A matrix method for chromatic polynomials - II

1. Introduction

The subject of this paper is the calculation of the chromatic polynomials of families of graphs that have cyclic symmetry. Generally speaking, there are no elegant methods in this field. The standard method of deletion-and-contraction is both inefficient and inelegant: it requires exponentially many steps, and any symmetry that the graph possesses is destroyed at the very first step.

In this paper we consider families of graphs $\{G_n\}$, where G_n has n-fold cyclic symmetry, and we shall develop a method, introduced in [2], that uses this symmetry in a crucial way. There are two basic steps. First, we introduce a 'compatibility operator' T, and apply the sieve principle to obtain an explicit formula for its action. Then we show that, in certain circumstances, it is possible to use this formula to construct invariant subspaces for T. Furthermore, the spectral decomposition of the action of T on these subspaces can be calculated (in principle). The resulting eigenvalues λ_i and their multiplicities m_i correspond to terms in the chromatic polynomial of G_n, which takes the form

$$P(G_n; z) \;=\; \sum_i m_i(z)\lambda_i(z)^n.$$

It is significant that the eigenvalues occur in 'levels', in such a way that the top levels are the simplest to compute and also the most important.

It has been known for many years that results of this kind provide insight into physical processes. In this context, the behaviour of the zeros of $P(G_n; z)$ as $n \to \infty$ is of paramount importance. A result of Beraha, Kahane and Weiss [1] implies that the zeros approach curves defined by equations of the form

$$|\lambda_i(z)| \;=\; |\lambda_j(z)| \quad (i \neq j).$$

Shrock and Tsai [8] point out that these curves divide the complex plane into regions, in each of which the *thermodynamic limit*

$$\lim_{n\to\infty} \{P(G_n; z)\}^{1/n}$$

is a well-defined analytic function. A series of papers by Shrock and his colleagues (see [9] and the references given there) discusses the relationship between these ideas and the critical behaviour of 'antiferromagnets'. It appears that the curves that determine the critical regions are those corresponding to the eigenvalues at the top levels.

The key elements of the method are described in Sections 2, 3, and 4. In Section 3 we obtain a general sieve formula for the action of T, and in Section

4 we describe, in general terms, how it can be used to construct invariant subspaces. Three applications of the method will be given in Sections 5, 6, and 7, where we study families of graphs D_n, I_n, $B_n(b)$, and obtain the following results.

1. The graph D_n is a cubic graph with $4n$ vertices, and D_5 is the graph of the regular dodecahedron. We use the matrix method to determine the terms of the chromatic polynomial of D_n with degree d satisfying $4n \geq d \geq 3n+2$. These correspond to eigenvalues at level 0.

2. The graph I_n is a regular graph of degree 4 with $3n$ vertices, and I_2 is the graph of the regular icosahedron. Here we determine the entire chromatic polynomial.

3. For each integer $b \geq 2$ the graph $B_n(b)$ is a regular graph of degree $b+1$ with bn vertices. The graph $B_n(2)$ is a *cyclic ladder graph*, whose chromatic polynomial was originally determined by the deletion-contraction method [5], and more recently by the matrix method [2]. The graph $B_n(3)$ is a $3 \times n$ *toroidal square lattice graph*, the entire chromatic polynomial of which has also been determined [3,6]. Here we shall obtain a general formula that can, in principle, be used to determine the entire chromatic polynomial of $B_n(b)$ for all $b \geq 2$. We shall give explicit formulae for the terms corresponding to eigenvalues at levels 0, 1, and 2, that is, the terms with degree d in the range $bn \geq d \geq (b-2)n+2$.

In each case we shall indicate how the results obtained can be used to provide information about the location of the zeros of the chromatic polynomial.

2. The compatibility operator

Throughout this paper we deal with two natural numbers b and k. We regard b as 'fixed' and take $V = \{1, 2, \ldots, b\}$ to be the vertex-set of a given graph B. On the other hand, we shall think of k as 'variable', and consider functions $\alpha : V \to \{1, 2, \ldots, k\}$ that are (proper) k-colourings of B. We denote by P_k the set of all such k-colourings, and by $\mathcal{V}_k$ the vector space of real-valued functions defined on P_k.

