs [5] corresponds to our weak resonance in the special case where  $A$  is partitioned into one-element sets; in fact the partition function of a weakly resonant model can easily be expressed in terms of that of a resonant model if we take into account the number of components of the graph concerned.

If we have additional structure on the set  $A$  then we may obtain further conditions on the model. For instance, if we know that  $A$  is a group and that  $x(a,b) = z(a-b)$  for some function  $z$  then we infer that  $A$  must be partitioned into cosets of a subgroup. In the definitions used by Biggs [4,5] this may be applied; however, whereas the dual model (see [5]) of a resonant model is also resonant, that of a weakly resonant model is not necessarily weakly resonant. Alternatively, in some cases when we have information about the function  $x$  we can provide a more elementary proof of the theorem without appealing to the Perron-Frobenius theorem.

### 4.3 The extension to hypergraphs

The additive property is a strong requirement for an interaction model, so it is not surprising that we can determine necessary and sufficient conditions from consideration of just the two families of graphs described. If we further demand that our interaction function be defined for more than two parameters, and have a generalization of the additive property for this case too, the function is further restricted. To establish this we define interaction models over hypergraphs.

The basic ideas for the hypergraph case are the same as for graphs. We require an interaction function  $x: \bigcup_{r=1}^{\infty} A^r \rightarrow \mathcal{C}$  whose values we shall write as  $x(r; a_1, \dots, a_r)$ , and a consistent order, say  $v_1, \dots, v_s$ , of the vertices in any particular edge; then we define  $x * \omega(e) = x(|e|; \omega(v_1), \dots, \omega(v_{|e|}))$  and the partition function as before, where  $|e|$  signifies the size of the edge  $e$ . Other notation will carry through from the graph case, but we must remember that contracting an edge involves deleting it and identifying all its vertices; of course, this may reduce the sizes of some other edges. This is the most apt interpretation of contraction not only due to its symmetry but also because this definition is the one required to make the weak chromatic polynomial of a hypergraph (see Jones [15]) satisfy the linear relation for the chromatic polynomial of a graph, with the same coefficients (Chvátal [9], referred to by Jones). Since we have ordered the vertices occurring in any particular edge, we should also specify their order in the event of two or more of them being identified by a contraction, say by placing the new vertex in the position of the earliest of the identified ones, and removing the others; however, as in the graph case this clearly can make no difference and in fact we discover

once again that the interaction function must be symmetric.

The proof of the hypergraph version of theorem 1 of the previous section is basically the same, and of course will have that theorem as a corollary, but the extra complexity involved in the the hypergraph case makes it worthwhile to present the proofs separately. We need to consider several families of hypergraphs this time, but start by restating lemmas 2 and 3 of the previous section in their hypergraph forms.

LEMMA 1: If  $x, y$  are interaction functions defined for a set  $A$  and related by  $x(z; a_1, \dots, a_z) = py(z; a_1, \dots, a_z) + q \quad \forall z \in \mathbb{Z}^+$ ,  $a_1, \dots, a_z \in A$  for some  $p, q \in \mathbb{C}$  with  $q \neq 0$ , then their partition functions are related by  $Z(\Gamma; x) = q^{|\mathbb{E}\Gamma|} \sum_{\Delta \in \Gamma} (p/q)^{|\mathbb{E}\Delta|} Z(\Delta; y)$ .

Proof. Identical to that for the graph form.  $\blacksquare$

LEMMA 2: If  $Z(\Delta; y) = dZ(\Delta'_e; y) + cZ(\Delta''_e; y)$  for all hypergraphs  $\Delta$  and all edges  $e$  thereof of size  $z$ , and if  $x$  and  $y$  are related as in lemma 1, then for all hypergraphs  $\Gamma$  and edges  $e$  thereof of size  $z$ ,  $Z(\Gamma; x) = (dp+q)Z(\Gamma'_e; x) + cpZ(\Gamma''_e; x)$ .

Proof. Identical to that for the graph form.  $\blacksquare$

We shall call a model weakly resonant to size  $z$  if  $A = A_1 \cup \dots \cup A_n$  is a partition into equal-sized subsets and the interaction function  $x$  has the property that for  $1 \leq w \leq z$ ,  $x(w; a_1, \dots, a_w)$  takes one value when  $a_1, \dots, a_w$  lie in the same subset  $A_i$  and a second (which might be the same) whenever they do not.

THEOREM 1: If  $Z(\Delta; y) = dZ(\Delta'_e; y) + cZ(\Delta''_e; y)$  with  $c \neq 0$  for all hypergraphs  $\Delta$  and all edges  $e$  thereof of size  $z$ , then the interaction model is weakly resonant to size  $z$ ; moreover the

two values referred to above are  $d + c/k$  and  $d$ , respectively; and conversely.

Proof. Since  $c \neq 0$  we may transform as in theorem 1 of the previous section to obtain  $Z(\Delta; x) = Z(\Delta''; x)$  for suitably-sized edges. Now we consider the hypergraph with  $r$  edges, each

containing the same  $z$  vertices in the same order (see figure 1 below). This yields 
$$\sum_{a_1, \dots, a_z \in A} x(z; a_1, \dots, a_z)^r = \sum_{a \in A} x(1; a)^{r-1}$$

which by lemma 1 of section 4.2 and the special case  $r=1$  implies that  $x(1; a) = m \quad \forall a \in A$ , and that  $x(z; a_1, \dots, a_z)$  takes the value  $m$  on  $|A|/m$  occasions and 0 on the others.

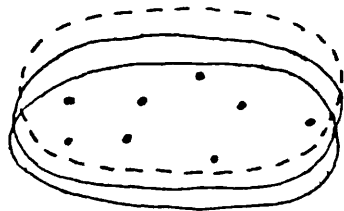


fig. 1

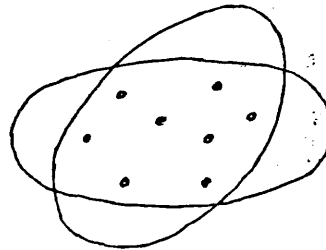


fig. 2

Next we consider the hypergraph with two edges each containing the same  $z$  vertices, the former in the order  $v_1, \dots, v_z$  and the latter in the order  $v_{\rho_1}, \dots, v_{\rho_z}$  for some permutation  $\rho$  (see figure 2 above).

Then the contracted graph is the same as in the previous case for

$r=2$ , so that 
$$\sum_{a_1, \dots, a_z \in A} x(z; a_1, \dots, a_z) x(z; a_{\rho_1}, \dots, a_{\rho_z}) =$$

$$\sum_{a_1, \dots, a_z \in A} x(z; a_1, \dots, a_z)^2$$
, and this now requires that  $x(z; a_1, \dots, a_z)$

$= m \Leftrightarrow x(z; a_{\rho_1}, \dots, a_{\rho_z}) = m$ .

Next we examine an analogue to the circuit graph, namely the  $z$ -uniform hypergraph with  $r(z-1)$  vertices and  $r$  edges  $e_1, \dots, e_r$  where the pairs of edges  $e_v$  and  $e_1, e_1$  and  $e_2$ , etcetera have precisely one vertex in common and no other pairs of edges have any common vertices (see figure 3 below). Calling this hypergraph

$C_r$  we have  $C_r = C_{r-1}$  and we may again use the transfer matrix method by defining  $T_{a,b} = \sum_{a_2, \dots, a_{z-1} \in A} x(z; a, a_2, \dots, a_{z-1}, b)$  and

obtaining  $Z(C_r; x) = \text{trace}(T^r)$  for  $r \geq 2$ . Now, if we knew that  $T_{a,b}$  could only take one of two values, one of which was zero, we could obtain as before the result that  $A$  must be partitioned into equal-sized subsets  $A_i$ ,  $i=1, \dots, |A|/k$ , with  $T_{a,b} = 1/k$  if  $a, b$  are in the same subset and 0 otherwise. However, consideration

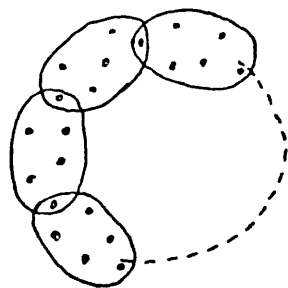


fig. 3

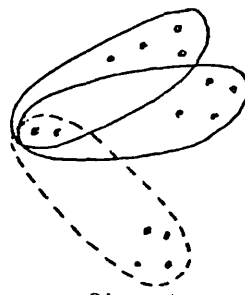


fig. 4

of the family of  $z$ -uniform hypergraphs whose  $r$ th member has  $r$  edges and  $r(z-2)+2$  vertices, two of which occur in all the edges and the rest of which occur in only one edge (see figure 4 above), indicates that  $\sum_{a,b \in A} (T_{a,b})^r = \sum_{a \in A} \left( \sum_{a_2, \dots, a_{z-1} \in A} x(z-1; a, a_2, \dots, a_{z-1}) \right)^{r-1}$ , which implies the desired result by lemma 1 of section 4.2.

Furthermore, it informs us by the same lemma that  $|A|k = k \left| \left\{ a \in A \mid \sum_{a_2, \dots, a_{z-1} \in A} x(z-1; a, a_2, \dots, a_{z-1}) = 1/k \right\} \right|$ , so that we have

$$\sum_{a_2, \dots, a_{z-1} \in A} x(z-1; a, a_2, \dots, a_{z-1}) = 1/k \quad \forall a \in A.$$

Now we examine another family of hypergraphs; for this the  $r$ th member will have  $2z-2$  vertices and  $r+1$  edges,  $r$  of which contain the same  $z$  vertices and the other contains two of these plus the remaining  $z-2$  (see figure 5 below). There are two sorts of edge we can contract, and equating the partition functions for the two resultant hypergraphs we get

$$\sum_{a, a_2, \dots, a_{z-1} \in A} x(z-1; a, a_2, \dots, a_{z-1})^r =$$

$$\sum_{a \in A} x(1; a)^{r-1} \sum_{a_2, \dots, a_{z-1} \in A} x(z-1; a, a_2, \dots, a_{z-1}) = m^{r-1} \sum_{a, a_2, \dots, a_{z-1} \in A} x(z-1; a, a_2, \dots, a_{z-1}).$$

Consequently, using lemma 1 of section 4.2 again,  $x(z-1; a, a_2, \dots, a_{z-1})$  can take only the two values 0 and  $m$ , as we wished.