The *standard basis* for $\mathcal{V}_k$ contains, for each α in P_k, the function $[\alpha]$ defined by

$$[\alpha](\beta) = \begin{cases} 1, & \text{if } \alpha = \beta; \\ 0, & \text{otherwise.} \end{cases}$$

We shall consider families of graphs constructed as follows. Given an integer $n \geq 3$ and a subset L of $V \times V$, take n disjoint copies of B and link them by extra edges as follows. For $i = 1, 2, \ldots, n$ and each pair $(v, w) \in L$, join vertex v in the ith copy to vertex w in the $(i+1)$th copy, with the convention that $n+1 = 1$. We obtain a 'ring' of n copies of B linked by edges in the manner prescribed. The resulting graph will be denoted by $\mathcal{C}_n(B, L)$.

It is often convenient to write vw instead (v, w) for a pair in L. With this convention, for example, when $B = K_2$ and $L = \{11, 22\}$, then $\mathcal{C}_n(B, L)$ is the cyclic ladder graph mentioned in the Introduction.

Suppose that B and L are given. We say that an ordered pair (α, β) of members of P_k is *compatible with* L if

$$(v, w) \in L \implies \alpha(v) \neq \beta(w).$$

The idea is that if two disjoint copies of B are linked by edges, as prescribed by L, then the colourings α and β combine to form a (proper) colouring of the linked graph.

We define the *compatibility matrix* $T = T_L(k)$ as follows. The rows and columns of T correspond to the elements of P_k, and the entries are given by:

$$T_{\alpha\beta} \;=\; \begin{cases} 1 & \text{if } (\alpha, \beta) \text{ is compatible with } L; \\ 0 & \text{otherwise.} \end{cases}$$

It is convenient to use the same symbol T for the linear operator represented by the matrix T, with respect to the standard basis on the space $\mathcal{V}_k$.

The connection between $T_L(k)$ and the chromatic polynomial arises from the formula [2]:

$$P(\mathcal{C}_n(B, L); k) \;=\; \operatorname{trace}\bigl(T_L(k)^n\bigr).$$

So if the eigenvalues of $T_L(k)$ are $\lambda_1(k), \lambda_2(k), \ldots, \lambda_s(k)$, with multiplicities $m_1(k), m_2(k), \ldots, m_s(k)$ respectively, we have

$$P(\mathcal{C}_n(B, L); k) \;=\; \sum_{r=1}^{s} m_r(k)\lambda_r(k)^n.$$

As a consequence of this formula, the calculation of $P(\mathcal{C}_n(B, L); k)$ is reduced to the calculation of the eigenspaces of T.

Note that k is any positive integer, and the left-hand side of the formula displayed above is known to be a polynomial function. The individual eigenvalues $\lambda_r(k)$ are not necessarily polynomials, but by collecting them together in sets that are algebraically conjugate, we can express the right-hand side as a sum of polynomials. It follows that we can replace k by a complex variable z.

3. The sieve formula

We shall require that the pair (B, L) satisfies the following condition:

Condition C For each $w \in V$ the set of $v \in V$ such that $(v, w) \in L$ is a complete subgraph of B.

The significance of the condition will appear in the proof of Theorem 1, but it may be helpful to mention that it holds in the important cases when

(i) B is a complete graph; or

(ii) for each $w \in V$ there is at most one $v \in V$ with $(v, w) \in L$.

Our first result (Theorem 1) is a formula for the action of T that is essentially a version of the sieve principle. Some preparatory machinery is needed.

Let X be a non-empty subset of V and let θ be a k-colouring of the subgraph of B induced by X. For any $\gamma \in P_k$, denote by γ_X the restriction of γ to X. We define $[X|\theta]$ to be the element of $\mathcal{V}_k$ given by

$$[X|\theta] = \sum_{\gamma_X = \theta} [\gamma].$$

In other words, it is the function that takes the value 1 on the colourings that agree with θ on X, and 0 otherwise.

To cover the case $X = \emptyset$ we define $[-|-] = \sum_\gamma [\gamma]$, where the sum is taken over all $\gamma \in P_k$. So $[-|-]$ is the function which takes the constant value 1 on every element of P_k. We also denote $[-|-]$ by u.

Given $X \subseteq V$ we say that an injection l of X into V is *induced* by L if

$$(l(x),\ x) \in L \quad \text{for all } x \in X.$$

The set of all such injections will be denoted by L_X.

Theorem 1 Suppose that k, B, and L are given, satisfying Condition C, and let $T = T_L(k)$ be the associated compatibility operator. For any given $\alpha \in P_k$ and $X \subseteq V$ let

$$\sigma_L(X, \alpha) = \sum_{l \in L_X} [X|\alpha l].$$

Then

$$T[\alpha] \ = \ \sum_{X \subseteq V} (-1)^{|X|} \sigma_L(X, \alpha).$$

Proof Denote the expression on the right-hand side by Σ. We have to show that $\Sigma(\beta)$ is 1 when β is such that (α, β) is compatible with L, and 0 otherwise.

Considering α as given, let

$$W_L(\beta) \ = \ \{w \in V \mid \beta(w) = \alpha(v) \text{ for some } v \text{ such that } (v, w) \in L\}.$$

We show that, when Condition C holds, $\sigma_L(X, \alpha)(\beta) = 1$ or 0, according as X is or is not a subset of $W_L(\beta)$.

By definition

$$[X|\alpha l](\beta) = 1 \quad \Longleftrightarrow \quad \alpha(l(x)) = \beta(x) \quad \text{for all } x \in X.$$

It follows that

$$\sigma_L(X,\alpha)(\beta) \;=\; \sum_{l \in L_X} [X|\alpha l](\beta)$$

is equal to the number of $l \in L_X$ such that $\alpha(l(x)) = \beta(x)$ for all $x \in X$.

Suppose that X is not a subset of $W_L(\beta)$. Then there is some $x' \in X$ for which $\beta(x')$ is not equal to any $\alpha(v)$, and hence there can be no injection $l : X \to V$ such that $\alpha(l(x)) = \beta(x)$ holds for all $x \in X$. In this case the sum is zero.

On the other hand, suppose that $X \subseteq W_\beta$. Then, since Condition C holds, for each $w \in V$ there is exactly one $v \in V$ such that $\alpha(v) = \beta(w)$. It follows that there is exactly one $l \in L_X$ satisfying the required condition, and so the sum is 1.

It follows that

$$\Sigma(\beta) = \sum_{X \subseteq V} (-1)^{|X|} \sigma_L(X,\alpha)(\beta) = \sum_{X \subseteq W_L(\beta)} (-1)^{|X|}.$$

If (α, β) is compatible with L, $W_L(\beta)$ is empty. So $\Sigma(\beta)$ has just the one term, corresponding to $X = \emptyset$, and the result is 1. On the other hand, if (α,β) is not compatible with L, $W_L(\beta)$ is not empty and $\Sigma(\beta) = (1 + (-1))^{|W_l(\beta)|} = 0$. The result follows. $\square$

4. Finding T-invariant subspaces

For any $x \in \mathcal{V}_k$ the space $\langle x \rangle_T$ spanned by $x, Tx, T^2x, T^3x, \ldots$ is a finite-dimensional subspace of $\mathcal{V}_k$, and clearly it is invariant under T. For our purposes, it is appropriate to take x to be a function of the form $[X|\theta]$.

Generally speaking, if the set $S = \theta(X)$ of colours specified is given, the elements $T^i[X|\theta]$ are linear combinations of terms $[X'|\theta']$ with $\theta'(X')$ a subset of S. (See, for example, Theorem 2.) Thus these elements span the invariant subspace $\langle [X|\theta] \rangle_T$, and the action of T on this subspace can be calculated. The spaces corresponding to sets S of size ℓ are the ones that produce eigenvalues at level ℓ, in the terminology of the Introduction. In the next section we shall see that even the 'trivial' case $S = \emptyset$ produces useful results.

5. First application: generalised dodecahedra

Let B be a path with vertex-set $V = \{1, 2, 3, 4\}$ (1 and 4 being the end-vertices), and let $L = \{11, 32, 44\}$. Then $D_n = \mathcal{C}_n(B, L)$ is a cubic graph with $4n$ vertices, and in particular D_5 is the graph of the regular dodecahedron.

In specific examples it is convenient to use a more explicit notation for the functions denoted by $[X|\theta]$ in Section 3. We shall write, for example

$$[1|h] \;=\; \sum_{\gamma(1)=h} [\gamma].$$

Thus $[1|h]$ is the function which takes the value 1 on the colourings that assign the colour h to vertex 1, and the value 0 otherwise. Similarly, we write $[1, 2|h, i]$ for the sum of all $[\gamma]$ with $\gamma(1) = h$ and $\gamma(2) = i$; and so on. If $\alpha \in P_k$ is defined by $\alpha(i) = \alpha_i$ $(1 \le i \le 4)$, then, in this notation, $[\alpha] = [1, 2, 3, 4|\alpha_1, \alpha_2, \alpha_3, \alpha_4]$. (Note that $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ are not necessarily all distinct.) Finally, $u = [-|-]$ is the sum of all $[\gamma]$ without restriction, that is, the function which takes the value 1 on all colourings.