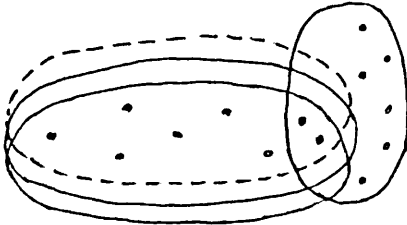


fig. 5

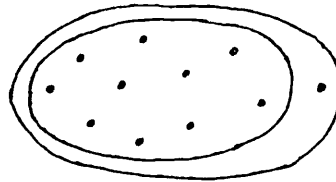


fig. 6

Next we turn our attention to the hypergraph with two edges, one containing  $z$  vertices and the other, of size  $z-1$ , containing all but one of these (see figure 6 above). When we contract the edge of size  $z$  we obtain a single vertex, in a loop; on equating the partition functions for these two hypergraphs we have

$$\sum_{a_1, \dots, a_{z-1} \in A} x(z-1; a_1, \dots, a_{z-1}) \sum_{a_z \in A} x(z; a_1, \dots, a_{z-1}, a_z) = \sum_{a \in A} x(1; a)$$

$= m|A|$ . However, we know the LHS  $\leq |A|k(1/k)m$ , because

$$x(z-1; a_1, \dots, a_{z-1}) \leq m \text{ and } \sum_{a_1, \dots, a_z \in A} x(z; a_1, \dots, a_z) = |A|k(1/k);$$

so the actual equality of the expression requires that

$$x(z; a_1, \dots, a_z) = m \Rightarrow x(z-1; a_1, \dots, a_{z-1}) = m.$$

$$x(z-1; a_1, \dots, a_{z-1}) \leq m \text{ and } \sum_{a_1, \dots, a_{z-1} \in A} x(z-1; a_1, \dots, a_{z-1}) = |A|/k \text{ we}$$

know the LHS  $\leq |A|(1/k)mk$ , because  $x(z; a_1, \dots, a_z) = 0$  if  $a_1, \dots, a_z$  are not all in the same subset  $A_i$ . So, again, the equality

necessitates  $x(z-1; a_1, \dots, a_{z-1}) = m$  only when  $a_1, \dots, a_{z-1}$  are all

in the same subset; and that  $x(z-1; a_1, \dots, a_{z-1}) = m, a_z$  in the

same subset as  $a_1, \dots, a_{z-1} \Rightarrow x(z; a_1, \dots, a_z) = m$ . These last two

results then combine to tell us that  $x(z; a_1, \dots, a_z) = m$  if and

only if  $a_1, \dots, a_z$  are in the same subset  $A_i$  of  $A$ , since any subset

must give rise to some nonzero terms, and we can then reach any other term by changing one argument at a time, and at each stage the new term is also nonzero.

Now an evaluation of  $T_{a,b}$  when  $a$  and  $b$  are in the same subset yields  $1/k = k^{z-2}m$ , and so  $m = k^{1-z}$ . Then a transformation back from  $x$  to  $y$  will give the values as stated in the proposition of the theorem, for edges of sizes  $z$ ,  $z-1$  and  $1$ .

Finally, we may establish that if the additive property holds for edges of size  $z$  it does so for smaller edges too. If we have any hypergraph  $\Gamma$  with an edge  $e$  of size  $w$  ( $1 < w < z$ ), form a new hypergraph  $\Delta$  that has the same edges and vertices except that  $e$  is replaced by an edge of size  $z$  containing the  $w$  vertices and  $z-w$  new ones, plus  $z-w$  other edges of size  $z$  each containing a different one of the  $z-w$  new vertices, any one of the  $w$  vertices originally contained in  $e$ , and  $z-2$  further new ones (see figure 7 below).

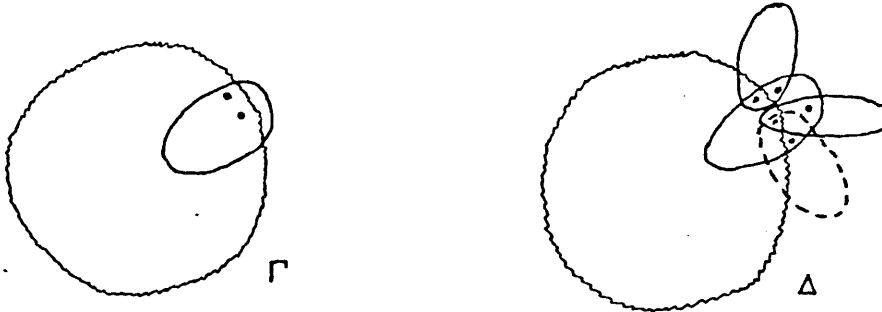


fig. 7

On contracting these last  $z-w$  edges of  $\Delta$  we simply recover  $\Gamma$ , so  $Z(\Delta; x) = Z(\Gamma; x)$ . Alternatively, if we contract the other new edge we obtain  $\Gamma''_e$  with  $z-w$  edges of size  $z-1$  joined at a single vertex, and we already know that each of these will contribute a factor of  $1/k$ ; so we establish that  $Z(\Delta; x) = k^{w-z}Z(\Gamma''_e; x)$ . Combining these two results we have  $Z(\Gamma; x) = k^{w-z}Z(\Gamma''_e; x)$  for any hypergraph and any edge of size  $w \leq z$ ; note that this formula works for edges of size  $1$  also.



Therefore we can show that the positive proposition of the theorem holds in full, since we have determined the values  $x$  can assume for edges of sizes  $z$ ,  $z-1$  and  $1$  by assuming the additive property holds for edges of size  $z$ ; consequently the values of  $x$  for edges of size  $w$ ,  $w-1$  and  $1$  for any  $w < z$  have now been determined, and these values will of course be consistent.

Conversely, if we have an interaction that is weakly resonant to size  $z$ , then make the transformation from  $y$  to  $x$  as before. Then clearly  $Z(\Gamma; x) = (|A|/k)^{k|\Gamma|} k^{|\Gamma|} (1-z)^{|\mathbb{E}\Gamma|}$  and so  $Z(\Gamma''; x) = Z(\Gamma; x)$  for an edge of size  $z$ , since then  $|\mathbb{V}\Gamma''| = |\mathbb{V}\Gamma| - (z-1)$  and  $|\mathbb{E}\Gamma''| = |\mathbb{E}\Gamma| - 1$ .  $\blacksquare$

We mention two corollaries to the theorem, before giving partial results concerning edges of size greater than  $z$ .

COROLLARY 1: For  $c \neq 0$ , if  $Z(\Delta; y) = dZ(\Delta'_e; y) + cZ(\Delta''_e; y)$  for all hypergraphs  $\Delta$  and all edges  $e$  of size  $z$ , then  $Z(\Delta; y) = dZ(\Delta'_e; y) + ck^{w-z}Z(\Delta''_e; y)$  for all edges  $e$  of size  $w \leq z$ , for some integer  $k$  dividing  $|A|$ .

Proof. Direct from the proof of the theorem.  $\blacksquare$

COROLLARY 2: If an interaction model has the additive property with the same coefficients for edges of two different sizes then the model is resonant, if  $c \neq 0$ .

Proof. If the two sizes concerned are  $z$  and  $w$ , then from corollary 1 we have  $c = ck^{w-z}$ , which implies  $k = 1$  as required.  $\blacksquare$

The above corollary indicates why the additive property in graphs for edges which may be loops is restrictive. Note that if  $c = 0$  in the statement of the theorem we can deduce (from consideration of the hypergraph diagrammed in figure 1) that

$y(z; a_1, \dots, a_z) = d \forall a_1, \dots, a_z \in A$  but we can obtain no information at all about edges of other sizes.

In the following two theorems we use the hypothesis of theorem 1, which we have seen implies that there is a partition of  $A$  into equal-sized subsets, with a certain property; this is implicitly assumed in their statements.

THEOREM 2: Given that  $c \neq 0$ ,  $z > 1$ , and  $Z(\Delta; y) = dZ(\Delta'; y) + cZ(\Delta''; y)$  for all hypergraphs and all edges of size  $z$ , then for all values of  $w$ , if  $a_1, \dots, a_w$  are in the same subset  $A_i$  we have  $y(w; a_1, \dots, a_w) = d + ck^{1-z}$ .

Proof. Form a hypergraph consisting of  $w$  vertices and  $w-1$  edges of size 2 which make a tree; add  $r$  edges of size  $w$ , containing these vertices, all in the same order (see figure 8 below).