In the case of the family $D_n = \mathcal{C}_n(B, L)$ defined above, it is clear that Condition C holds. For each $X \subseteq V$ the set L_X contains at most one injection, and according to Theorem 1 the formula for $T[\alpha]$ is

$$\begin{aligned} T[\alpha] = u - &[1|\alpha_1] - [2|\alpha_3] - [4|\alpha_4] + [1, 2|\alpha_1, \alpha_3] + [1, 4|\alpha_1, \alpha_4] \\ &+ [2, 4|\alpha_3, \alpha_4] - [1, 2, 4|\alpha_1, \alpha_3, \alpha_4]. \end{aligned}$$

Following the approach outlined in Section 4 we shall study the action of T on the invariant subspace at 'level 0', that is

$$\langle u \rangle_T = \langle u, Tu, T^2u, \dots \rangle.$$

Since

$$Tu = T\left(\sum_{\alpha \in P_k} [\alpha]\right) = \sum_{\alpha \in P_k} T[\alpha],$$

it is necessary to evaluate the sum over all $\alpha \in P_k$ for each of the 8 terms in the formula for $T[\alpha]$ displayed above. Clearly

$$\sum_{\alpha \in P_k} u = k(k-1)^3 u,$$

and

$$\sum_{\alpha \in P_k} [1|\alpha_1] = \sum_{\alpha \in P_k} [2|\alpha_3] = \sum_{\alpha \in P_k} [4|\alpha_4] = (k-1)^3 u.$$

Next, consider the sum over $\alpha \in P_k$ of the terms $[1, 2|\alpha_1, \alpha_3]$. In any colouring the colours i and j assigned to vertices 1 and 2 must be different, and hence the sum of $[1, 2|i, j]$ over all pairs with $i \neq j$ is just u. For each such pair the number of $\alpha \in P_k$ such that $\alpha_1 = i$ and $\alpha_3 = j$ is $(k-1)(k-2)$. Hence

$$\sum_{\alpha \in P_k} [1, 2|\alpha_1, \alpha_3] = (k-1)(k-2)u.$$

For the remaining terms, it is helpful to define

$$E_{14} = \{\gamma \in P_k \mid \gamma(1) = \gamma(4)\}, \quad E_{24} = \{\gamma \in P_k \mid \gamma(2) = \gamma(4)\}.$$

(Note that the analogous set E_{12} is empty.) Let e_{14} and e_{24} be the characteristic functions of the sets E_{14} and E_{24}.

Now consider the sum over $\alpha \in P_k$ of the terms $[1, 4|\alpha_1, \alpha_4]$. We split P_k into two parts, E_{14} and $P_k \setminus E_{14}$. For the first part, the sum of $[1, 4|i, i]$, taken over all colours i, is e_{14}, and the number of α such that $\alpha_1 = \alpha_4 = i$ is $(k-1)(k-2)$. For the second part, the sum of $[1, 4|i, j]$, taken over all pairs $i \neq j$, is $u - e_{14}$, and the number of α such that $\alpha_1 = i, \alpha_4 = j$ is $k^2 - 3k + 3$. Hence

$$\sum_{\alpha \in P_k} [1, 4|\alpha_1, \alpha_4] = (k-1)(k-2)e_{14} + (k^2 - 3k + 3)(u - e_{14}).$$

Similarly we find

$$\sum_{\alpha \in P_k} [2, 4|\alpha_1, \alpha_4] = (k-1)^2(u - e_{24}).$$

$$\sum_{\alpha \in P_k} [1, 2, 4|\alpha_1, \alpha_3, \alpha_4] = (k-2)(u - e_{24}).$$