Transform  $y$  to  $x$  as before; the partition function then equals  $k^{(1-z)(w-1)} \sum_{a_1, \dots, a_w \in A_i} x(w; a_1, \dots, a_w)^r$  since if there are two

$a_j$ s in different subsets there must be two such representing adjacent vertices, which means that the factor provided by the edge between them is zero. However, if we contract all the edges of size 2 we obtain a hypergraph with  $r$  edges containing just one vertex, and so the above expression equals  $k^{(2-z)(w-1)} |A| k^{(1-z)r}$ , using corollary 1. Now we note that there are  $|A| k^{w-1}$  terms in the sum which must total  $|A| k^{(2-z)(w-1) + (1-z)r - (1-z)(w-1)} = |A| k^{w-1 + (1-z)r}$ , so by lemma 1 of section 4.2 we must have  $x(w; a_1, \dots, a_w) = k^{1-z}$  for all  $a_1, \dots, a_w$  in the same subset. Lastly transform back from  $x$  to  $y$  for the result.  $\blacksquare$

THEOREM 3: Given that  $c \neq 0$ ,  $z > 1$ , and  $Z(\Delta; y) = dZ(\Delta'; y) + cZ(\Delta''; y)$  for all hypergraphs and all edges of size  $z$ , then for all values of  $w$ , if  $a_1, \dots, a_w$  are in  $t$  different subsets  $A_i$  with  $1 < t \leq z$  we

have  $y(w; a_1, \dots, a_w) = d$ .

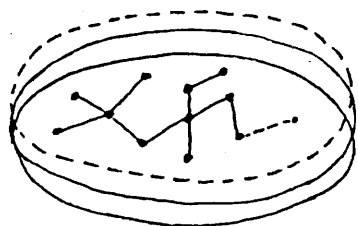


fig. 8

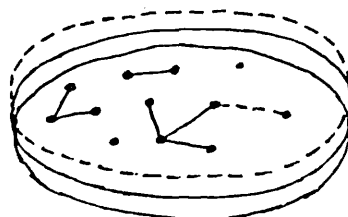


fig. 9

Proof. We have already shown this in theorem 1 for  $w \leq z$ ; if  $w > z$  then consider the hypergraph on  $w$  vertices with  $w-z$  edges of size 2 forming a forest, plus  $r$  edges containing all  $w$  vertices in the same order (see figure 9 above). Transform  $y$  to  $x$  as usual, and relate the partition functions for the hypergraph as it stands and after all the edges of size 2 have been contracted, to obtain  $k^{(1-z)(w-z)} \sum x(w; a_1, \dots, a_w)^r = k^{(2-z)(w-z)} |A| k^{z-1} k^{(1-z)r}$ , where the summation is over all  $a_1, \dots, a_w$  not lying in more than  $z$  subsets, since all other terms will be zero (as in theorem 2). So we infer  $\sum x(w; a_1, \dots, a_w)^r = |A| k^{w-1+(1-z)r}$ ; but this equals the sum in the last theorem, when  $a_1, \dots, a_w$  all lay in one subset; therefore terms in the sum corresponding to  $a_1, \dots, a_w$  in  $t$  different subsets (with  $1 < t \leq z$ ) must all be zero, using lemma 1 of section 4.2. By choosing different forests to start our hypergraph with we can demonstrate that whichever of the  $a_j$ s are in the same subsets the corresponding  $x(w; a_1, \dots, a_w)$  will be zero unless they are all in one subset. Finally, transform back from  $y$  to  $x$  to obtain the result.  $\blacksquare$

We cannot in general say any more than this because if we wish to be able to contract edges of sizes less than or equal to  $z$  in order to reduce the sizes of other edges, this will in fact necessitate certain of the vertices having images under  $\omega$  in the same subset, to contribute nonzero terms.

The definition of an interaction model on a hypergraph used here is the straightforward generalization of that for a graph, and is effectively (apart from the absence of symmetry as a prerequisite) the same as that used by Grimmett [13], except that he utilises cliques in a graph instead of edges of sizes greater than two in a hypergraph.

#### 4.4 The rank polynomial for hypergraphs

Any graph function with the additive property for every edge that is not a loop can be expressed, as in [24], as a sort of rank polynomial; and conversely. We can obtain corresponding results for hypergraphs.

LEMMA 1: If  $Z(\Gamma; y) = dZ(\Gamma'; y) + cZ(\Gamma''; y)$  for all hypergraphs and all edges of size  $z$ , then, writing  $R_\Delta$  for the rank of the hypergraph  $\Delta$ ,  $Z(\Gamma; y) = d^{|E\Gamma|} |A|^{|\Gamma|} \sum_{\Delta \in \Gamma} (ck^{1-z}/d)^{|E\Delta|} (k/|A|)^{R_\Delta}$ .

Proof. From lemma 1 of section 4.3, and using the usual relation between  $y$  and  $x$ ,  $Z(\Gamma; y) = d^{|E\Gamma|} \sum_{\Delta \in \Gamma} (c/d)^{|E\Delta|} Z(\Delta; x)$ ; but  $Z(\Delta; x) = k^{(1-z)|E\Delta|} |A|^{k\Delta} |V\Delta|^{-k\Delta}$ , so the result follows. Note that the result holds even for  $d=0$  if we agree to rewrite the expression with  $d^{|E\Gamma| - |E\Delta|}$  inside the summation.  $\blacksquare$

LEMMA 2: If  $Z(\Gamma; y) = f^{|E\Gamma|} g^{|\Gamma|} \sum_{\Delta \in \Gamma} h^{|E\Delta|} j^{R_\Delta}$  then  $Z(\Gamma; y) = fZ(\Gamma'; y) + (gj)^{|e| - 1} fhZ(\Gamma''; y)$ .

Proof. We may split the summation into two, according as the edge  $e$  is or is not in the subhypergraph  $\Delta$ ; then  $Z(\Gamma; y) = f^{|E\Gamma| + 1} g^{|\Gamma|} \sum_{\Delta \in \Gamma'} h^{|E\Delta|} j^{R_\Delta} + f^{|E\Gamma''| + 1} g^{|\Gamma''| + |e| - 1} \sum_{\Delta \in \Gamma''} h^{|E\Delta| + 1} j^{R_\Delta + |e| - 1} = fZ(\Gamma'; y) + (gj)^{|e| - 1} fhZ(\Gamma''; y)$ .  $\blacksquare$

In the above, lemma 1 applies to hypergraphs with no edge of size greater than  $z$ , and we may restrict both the condition and the conclusion of lemma 2 similarly. Combining these two and an earlier theorem results in the following.

THEOREM 1: The following conditions are equivalent for an interaction model on hypergraphs: (i) it is weakly resonant

to size  $z$ ; (ii) it has the additive property for edges of sizes greater than 0 and not greater than  $z$ ; (iii) it is expressible as a sort of rank polynomial (as in lemma 2) on hypergraphs with no edge of size greater than  $z$ .

Proof. Conditions (i) and (ii) are equivalent by theorem 1 of section 4.3; if  $c=0$  in condition (ii) then the comment after corollary 2 of that section implies (i) since the additive property exists for all sizes of edges up to  $z$ . Condition (ii) implies (iii) by lemma 1, with the case  $c=0$  easily being true. Finally, condition (iii) implies (i) by lemma 2.  $\blacksquare$

## CHAPTER 5

### AVITOIDS; FUNCTIONS AND DUALS

Section 5.1 Diagramming by hypergraphs

Section 5.2 The rank function for avitoids

Section 5.3 The dual function

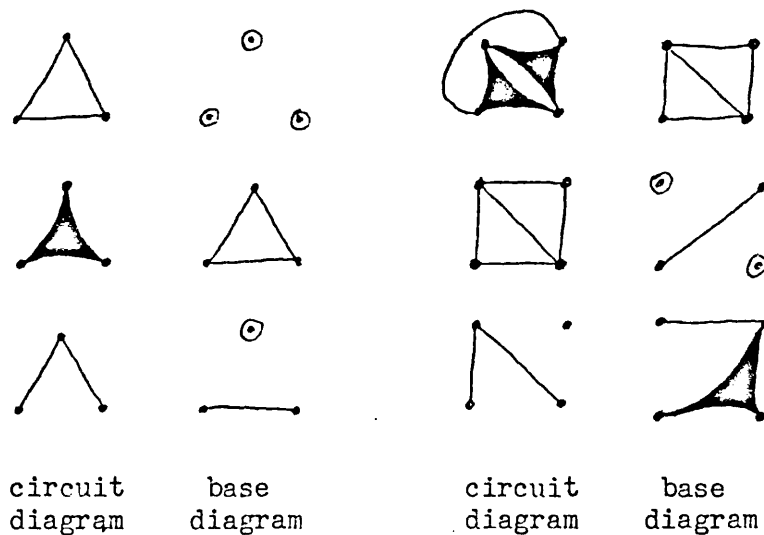
In this chapter we pursue the idea of avitoids introduced in section 3.4, and see how far some results on rank polynomials for graphs can be generalized to these structures, particularly those relating to duality.

## 5.1 Diagramming by hypergraphs

It is helpful to diagram avitoids using hypergraphs so that each (isomorphism class of) avitoid is represented by a unique (isomorphism class of) hypergraph. There are two simple ways of doing this: we represent elements of the avitoid by vertices of a hypergraph and then allow a hyperedge whenever the relevant vertices represent elements forming a circuit, or alternatively a base. We call these the circuit diagram and base diagram respectively of the avitoid. The interpretation of a null hypergraph will differ in the two cases, representing no circuits in the former and the empty base in the latter.

The circuit diagram is usually more helpful; we find that an avitoid is nonseparable if and only if its circuit diagram is connected. Also, when we delete an element from an avitoid we simply delete the corresponding vertex from the circuit diagram; this makes the identifying of subavitoids straightforward. Both of these facts follow immediately from the definitions.

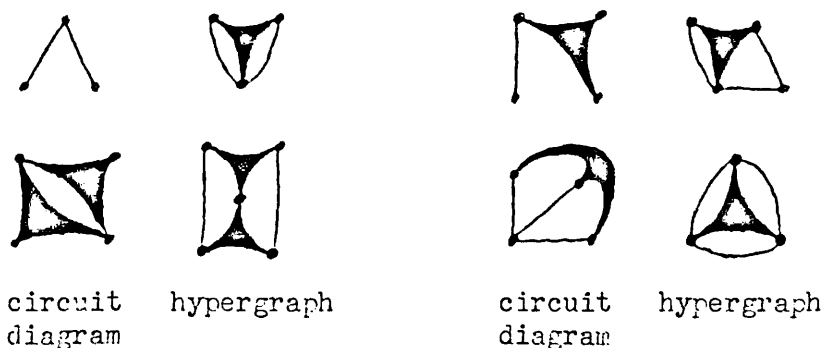
From the definitions of circuits and bases we see that the diagramming hypergraphs of avitoids must be elementary. Conversely, every elementary hypergraph will be a diagram of either type. We list a few avitoid diagrams below.