Collecting up the terms, and writing $c = k - 2$, we get

$$T(u) = (c^4 + 2c^3 + 3c^2 + c + 1)u - e_{14} - (c^2 + c + 1)e_{24}.$$

Expressions for $T(e_{14})$ and $T(e_{24})$ can be obtained in a similar fashion, and it turns out that they are linear combinations of u, e_{14}, and e_{24}. It follows that $\langle u \rangle_T$ is the 3-dimensional space $\langle u, e_{14}, e_{24} \rangle$. The action of T on this subspace is represented by the matrix

$$\hat{T} = \begin{pmatrix} c^4 + 2c^3 + 3c^2 + c + 1 & c^3 + c & c^3 + c^2 + 2c \\ -1 & c^2 & -c \\ -(c^2 + c + 1) & -c & -c \end{pmatrix}.$$

The eigenvalues $\lambda_1, \lambda_2, \lambda_3$ are the the roots of the characteristic equation:

$$\det(\lambda I - \hat{T}) = \lambda^3 - a_1\lambda^2 + a_2\lambda - a_3 = 0,$$

where

$$\begin{aligned} a_1 &= c^4 + 2c^3 + 4c^2 + 1 \\ a_2 &= c(c+1)(c^4 + c^3 + 2c^2 + 2) \\ a_3 &= c^2(c+1)^2. \end{aligned}$$

The terms of the chromatic polynomial at level 0 are $A_n = \lambda_1^n + \lambda_2^n + \lambda_3^n$. This is equal to the trace of $\hat{T}^n$, which is clearly a polynomial function of c. In fact, A_n is more easily evaluated recursively by Newton's formulae, thus:

$$A_0 = 3, \quad A_1 = a_1, \quad A_2 = a_1^2 - 2a_2,$$

$$A_n = a_1 A_{n-1} - a_2 A_{n-2} + a_3 A_{n-3} \quad (n \geq 3).$$

It follows that A_n is a monic polynomial of degree $4n$ in $k = c + 2$. In fact, this polynomial determines the leading terms of the chromatic polynomial of D_n: specifically, replacing k by a complex variable z, we have

$$P(D_n; z) = A_n(z) + R_n(z),$$

where $R_n(z)$ is a polynomial of degree $3n + 1$.

The motivation for studying the family $\{D_n\}$ is the question of whether chromatic roots can have negative real parts. Many years ago it was thought that two of the chromatic roots of D_5 (the dodecahedron) had this property, but there was a small error in the computation, and in fact the real parts of the roots are just positive. Subsequently, empirical work by Read and Royle [7] showed that cubic graphs with large numbers of vertices can have chromatic zeros with negative real parts. But examples are scarce, and all of them have girth at least five, which is the girth of D_n. This suggests that the behaviour, as $n \to \infty$, of the smallest real part of a chromatic zero of a graph D_n is worth studying.

Our results show that, in general terms, the limiting behaviour of the zeros of $P(D_n; z)$ is determined by $A_n(z)$. The next step would be to obtain an expression of the form

$$P(D_n; z) = A_n(z) + (z - 1)B_n(z) + S_n(z).$$

Here $B_n(z)$ should be a polynomial of degree $3n$, given by a recurrence like that which determines $A_n(z)$, and $S_n(z)$ should be a polynomial of degree $2n + 2$. Analysis of this formula, using the methods outlined at the end of the next section, should help to determine the asymptotic behaviour of the zeros.

6. Second application: cyclic octahedra

In this section and the next one we shall investigate the situation when the base graph B is a complete graph K_b. In these cases the invariant subspace $\langle u\rangle_T$ is one-dimensional. This can be established by the method used in the previous section, but it is simpler to observe that $Tu = \lambda u$, where λ is the number of k-colourings β of K_b such that (α, β) is compatible with L, for any given α. In other words, λ is the number of 1's in each row of in the standard matrix representation of T.

It follows that, in the chromatic polynomial of $\mathcal{C}_n(K_b, L)$, the 'level 0' term is simply λ^n. The terms at lower levels arise from the action of T on invariant subspaces associated with non-empty sets of colours, which we shall study in the next two sections.

In this section we fix $b = 3$, so the base graph B is K_3, with vertex-set $\{1, 2, 3\}$. When the linking set is $L = \{11, 22, 33\}$, the graph $\mathcal{C}_n(K_3, L)$ is a *toroidal square lattice graph*. This has been studied fully [3,6], and it is a special case of the situation covered in the next section. When the linking set is

$$L^* = \{12, 13, 21, 23, 31, 32\},$$

we shall refer to the resulting graph $\mathcal{C}_n(K_3, L^*)$ as a *cyclic octahedron*, the subject of this section. The name is suggested by the fact that in the case $n = 2$ the resulting graph reduces to the regular octahedron, $K_{2,2,2}$. Note also that I_3 is the complete tripartite graph $K_{3,3,3}$.

Since the base graph B is complete, Theorem 1 applies and we have the sieve formula

$$T[\alpha] = \sum_{X\subseteq V} (-1)^{|X|} \sum_{l\in L^*_X} [X\,|\,\alpha l].$$

Each set L^*_X contains several different injections. For example, when $X = \{1, 2\}$, there are three possible injections $l : X \to V$ induced by L; the possible values of $(l(1), l(2))$ being $(2, 1)$, $(2, 3)$, and $(3, 1)$. So the formula for the effect of T on $\alpha = [1, 2, 3|h, i, j]$ contains three terms corresponding to $X = \{1, 2\}$:

$$[1, 2|i, h], \quad [1, 2|i, j], \quad [1, 2|j, h].$$

When all the terms called for in Theorem 1 are listed, we obtain the following formula

$$
\begin{aligned}
T[1,2,3|h,i,j] = u - \Big(&[1|i] + [1|j] + [2|h] + [2|j] + [3|h] + [3|i]\Big) \\
+\Big(&[1,2|i,h] + [1,2|i,j] + [1,2|j,h] \\
&+ [2,3|h,i] + [2,3|j,h] + [2,3|j,i] \\
&+ [1,3|i,h] + [1,3|j,h] + [1,3|j,i]\Big) \\
-\Big(&[1,2,3|i,j,h] + [1,2,3|j,h,i]\Big).
\end{aligned}
$$

In order to apply the method outlined in Section 4, consider first the subspace $\langle u\rangle_T$. As we have already noted, this space is one-dimensional, and here $Tu = \lambda u$, where $\lambda = k^3 - 9k^2 + 29k - 32$. It is a standard result of 'Perron-Frobenius' theory that this eigenvalue has multiplicity 1.

Next, fix a colour h, and let F_{vh} $(v = 1,2,3)$ be the set of colourings γ such that $\gamma(v) = h$. The characteristic function of the set F_{vh} is $f_{vh} = [v|h]$. We shall show that the invariant subspace $\langle f_{1h}\rangle_T$ is spanned by $u, f_{1h}, f_{2h}, f_{3h}$.

It is convenient to abbreviate the function $[1,2,3|h,i,j]$ to $[hij]$. Then we can write the definition of f_{1h} as

$$
f_{1h} = \sum_{\alpha\in F_{1h}} [\alpha] \;=\; \sum_{ij\in N(h)} [hij],
$$

where the notation $ij \in N(h)$ means that the sum is taken over ordered pairs (i,j) with $i \neq j$ such that $i \neq h$ and $j \neq h$. Thus

$$
T(f_{1h}) \;=\; T\left(\sum_{ij\in N(h)} [hij]\right) \;=\; \sum_{ij\in N(h)} T[hij].
$$

The formula for $T[hij]$ displayed above has eighteen terms, and we can calculate the sum over $ij \in N(h)$ for each one of them. Many of the calculations are similar, and we need only work out a few examples, as follows.

$$
\begin{aligned}
\sum_{ij\in N(h)} u &= (k-1)(k-2)u \\
-\sum_{ij\in N(h)} [1|i] &= -(k-2)(u-[1|h]) \\
-\sum_{ij\in N(h)} [2|h] &= -(k-1)(k-2)[2|h] \\
\sum_{ij\in N(h)} [1,2|i,h] &= (k-2)[2|h] \\
\sum_{ij\in N(h)} [1,2|i,j] &= u-[1|h]-[2|h] \\
-\sum_{ij\in N(h)} [ijh] &= -[3|h].
\end{aligned}
$$

The important point is that all the terms are linear combinations of the four functions u, $f_{1h}=[1|h]$, $f_{2h}=[2|h]$, and $f_{3h}=[3|h]$. Collecting up the terms, we obtain

$$T(f_{1h}) = (k^2-7k+13)(u-f_{2h}-f_{3h}) + (2k-6)f_{1h}.$$

There are similar formulae for $T(f_{2h})$ and $T(f_{3h})$. Writing $x=k^2-7k+13$ and $y=2k-6$, we have

$$
\begin{aligned}
T(f_{1h}) &= xu + yf_{1h} - x(f_{2h}+f_{3h}) \\
T(f_{2h}) &= xu + yf_{2h} - x(f_{1h}+f_{3h}) \\
T(f_{3h}) &= xu + yf_{3h} - x(f_{1h}+f_{2h}).
\end{aligned}
$$