When we take the dual of an avitoid it is clearly easier to work with the base diagram, for then each new hyperedge is just the complement of the corresponding old one. When we delete an element the base diagram is modified as follows: we remove the associated vertex, and any hyperedges that contained it are diminished by that vertex. This may result in a non-elementary hypergraph, though, and we resolve this by deleting all edges properly contained in others, and deleting all but one of a family of equal edges. Contraction of an element is superficially similar: we again remove the associated vertex and diminish any hyperedges that contained it. If we now have a non-elementary hypergraph we delete all edges properly containing others, and all but one of a family of equal edges. We must momentarily remember that diminishing a hyperedge of size  $l$  will result in a hyperedge of size  $0$ , which will be contained in all other hyperedges.

We can also use hypergraphs as examples of avitoids, with circuits being defined in a way that is nonstandard, but uses the same basic idea. For a hypergraph we define a circuit as a minimal (by inclusion) set of edges  $\{e_1, \dots, e_c\}$  such that  $c=1$  and  $e_1$  is a loop, or  $c > 1$  and there are distinct vertices  $v_1, \dots, v_c$  such that  $e_1 \ni v_1 \in e_2 \ni v_2 \in \dots \in e_c \ni v_c \in e_1$ . Then some avitoids that cannot be realized as graphs may be as hypergraphs, as shown below. However, we cannot provide examples of all avitoids in this way; for instance, the avitoid whose only circuits are  $\{a, b, c, d\}$  and  $\{a, b, c, e\}$  is not realizable.



## 5.2 The rank function for avitoids

In this section we present a rank function for avitoids, preserving as far as possible the properties that hold for graphs (and, more generally, for matroids). The main problem lies in defining the rank of an avitoid usefully, since an avitoid may have bases of different sizes.

The rank of an avitoid is defined as the size of its smallest bases. Following from that definition, we let the rank function  $H(\Gamma; a, b)$ , or simply  $H(\Gamma)$ , of an avitoid  $\Gamma$  equal  $\sum_{\Delta \in \Gamma} a^{|\mathcal{E}\Delta|} b^{R\Delta}$  where  $R\Delta$  is the rank of  $\Delta$ . The cycle number will be defined as  $C\Gamma = |\mathcal{E}\Gamma| - R\Gamma$ , and the chromatic function will be  $H(\Gamma; -1, 1/n)$ .

We introduce two more notions before proceeding. An element  $e$  of an avitoid  $\Gamma$  will be said to commute if  $\Gamma_{eA}^{\prime\prime} = \Gamma_{Ae}^{\prime\prime} \forall A \in \mathcal{E}\Gamma \setminus \{e\}$ ; and an element  $e$  is regular if it occurs in a smallest base of  $\Gamma_A \forall A \in \mathcal{E}\Gamma \setminus \{e\}$ .

LEMMA 1: If  $e$  is in a smallest base of  $\Delta$  then  $R\Delta_e^{\prime\prime} = R\Delta - 1$ .

Proof. The set of bases for  $\Delta_e^{\prime\prime}$  includes those bases of  $\Delta$  that contain  $e$ , less it; therefore on contracting  $e$  some smallest base of  $\Delta$  diminishes in size by one element and since no base can decrease by more than this it is still a smallest base.  $\blacksquare$

THEOREM 1: If  $e \in \mathcal{E}\Gamma$  is regular and commutes, then the rank function satisfies  $H(\Gamma) = H(\Gamma_e^{\prime\prime}) + ab H(\Gamma_e^{\prime\prime\prime})$ .

Proof. Write  $h(\Delta) = a^{|\mathcal{E}\Delta|} b^{R\Delta}$ ; then  $H(\Gamma) = \sum_{\Delta \in \Gamma} h(\Delta)$  and from lemma 1 we have  $h(\Delta) = ab h(\Delta_e^{\prime\prime})$  if  $e \in \mathcal{E}\Delta$  since  $e$  is regular. We may put  $H(\Gamma) = \sum_{A \in \mathcal{E}\Gamma} h(\Gamma_A^{\prime\prime})$  and then split the summation according as

$e$  is or is not contained in  $A$ ; then expressing the summations

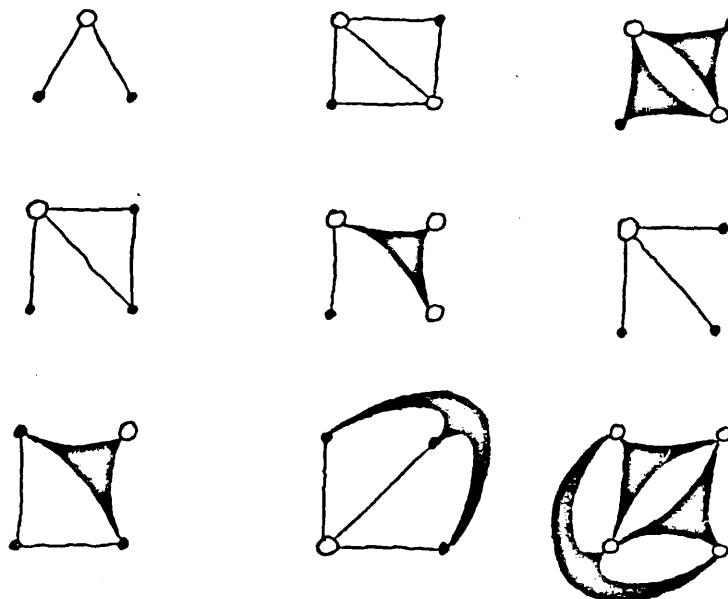
differently gives  $H(\Gamma) = \sum_{B \in E\Gamma'_e} h(\Gamma'_{eB}) + \sum_{D \in E\Gamma''_e} h(\Gamma'_D)$ , which equals

$H(\Gamma'_e) + \sum_{D \in E\Gamma''_e} ab h(\Gamma''_{De})$  by the above. Now, since  $e$  commutes, the

(remaining) summation equals  $ab \sum_{D \in E\Gamma''_e} h(\Gamma''_{De}) = ab H(\Gamma''_e)$ ; therefore

$H(\Gamma) = H(\Gamma'_e) + ab H(\Gamma''_e)$ , as required.  $\blacksquare$

The definitions of rank, commuting and regularity are made to generalize as much as possible the results for graphs. In graphs, or more generally matroids, every element that is not a loop is regular, so the prohibition of non-regular elements is necessary there too. Below we show the circuit diagrams of some aroids that are not matroids with elements that are regular and commute being denoted by white rather than black vertices; it is only for the last of these that all the vertices possess this property.



### 5.3 The dual function

In this section we investigate the function dual to a given one; we define the dual function as  $F^*(\Gamma) = F(\Gamma^*)$ , and can establish a relationship in terms of the summation expression.

**THEOREM 1:** If  $F(\Gamma) = \sum_{\Delta \subseteq \Gamma} f(\Delta)$  then the dual function satisfies  $F^*(\Gamma) = \sum_{\Delta \subseteq \Gamma} f^*(\Delta)$  where  $f^*(\Delta) = \sum_{\substack{A, B \subseteq E\Delta \\ \text{st. } A \wedge B = \emptyset}} (-1)^{|A|} f(\Delta_{AB}^{**})$ .

**Proof.** Note that we are writing  $f^*(\Delta)$  for notational convenience, and that it is not defined as  $f(\Delta^*)$ ; that is only for the capital letter functions. Now, the relation  $F^*(\Gamma) = \sum_{\Delta \subseteq \Gamma} f^*(\Delta) = \sum_{A \subseteq E\Gamma} f^*(\Gamma_A')$  has the simple inversion formula  $f^*(\Gamma) = \sum_{A \subseteq E\Gamma} (-1)^{|A|} F^*(\Gamma_A')$ . Therefore  $f^*(\Delta) = \sum_{A \subseteq E\Delta} (-1)^{|A|} F(\Delta_A^{**}) = \sum_{\substack{A \subseteq E\Delta \\ B \subseteq E\Delta^{**} \\ A \wedge B = \emptyset}} (-1)^{|A|} f(\Delta_{AB}^{**})$ , and when the summation

conditions are rewritten this is the desired result.  $\blacksquare$

For graphs, it is known that the flow polynomial is just a multiple of the dual function of the chromatic polynomial, and both are evaluations of the rank polynomial (see, for instance, Biggs [3]). We may pursue this relationship for avitoids in general; firstly we do so for matroids.

**LEMMA 1:** For a matroid,  $CA_A' + CA_{A^*B}' = |E\Delta| - |A| - |B| + CA_{E\Delta \setminus B}'$  when  $A \wedge B = \emptyset$ .

**Proof.** Firstly, note that  $CA_A' = CA_{AB}^{**} + CA_{E\Delta \setminus B}'$  because when we start with the matroid  $\Delta_A'$  and contract the elements of B one by one we leave the cycle number unchanged except when we contract a loop, which decreases the cycle number by 1; so the total number

of times we have to contract a loop is simply the cycle number of the submatroid induced by the elements of B, that is, the matroid  $\Delta'_{E\Delta \setminus B}$ . Using this,  $C\Delta'_A + C\Delta'_{A^*B} = C\Delta'_{AB} + C\Delta'_{E\Delta \setminus B} + C\Delta'_{AB} = |E\Delta'_{AB}| + C\Delta'_{E\Delta \setminus B}$ , because the sum of the cycle numbers of a matroid and its dual is the number of elements; and now expanding  $|E\Delta'_{AB}|$  yields the result.  $\blacksquare$

THEOREM 2: If  $F(\Gamma) = \sum_{\Delta \in \Gamma} f(\Delta)$  where  $f(\Delta) = a^{|E\Delta|} b^{R\Delta}$ , and  $G(\Gamma) = a^{-|E\Gamma|} b^{-C\Gamma} F(\Gamma^*)$ , then  $G(\Gamma) = \sum_{\Delta \in \Gamma} g(\Delta)$  where  $g(\Delta) = a^{-|E\Delta|} b^{-C\Delta}$ .

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matroids

Proof. By simple inversion  $g(\Delta) = \sum_{A \subseteq E\Delta} (-1)^{|A|} G(\Delta'_A) = \sum_{A \subseteq E\Delta} (-1)^{|A|} a^{-|E\Delta'_A|} b^{-C\Delta'_A} F(\Delta'_A)$ , and replacing  $F(\Delta'_A)$  with  $\sum_{B \subseteq E\Delta \setminus A} a^{|E\Delta'_{AB}|} b^{R\Delta'_{AB}}$  and rearranging the summation gives  $g(\Delta) = \sum_{A, B \subseteq E} (-1)^{|A|} a^{|E\Delta'_{AB}| - |E\Delta'_A|} b^{R\Delta'_{AB} - C\Delta'_A}$  which, by the lemma, is equal to  $\sum_{\substack{A, B \subseteq E \\ \text{st. } A \cap B = \emptyset}} (-1)^{|A|} a^{-|B|} b^{-C\Delta'_{E\Delta \setminus B}}$ . Now we sum over  $A \subseteq E\Delta \setminus B$

and the only nonzero contribution occurs when  $E\Delta \setminus B = \emptyset$ ; hence  $g(\Delta) = a^{-|E\Delta|} b^{-C\Delta}$ .  $\blacksquare$

We would like to know if a similar property holds for some class of avitoids other than matroids; however, the following theorem shows that this does not happen.

THEOREM 3: If  $a^{|E\Gamma|} b^{C\Gamma} \sum_{\Delta \in \Gamma} a^{-|E\Delta|} b^{-C\Delta} = \sum_{\Delta \in \Gamma^*} a^{|E\Delta|} b^{R\Delta}$  for an avitoid  $\Gamma$  and all  $a, b$  then  $\Gamma$  is a matroid.

Proof. Since the equation holds for all  $a, b$  we may compare coefficients in the two expressions. We do so firstly by the powers of  $a$ .

Note that  $\Delta = \Gamma$  in the summation on the left-hand side of the equation corresponds to  $\Delta = \emptyset$  on the right-hand side, both

providing the only constant, 1. For the terms arising from  $\Delta = \emptyset$  and  $\Lambda = \Gamma^*$ , the only ones concerning  $a^{|\Sigma\Gamma|}$ , to be equal we need  $b^{C\Gamma} = b^{R\Gamma^*}$ , that is,  $|\Sigma\Gamma| - R\Gamma = R\Gamma^*$ . The only way for this to happen is for  $\Gamma$  to have all its bases the same size.

Next, since both sides of the equation in the statement of the theorem are multiplicative, we need only verify the result for nonseparable  $\Gamma$ . In such cases the terms with  $a^{|\Sigma\Gamma|-1}$ , resulting from  $\Delta$  comprising a single element, sum to  $|\Sigma\Gamma| a^{|\Sigma\Gamma|-1} b^{C\Gamma}$  on the left-hand side and so for equality we require  $R\Gamma_e^* = R\Gamma \forall e$ .

Similarly, comparing the coefficients of  $a^1$  gives  $|\Sigma\Gamma^*| ab$  on the right-hand side and so we need  $C\Gamma_e^* = C\Gamma - 1 \forall e$ , that is,

$$R\Gamma_e^* = R\Gamma \forall e.$$

Also

$$R\Gamma^* = R\Gamma_e^* (ve)$$

Restating the above information in terms of bases, we see that any base less an element must be contained in another base, and that any base plus a new element must contain another base.

Now we examine the two sums term by term, letting  $\Lambda \subseteq \Gamma^*$  correspond to that  $\Delta \subseteq \Gamma$  such that  $\Delta = \Gamma_{EA}^*$ ; the contribution to the right-hand side will be  $a^{|\Sigma\Lambda|} b^{R\Lambda}$ . Now suppose, inductively, that deleting from  $\Gamma$  a set of size less than  $|\Sigma\Lambda|$  of elements that is independent in  $\Gamma^*$  does not change the rank. Accordingly we delete from  $\Gamma$  a base, say  $B$ , of  $\Lambda$ ; then  $R\Gamma_B^* = R\Gamma$ . Next observe that for any element  $x \in E\Lambda \setminus B$  there is a subset  $C \subseteq B$  such that  $C \cup \{x\}$  is a circuit, because  $B$  is a base; but, by a property relating bases of  $\Gamma$  to circuits of  $\Gamma^*$ , this means that every base of  $\Gamma$  contains at least one member of  $C \cup \{x\}$ ; and since the remaining bases, of  $\Gamma_B^*$ , cannot contain any elements of  $C$ , we deduce that every remaining base contains  $x$ , and this holds for all  $x \in E\Lambda \setminus B$ . Consequently, when we delete all the elements of  $E\Lambda$  we reduce the rank by  $|\Sigma\Lambda \setminus B|$ ; note that this is true for any base  $B$ , so we have incidentally

established that all bases of  $\Lambda$  have the same size, but all that we shall use is that  $R\Gamma'_{E\Lambda} = R\Gamma - C\Lambda$  since every base  $B$  is a smallest base. Hence  $C\Gamma'_{E\Lambda} = C\Gamma - R\Lambda$  and so the contribution to the left-hand side is  $a^{|\Gamma| - (|\Gamma| - |E\Lambda|)} b^{C\Gamma - (C\Gamma - R\Lambda)} = a^{|E\Lambda|} b^{R\Lambda}$ .

The only problem remaining is if the set  $E\Lambda$  is independent in  $\Gamma^*$ , when we might obtain  $R\Gamma'_{E\Lambda} < R\Gamma$ . In order to ensure that this does not happen we must place further restrictions on the bases of the avitoid. Accordingly, suppose that we are given bases  $B_1, B_2$  with  $x \in B_1 \setminus B_2$ , and look at the set  $D$  defined as  $\{d \in E\Gamma \mid (B_1 \setminus x) \cup d \text{ is a base of } \Gamma\}$ ; we have already seen that this must have size at least 2. Deleting  $D$  from  $\Gamma$  will certainly reduce the rank by at least 1, so we must insist that  $D$  be a dependent set in  $\Gamma^*$ ; that is,  $D$  contains a circuit in  $\Gamma^*$ , which implies that at least one element of  $D$  occurs in any base of  $\Gamma$ . However,  $B_2$  does not contain  $x$  so it must contain another element, say  $y$ , of  $D$ ; and then  $y \in B_2 \setminus B_1$ , and  $(B_1 \setminus x) \cup y$  is a base, which satisfies one way of stating the additional axiom which converts an avitoid into a matroid.

To recap the argument: it is necessary to have the inductive hypothesis that deleting a set of elements independent in  $\Gamma^*$  does not change the rank in  $\Gamma$ ; we showed that this was necessary for one-element sets, and that it was inductively necessary for sets of increasing sizes. In the above paragraph, though, we have established that this requirement for all sizes implies that the avitoid be in fact a matroid.  $\blacksquare$

If we write  $\tilde{H}(\Gamma) = \tilde{H}(\Gamma; a, b) = a^{|\Gamma|} b^{C\Gamma} \sum_{\Delta \in \Gamma} a^{-|\Delta|} b^{-C\Delta}$  then the results of theorems 2 and 3 state that  $\tilde{H}(\Gamma) = H(\Gamma^*) \quad \forall a, b$  if and only if  $\Gamma$  is a matroid.

Nagle, in [17], showed how the chromatic polynomial of a graph could be expressed as a suitably adjusted sum of the flow polynomials of its subgraphs (although he did not remark that his weight function was virtually the flow polynomial). This can be generalized to our formulation for avitoids.

$$\text{THEOREM 4: } H(\Gamma) = (1 - a^2b)^{|\Gamma|} \sum_{\Delta \subseteq \Gamma} \tilde{H}(\Delta) a^{|\Delta|} b^{R\Delta} (1 - a^2b)^{-|\Delta|}.$$

Proof. On expanding  $\tilde{H}(\Delta)$  the right-hand side equals

$$\begin{aligned} & \sum_{\Delta \subseteq \Gamma} \sum_{\Lambda \subseteq \Delta} a^{|\Delta|} b^{R\Delta} (1 - a^2b)^{|\Gamma| - |\Delta|} a^{|\Delta|} b^{C\Delta} - |\Delta| b^{-C\Delta} = \\ & \sum_{\Lambda \subseteq \Gamma} a^{|\Lambda|} b^{R\Lambda} \sum_{\substack{\Delta \subseteq \Gamma \\ \Delta \supseteq \Lambda}} (a^2b)^{|\Delta| - |\Lambda|} (1 - a^2b)^{|\Gamma| - |\Delta|} = \sum_{\Lambda \subseteq \Gamma} a^{|\Lambda|} b^{R\Lambda}, \end{aligned}$$

which equals  $H(\Gamma)$ , as required.  $\blacksquare$



## CHAPTER 6

### MOLECULES; EVALUATION OF THE MATRICES

Section 6.1 The formulae

Section 6.2 General results

Section 6.3 Practical evaluation

This chapter follows through the properties of molecules as defined in section 3.5. The evaluation of the  $B^{-1}$  matrix needed in chapter 2 is investigated in a general setting for which the basic results hold even though we may not have molecules that represent graph types.

## 6.1 The formulae

The procedure described by Biggs [3] using results by Tutte [22] makes it evident that we can evaluate the B-matrix of chapter 2 simply by knowing the (numbers of) nonseparable graphs contained in a given graph, without any structural information on how these may fit together. All that we need is the entries in the N-matrix for nonseparable graphs to generate B recursively; this is precisely what allows us to apply these results to the graph reconstruction problem as Tutte [25] noted, since the set of subgraphs we are provided with in the problem contains more than enough information for this method. However, we do not need to go to the length of deriving the successive  $q$  (or even  $\log q$ ) functions by manipulating previous ones; the process we shall describe, in the more general setting of molecules, for determining the B-matrix and the consequent M-matrix is much simpler.

The operation is as follows: given the N-matrix for atoms we extend it to cover molecules as described in section 3.5. We then progressively define, for increasing  $m$ , the entries of B and M by:

$$M_{m,n} = (N_{m,n} - \sum_{r < m} B_{m,r} M_{r,n}) / B_{m,m} \text{ for } m < n; M_{m,m} = 1; M_{m,n} = 0 \text{ for } m > n;$$

$$B_{m,n} = N_{m,n} - \sum_{r < n} B_{m,r} M_{r,n} \text{ for } m \geq n; B_{m,n} = 0 \text{ for } m < n.$$

The fact that this is well-defined (i.e. that  $B_{m,m}$  is never zero) will be established in the next section, but for the time being we just note the following result.

**THEOREM 1:** If the atoms correspond to nonseparable graph types and the N matrix is as in chapter 2 then the B and M matrices are as defined there, if the weight function is the atomic number.

**Proof.** If the atoms do represent graph types then the B and M matrices exist, are lower and upper triangular matrices

respectively and  $M$  has 1's along the diagonal, all by definition; so the entries of both must be determined by the above relations since  $N = BM$ .     ■

The fact that we can generalize graph types to regular clusterings leads to other elementary results. Given a regular clustering we can represent all isomorphic sub-clusterings by the same molecule; where, in the obvious way, two subsets of a clustering are isomorphic if there is a correspondence between elements which preserves 'clusterhood'. We might also distinguish some isomorphic subsets if necessary, as we suggested in section 3.5.

**THEOREM 2:** If the atoms correspond to types of isomorphic clusters and the  $N$  matrix is derived as before, then the  $B$  and  $M$  matrices have the same meanings as for graphs. In particular,  $B$  and  $M$  are integral and nonnegative, and the columns of  $M$  sum to powers of 2, providing the weight function equals the atomic number.

**Proof.** This is trivial because  $B$  and  $M$  retain their meanings in the generalization to regular clusterings.     ■

In fact we can be less strict about the weight function and still obtain the above result. However, by other choices of the weight function we can produce negative entries in  $B$  and  $M$ , and stop columns of  $M$  summing to powers of 2. In the next section we investigate whether the integrality of the coefficients of  $M$  is maintained in the generalization to molecules.

## 6.2 General results

We commence this section by noting the values of the entries that we would derive for the B and M matrices using the procedure of the previous section if we started with a general N matrix, not necessarily one derived as in section 3.5. We shall, for the time being, use numerals as subscripts, and view the derivations as formal expressions. To shorten the expressions considerably, we shall use the notation  $|u,v w,x y,z|$  to mean the determinant of the submatrix of N with rows indexed by u,w and y and columns by v,x and z, in that order; and so on for determinants of other sizes. Thus, for instance,  $|1,2 2,4| = \begin{vmatrix} N_{1,2} & N_{1,4} \\ N_{2,2} & N_{2,4} \end{vmatrix}$ .

LEMMA 1: Deriving the B and M matrices from a general N gives

$$B_{i,j} = |1,1 2,2 \dots j-1,j-1 i,j| / |1,1 2,2 \dots j-1,j-1| \text{ and}$$

$$M_{j,k} = |1,1 2,2 \dots j-1,j-1 j,k| / |1,1 2,2 \dots j-1,j-1 j,j|.$$

Proof. Note, incidentally, that the above expressions subsume the zero values for  $B_{i,j}$  when  $i < j$  and  $M_{j,k}$  when  $j > k$ , and the unit value for  $M_{k,k}$ . Now, following the procedure for deriving the B and M matrices we obtain a unique expression for every term; therefore it is sufficient to verify that the values given satisfy  $N = BM$ . The resulting expressions are in effect the expansions of Schweins for quotients of determinants, as presented by Aitken [1].

Mimicking the proof used by Aitken, we write  $B_{i,j} M_{j,k} = (|1,1 \dots i,j| / |1,1 \dots j-1,j-1|) (|1,1 \dots j,k| / |1,1 \dots j,j|) = |1,1 2,2 \dots j-1,j-1 i,k| / |1,1 2,2 \dots j-1,j-1| - |1,1 2,2 \dots j-1,j-1 j,j i,k| / |1,1 2,2 \dots j-1,j-1 j,j|$ , because this equation is the extensional of the identity  $(|i,j|/1)(|j,k|/|j,j|) = |i,k|/1 - |j,j i,k|/|j,j|$ .

The expression we now have for  $B_{i,j}M_{j,k}$  holds as we have written it for  $j \leq i, k$ . When  $j=1$  we interpret the empty determinant as having the value 1, and the expression becomes  $B_{i,1}M_{1,k} = N_{i,k}/1 - \begin{vmatrix} N_{1,1} & N_{1,k} \\ N_{i,1} & N_{i,k} \end{vmatrix} / N_{1,1}$ ; when  $j$  equals  $i$  or  $k$  the last row or column (respectively) of the numerator of the second term in the expression is a repetition of the previous row or column. Hence on writing out  $\sum_{j \leq i, k} B_{i,j}M_{j,k}$  the terms cancel out in pairs except for the first, which is  $N_{i,k}$ , and the last, which equals 0. Thus the answers as given are the correct ones.  $\blacksquare$

Before proving the main result of this section we need one more lemma, for which we prepare with some terminology and notation. We shall consider polynomials in several variables  $x_1, x_2, \dots, x_d$  and denote the point in  $d$ -dimensional space with corresponding co-ordinates by  $x$ . We shall call a set  $S$  of points with non-negative integral co-ordinates star-shaped if  $\forall s \in S, 0 \leq r \leq s \Rightarrow r \in S$ , where ' $\leq$ ' has the usual meaning for vectors (i.e. that every co-ordinate must be less than or equal to the corresponding one). We shall write  $e_i$  for the point with  $i$ th co-ordinate 1 and all others 0.

The lemma is a simple consequence of a standard result in the calculus of finite differences, as for example stated by Fort [12]. We shall extend the notation slightly: given a function  $f$ , or just its values at suitable points, we define  $\Delta_{e_i}(x) = f(x+e_i) - f(x)$ . Then  $\Delta_{e_i e_j}(x) = f(x+e_i+e_j) - f(x+e_i) - f(x+e_j) + f(x) = \Delta_{e_j e_i}(x)$ , so that we may define  $\Delta_y(x)$  uniquely in the obvious way.

LEMMA 2: Given integral values on a star-shaped set of points  $S$

there is a unique polynomial with terms just in  $\prod_{i=1}^d x_i^{s_i}$  for  $s \in S$  that fits them; and this is always integer-valued for integral arguments.

Proof. Since  $S$  is star-shaped we can evaluate  $\Delta_s(0)$  for all  $s \in S$  and then assume that  $\Delta_r(0) = 0$  for all  $r \notin S$ . This leads to the expression  $\sum_{s \in S} \Delta_s(0) \prod_{i=1}^d x_i^{(s_i)} / s_i!$  for the unique polynomial of required degree, where  $x_i^{(s_i)}$  represents the 'falling factorial'  $x_i(x_i-1)\dots(x_i-s_i+1)$ . The details of this assertion are straightforward generalizations of the standard result.

However, we may derive the value at any desired point with non-negative integral co-ordinates as follows. Given such a point  $t \notin S$ , the equation  $\Delta_t(0) = 0$  expresses the value at  $t$  as an integral combination of the values at the points  $r$  with  $0 \leq r < t$ ; so that if we have already discovered these values in the same way (or from the original data if  $r \in S$ ) we know that the value at  $t$  must be integral. A suitable order for determining the values at points  $r < t$  would be their 'lexicographical' order when written out as vectors. ■

As an example, if we had to find a polynomial  $f(x,y)$  with terms in  $1, x, x^2, y$  and  $xy$  and satisfying  $f(0,0) = -1$ ,  $f(1,0) = 1$ ,  $f(2,0) = 4$ ,  $f(0,1) = 2$  and  $f(1,1) = 5$  we could derive the polynomial  $3y + \frac{1}{2}x^2 + \frac{3}{2}x - 1 + xy$ ; alternatively, if we only wished to know the value  $f(3,2)$  then we could recursively evaluate  $f(0,2) = 5$ ,  $f(1,2) = 9$ ,  $f(2,1) = 9$ ,  $f(2,2) = 14$ ,  $f(3,0) = 8$ ,  $f(3,1) = 14$  and finally  $f(3,2) = 20$ .

We now proceed to the main theorem of this section, on molecules.

THEOREM 1: For any system of molecules,  $B_{n,n}$  is always nonzero and  $M_{m,n}$  is integral.

Proof. From lemma 1 we know that  $M_{m,n}$  is equal to  $|1,1 2,2 \dots j-1,j-1 j,k|/|1,1 2,2 \dots j-1,j-1 j,j|$  where  $m$  is the  $j$ th molecule and  $n$  the  $k$ th. The denominator of this is an integer which we shall inductively suppose to be nonzero, and the numerator may be taken to be an integral polynomial in variables corresponding to the various atoms involved so far. In this way we shall have a term in  $\prod_a (\sum_b n_b N_{a,b})^r$  for each molecule  $r \leq n$ , and each such is multiplied by an appropriate minor. In particular, the relevant minor for the term with  $r=n$  is nonzero by the inductive hypothesis.

Now, if we consider just the numerator we see that it is a polynomial which is zero for  $j$  sets of values, namely when  $n$  comprises all zeros or represents any of the first  $j-1$  molecules. If we now know the value taken when  $n$  represents the  $j$ th molecule then a unique polynomial with appropriate terms is determined, by lemma 2, since the data points form a star-shaped set. However, this last value cannot also be zero for then the polynomial would be identically zero, which cannot be the case because the  $j$ th term is multiplied by a nonzero minor. Therefore the last value, which is in fact the denominator of  $M_{m,n}$ , is nonzero.

So we have established that  $|1,1 2,2 \dots j,j| \neq 0$  and so the inductive step is proved, as is the fact that  $B_{n,n} \neq 0$ ; the start of the induction is provided by the observation that  $N_{1,1} = 1 \neq 0$ . Furthermore we have shown that  $M_{m,n}$  regarded as a polynomial has the value 0 at  $j$  points and 1 at another, which form a star-shaped region; therefore by lemma 2 again,  $M_{m,n}$  must be integral at any point with integral co-ordinates, i.e. for any  $n$ . ■

### 6.3 Practical evaluation

For practical purposes of evaluating chromatic polynomials, interaction partition functions and the like we need to find the coefficients of the matrix  $B^{-1}$ ; and for theoretical purposes of showing that the obvious definition of the 'thermodynamic limit' of a suitable sequence of graphs of increasing size (see Biggs [5]) provides a convergent infinite series we want to be able to place bounds on the coefficients. We first note that a determinantal expression exists for the inverse of the B-matrix, similar to those in lemma 1 of the last section.

**THEOREM 1:**  $B_{j,k}^{-1} = |1,1 \dots j-1,j-1 j,\hat{k}| / |1,1 \dots j-1,j-1 j,j|$  for  $j \geq k$  and 0 otherwise, where we define the extra column  $\hat{k}$  of  $N$  by  $N_{k,\hat{k}} = 1$  and  $N_{i,\hat{k}} = 0$  for  $i \neq k$ .

*Proof.* We proceed as in the lemma referred to by writing  $B_{i,j} B_{j,k}^{-1} = |1,1 \dots j-1,j-1 i,\hat{k}| / |1,1 \dots j-1,j-1 i,j| - |1,1 \dots j-1,j-1 j,j i,\hat{k}| / |1,1 \dots j-1,j-1 j,j|$ . When we sum this over all  $j$  such that  $k \leq j \leq i$  all the terms except two cancel in pairs; the minus term with  $j=i$  is also zero because the last two rows of the numerator are equal, and the plus term with  $j=k$  is also zero unless  $i=k$  too for otherwise the last column is all zeros. In this last case the numerator equals the denominator, so that  $\sum_j B_{i,j} B_{j,k}^{-1} = 1$  if and only if  $i=k$ ; hence what we have written as  $B^{-1}$  is genuinely the inverse of  $B$ .  $\blacksquare$

It is a straightforward matter to write a computer programme to determine the coefficients of the  $N$ ,  $B$ ,  $M$  and  $B^{-1}$  matrices, and in fact the nature of the procedure allows us to re-use the same storage locations for these as we proceed (which is very useful if we wish to deal with large matrices). If we only want to



find the coefficients of  $B^{-1}$  given the  $N$ -matrix we may proceed as follows, putting  $N$  augmented by  $I$  into echelon form (see, for instance, Jones [14]): we write the  $N$  matrix and extend its rows to twice their length with a copy of the identity matrix; then we subtract from each row multiples of previous rows only, to make the  $N$  matrix upper triangular; lastly we divide each row by a suitable factor to ensure that  $B$  has unit elements on its main diagonal. By this process we have turned  $N$  into an upper triangular matrix with units on the diagonal by (in effect) premultiplying by a lower triangular matrix, so this latter, a copy of which now resides in the place formerly occupied by  $I$ , must have been  $B^{-1}$ . We can also re-use computer memory locations during this method, as before.

This operation could also be carried through for general  $N$  matrices, as long as their nullities are zero. We give an example below of the process for a system of molecules that represents simple graphs with up to 3 edges.

$$\begin{array}{cccccccc}
 1 & 2 & 3 & 3 & 1 & 0 & 0 & 0 \\
 1 & 4 & 9 & 9 & 0 & 1 & 1 & 1 \\
 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
 1 & 8 & 27 & 27 & 0 & 0 & 0 & 1 \\
 \hline
 1 & 2 & 3 & 3 & 1 & 0 & 0 & 0 \\
 0 & 2 & 6 & 6 & -1 & 1 & 0 & 0 \\
 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
 0 & 0 & 6 & 6 & 2 & -3 & 0 & 1
 \end{array}
 \quad
 \begin{array}{cccccccc}
 1 & 2 & 3 & 3 & 1 & 0 & 0 & 0 \\
 0 & 2 & 6 & 6 & -1 & 1 & 0 & 0 \\
 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
 0 & 6 & 24 & 24 & -1 & 0 & 0 & 1 \\
 \hline
 1 & 2 & 3 & 3 & 1 & 0 & 0 & 0 \\
 0 & 2 & 6 & 6 & -1 & 1 & 0 & 0 \\
 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
 0 & 0 & 0 & 6 & 2 & -3 & -6 & 1
 \end{array}
 \quad
 \begin{array}{cccccccc}
 & & & & 1 & 0 & 0 & 0 \\
 & & & & -\frac{1}{2} & \frac{1}{2} & 0 & 0 \\
 & & & & 0 & 0 & 1 & 0 \\
 & & & & \frac{1}{3} & -\frac{1}{2} & -1 & \frac{1}{6}
 \end{array}$$

## CHAPTER 7

### CONCLUSION

- Section 7.1 Comments
- Section 7.2 On paragraphs
- Section 7.3 On avitoids
- Section 7.4 On molecules

The first section of this chapter summarises the main theme of the thesis, and indicates lines of possible further development. The other three sections contain further results and conjectures on the corresponding structures that are not directly relevant to the central theme.

## 7.1 Comments

The original motivation for this thesis was the examination of graph theory models of physical phenomena, particularly interaction models. This suggested the problem studied in chapter 4, and the results obtained there allow us to limit the types of interaction model we might use to represent a particular additive physical system.

If we wish to provide approximations to very large systems it is natural to study an appropriate infinite model. This is effected by taking a suitable sequence of finite models; for instance, the infinite plane square lattice graph is often approximated by a sequence of increasingly large toroidal square lattice graphs. The problem connected with this is giving a useful meaning to the partition function for the infinite model; the standard device (see Biggs [5]) is to take an appropriate root of the function for each successive member of the sequence and examine the limit thereof. This leads to an investigation of the multiplicative expansion of a graph function, as in chapter 2.

Stemming from the multiplicative formulation is the practical problem of working out the parameters, which suggests the material of chapter 6. If we derive suitable approximations for the terms in the  $B^{-1}$  matrix we may be able to justify the following definition of the relevant function for an infinite structure. Using the terminology of section 2.5, we wish to examine  $\Phi(b)^{1/|Vb|}$  for large graph types  $b$ . Now we observe that for any nonseparable subgraph type  $p$ ,  $|Vp|M_{p,b}$  is simply equal to  $|Vb|$  times the average number of subgraphs of type  $p$  a vertex of  $b$  lies in; call this last number  $\beta_p$ ; therefore theorem 1 of section 2.5

tells us that  $\Phi(b)^{1/|Vb|} = \prod_P \beta_P^{1/|V_P|}$ . In this way it seems likely that a useful definition of the function for an infinite graph will be obtained by working out the averages  $\beta_P$  and substituting in the above expression. For a series of graphs to 'tend to' the infinite graph we might just require that their  $\beta$  vectors converge to its  $\beta$  vector in some suitable way. This would allow discrepancies that could make the function zero at points where we do not wish it to be; if we desire to we could place further restrictions on the values of the  $\beta$  vectors for the finite graphs.

The details of chapter 2 can be followed through for other set-systems, and this suggests the structures of chapter 5. They can then be used to see whether results on duals for functions on graphs can be carried through.

This thesis concludes with three sections which indicate that the structures we introduced in chapter 3 may prove interesting in their own right.

## 7.2 On paragraphs

Three processes described by Bloch [6] for determining an electrical network 'dual' to a given nonplanar one are a method due to Julia, its dual and the 'fictitious junction point' method. These correspond, in that order, to the following operations on graphs and paragraphs: contracting edges until a planar network is reached, dualizing, then introducing further edges in an appropriate way; deleting edges to obtain a planar network, dualizing and reversing the process of contraction to add the extra edges; and directly translating the network as it stands, usually using the process indicated in figure 1 below.

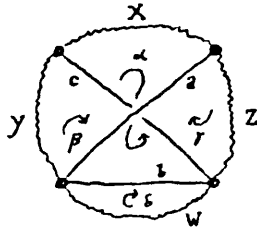


fig. 1a

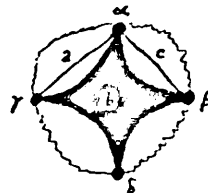


fig. 1b

In the paragraph formulation we may obtain a dual of any graph in much the same way as we would derive that of a planar graph. The definition of a dual assigns the status of vertices in the dual to circuits in the original, and the system of faces of a plane graph forms a suitable set of circuits. If we can draw a graph in the plane with just one crossing, and that of the sort in figure 1a, then we can obtain as its dual paragraph one that is planar and has only one edge of size greater than 2, as in figure 1b. If the edges in 1a are as labelled (a,b,c being single edges and w,x,y,z possibly paths) and we take as the faces those outside the region shown plus the circuits x-a-b-c, y-c-b, z-b-a and w-b (with the orientation as shown) which we denote by  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\delta$  respectively, then we derive the dual as shown.

The above operation suggests the problem of determining how 'near' to a graph we can make the dual of a nonplanar graph. If a graph cannot be drawn with just one crossing, and that of the sort shown above, then its dual cannot have just one 4-edge with other edges being 2-edges; for if we consider such a graph and its dual, then delete the 4-edge and contract the corresponding edge in the original, we are left with two graphs which are dual, and so they must both be planar. Hence we have obtained a planar graph by contracting one edge of a nonplanar one, and this could only have happened if we had contracted an edge adjacent to two edges that cross in some 'almost planar' drawing.

This now suggests the problem of characterising those graphs that have crossing number 1 but require more than one edge of size greater than 2 in their paragraph dual. Three small examples are given in figure 2 below.

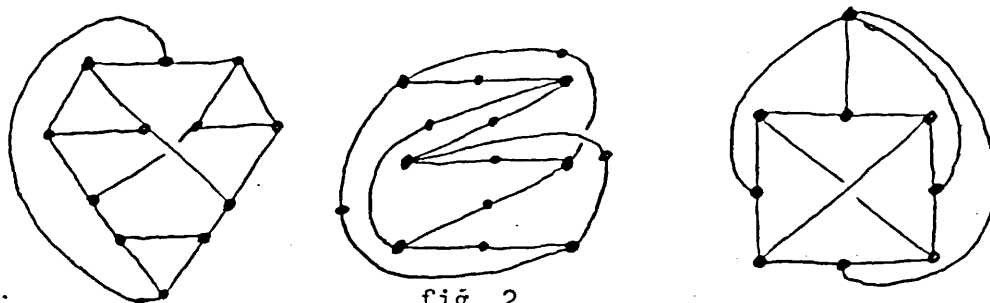


fig. 2

We can define several graph-theoretic notions for paragraphs as follows. A path from  $u$  to  $v$  is a vector  $(P_e)_{e \in E}$  such that  $\sum_e A_{w,e} P_e$  is zero for  $w \neq u, v$  and nonzero for  $w = u$  or  $v$ ; a cycle is a vector  $P$  such that  $\sum_e A_{w,e} P_e = 0 \quad \forall w$ . Then we can define connectedness suitably and therefore number of components, and also cycle number. We might also study linear dependence of paths and so on. If we wish to investigate colourings and flows for paragraphs we need to work over a suitable ring and redefine cycles accordingly; a colouring would be a vector  $(C_v)_{v \in V}$  such that  $\forall e \sum_v A_{v,e} C_v \neq 0$ , and a flow a vector  $(F_e)_{e \in E}$  with no co-ordinates zero such that

$\forall v \sum_c A_{v,e} F_e = 0$ . We can obtain the result that a paragraph has a colouring modulo 2 if and only if it has no cycle modulo 2 of odd weight, where the weight of a cycle  $P$  equals  $\sum_e P_e$ . Note that duality becomes complicated when we work over rings; we might try to restrict our paragraph matrix entries to  $\pm 1$ ,  $-1$  and  $0$ , but there are such paragraphs whose duals cannot be of that form.

The above notions often differ widely from the usual ones for hypergraphs.

### 7.3 On avitoids





















Our development of the subject of avitoids suggests some further avenues of investigation. One such is the study of the relationship between the derived avitoids  $\Gamma_{ab}''$  and  $\Gamma_{ba}''$  for general elements  $a, b$  of an avitoid  $\Gamma$ , or between their associated regular clusterings. Another is to see whether we can relax the conditions of theorem 1 of section 5.2 to the requirements that  $e$  commute and be in a smallest base of  $\Gamma$ ; that would be the case if  $e$  commuting and being in a smallest base of  $\Gamma$  implied that  $e$  was in a smallest base of  $\Gamma_A^1$  for any  $A \subseteq E\Gamma \setminus \{e\}$ .

In [7] Brylawski studied various functions on matroids, including rank polynomials and ones with an additive property. He also exhibited two pairs of different matroids with the same rank polynomials. We might search for smaller pairs of avitoids behaving like this, although there are none with fewer than five elements, and Brylawski's smaller examples contained six elements.

Below we list the circuit and base diagrams of all nonseparable avitoids with up to four elements, indicating their duals and whether they represent graphs or matroids.

graph			each other			graph	
graph			same	same			neither
graph			each other			graph	
graph			each other			graph	
graph			isom- orphic	same			matroid
	circuit diagram	base diagram	dual	dual	base diagram	circuit diagram	



neither			each	other			neither
neither			each	other			neither
neither			each	other			neither
neither			same	same			neither
neither			isom-	isom-			neither
	circuit	base	dual	dual	base	circuit	
	diagram	diagram			diagram	diagram	

#### 7.4 On molecules

As we remarked in section 6.1 we can easily devise systems of molecules that produce negative entries in the B and M matrices. A more interesting question is whether molecule systems producing nonnegative B and M entries, with columns of M summing to powers of 2, must always correspond to some set-theoretic structure.

If we restrict our attention to systems with only one particle and weight function equalling the atomic number, then we may examine the atoms satisfying the above by increasing weight. With weight 1 and 2 we obtain structures that correspond to graphs, being a single edge and two edges forming a circuit, respectively. For weight 3 we get two graphs (the triangle and three edges between the same two vertices), one avitoid (the example in section 3.4) and one clustering (also mentioned in section 3.4). Of course, any of the terms graph, matroid, avitoid, clustering, molecule includes all previous ones, but we are using the strongest possible names in the above cases. With weight 4 we appear to have a total of 41 atoms: 3 graphs, 1 matroid, 10 avitoids, 23 clusterings (2 of which represent the same atom) and 5 atoms. The five candidates to be suitable atoms are indicated in the table below (by the letters G, H, I, J and K), and the derived B and M matrices for that system satisfied our conditions for the first 160 molecules when tested on a computer. In the table we refer to the atoms with capital letters, with A, B, C, D, E, F being the six atoms of weight less than four mentioned above. The defining N matrix may be recovered from the M matrix by examining the entries with row and column subscripts both being atoms. In particular, G and H have the values 4, 5, 3, 0 and 0 in the A, B, C, D and E rows respectively, where I, J and K have entries 4, 4, 2, 2 and

C; and the entries in the F row for G, H, I, J and K are 0, 1, 0, 1 and 2 respectively.

	A	B	A <sup>2</sup>	C	D	E	F	BA	A <sup>3</sup>	G	H	I	J	K	FA	EA	DA	CA	B <sup>2</sup>	BA <sup>2</sup>	A <sup>4</sup>
A	1	2	2	3	3	3	3	3	3	4	4	4	4	4	4	4	4	4	4	4	4
B	0	1	0	3	0	2	1	1	0	5	5	4	4	4	1	2	0	3	2	1	0
A <sup>2</sup>	1	2	2	0	3	1	2	2	3	1	1	2	2	2	5	4	6	3	4	5	6
C	0	0	0	1	0	0	0	0	0	3	3	2	2	2	0	0	0	1	0	0	0
D	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
E	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
F	0	0	0	0	0	0	1	0	0	0	1	0	1	2	1	0	0	0	0	0	0
BA	0	2	0	3	0	2	1	1	0	1	0	2	1	0	1	2	0	3	4	2	0
A <sup>3</sup>	1	6	6	6	6	6	6	6	6	0	0	0	0	0	2	1	3	0	0	2	4
G	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
H	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
I	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
J	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
K	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
FA	0	0	0	0	0	0	3	0	0	0	1	0	1	2	1	0	0	0	0	0	0
EA	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
DA	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
CA	0	0	0	3	0	0	0	0	0	3	3	2	2	2	0	0	0	1	0	0	0
B <sup>2</sup>	0	1	0	6	0	2	0	0	0	2	2	0	0	0	0	0	0	0	2	0	0
BA <sup>2</sup>	0	4	0	15	0	10	5	5	0	10	10	8	8	8	2	4	0	6	4	2	0
A <sup>4</sup>	1	14	14	36	36	36	36	36	36	24	24	24	24	24	24	24	24	24	24	24	24

For the above table we superimposed the upper triangular M entries and the lower triangular B entries; the diagonal terms are those of B, because those of M are always 1. It is of course possible that we may be able to represent the atoms that cannot be clusterings as they stand by other structures with different weight functions. However, G, H, I, J and K cannot be represented by any set structure as they are, as may be seen from simple combinatorial arguments on the numbers of submolecules they contain.

In the above discussion we mentioned that two of the

clustering corresponded to the same atom; these have nontrivial clusters  $\{a,b\}$ ,  $\{c,d\}$ ,  $\{a,b,c\}$ ,  $\{a,b,d\}$  and  $\{a,b\}$ ,  $\{c,d\}$ ,  $\{a,b,c\}$ ,  $\{b,c,d\}$  respectively. This provides a very small counterexample to hopes of reconstruction of clusterings from their subset details alone. Brylawski, in [8], showed that matroids are not reconstructible but we can nevertheless obtain useful information about a structure in this way merely by knowing the numbers of the various atoms.

A problem suggested by the above is what extra conditions we must impose on a molecule system to ensure that it does represent some set structure. Note that we can obtain stronger results than we presented in section 6.2. For instance, the diagonal terms of  $B$  are given by  $B_{n,n} = \prod_a m_a!$ , but the proof we have of this is rather laborious; it should also be possible to establish the composition rules for the  $M$  matrix as in section 2.4 and similar ones for the  $B$  matrix.

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