We already know that $T(u)=(k^3-9k^2+29k-32)u$. It follows that

$$\langle f_{1h}\rangle_T = \langle u, f_{1h}, f_{2h}, f_{3h}\rangle.$$

The eigenvalues and eigenfunctions arising from the action of T on this 4-dimensional space can be deduced directly from the equations. For example, we have the equation

$$T(f_{1h}-f_{2h}) = (x+y)(f_{1h}-f_{2h}),$$

which implies that $x+y=k^2-5k+7$ is an eigenvalue with eigenfunction $f_{1h}-f_{2h}$. Clearly, $f_{2h}-f_{3h}$ and $f_{1h}-f_{3h}$ are also eigenfunctions for the same eigenvalue.

In order to determine the total multiplicity for the eigenvalue k^2-5k+7, observe first that there are three eigenfunctions $f_{1h}-f_{2h}$, $f_{2h}-f_{3h}$, and $f_{1h}-f_{3h}$, for each h in the range $1\le h\le k$. However, the third one is the sum of the first two, so there are only two linearly independent eigenfunctions for each of the k values of h. It is easily verified that the only linear relationships among these $2k$ eigenfunctions are the obvious ones

$$\sum_{h=1}^{k}(f_{1h} - f_{2h}) = 0, \quad \sum_{h=1}^{k}(f_{2h} - f_{3h}) = 0,$$

and so the eigenspace has total dimension $2(k-1)$.

Another piece of simple algebra shows that $k(f_{1h} + f_{2h} + f_{3h}) - 3u$ is an eigenfunction for the eigenvalue $y - 2x = -2(k-4)^2$. Here there are k eigenfunctions, one for each value of h in the range $1 \leq h \leq k$, but again the sum of all of them is identically zero, so they define an eigenspace of dimension $k-1$.

Similar calculations can be done at levels 2 and 3. At each level there are two steps. First, there is the analysis of an invariant subspace of the form $\langle [X|\theta] \rangle_T$, where $\theta(X)$ is a specified set of 2 (or 3) colours; this produces the required eigenvalues. Then there is the analysis of the multiplicities of the eigenvalues, given that the specified set of colours is allowed to be any subset of size 2 (or 3).

It turns out that, at level 2, the space splits in exactly the same way as for the $3 \times n$ toroidal square lattice [3,6]. That is, there are four eigenspaces, with dimensions $m_k, 2m_k, m_k + 1, 2(m_k + 1)$, where

$$m_k = \binom{k}{2} - \binom{k}{1} = \frac{1}{2}k(k-3),$$

giving the total dimension $3(k^2 - 3k + 1)$. At level 3, the total dimension is $k^3 - 6k^2 + 8k - 1$, which splits in this case into two spaces of dimensions $2n_k + k - 1$, and $2(2n_k + k)$, where

$$n_k = \binom{k}{3} - \binom{k}{2} = \frac{1}{6}k(k-1)(k-5).$$

In summary the eigenvalues and multiplicities are as follows.

Eigenvalue	Multiplicity
$k^3 - 9k^2 + 29k - 32$	1
$-2(k-4)^2$	$k-1$
$k^2 - 5k + 7$	$2(k-1)$
$3k - 14$	m_k
1	$2m_k$
$k-2$	$m_k + 1$
$-(2k-7)$	$2(m_k + 1)$
-2	$2n_k + k - 1$
1	$2(2n_k + k)$

Note that the eigenvalue 1 occurs at levels 2 and 3, and its total multiplicity is $k(k-1)(2k-7)/3$.

These results imply that the chromatic polynomial of $I_n = \mathcal{C}_n(K_3, L^*)$ is

$$\begin{aligned} P(I_n; z) &= (z^3 - 9z^2 + 29z - 32)^n \\ &\quad + (z-1)\Big((-2(z-4)^2)^n + 2(z^2 - 5z + 7)^n\Big) \\ &\quad + (1/2)z(z-3)(3z-14)^n \\ &\quad + (1/2)(z-1)(z-2)\Big((z-2)^n + 2(-2z+7)^n\Big) \\ &\quad + (1/3)(z^3 - 6z^2 + 8z - 3)(-2)^n + (1/3)z(z-1)(2z-7). \end{aligned}$$

In order to study the location of the roots of $P(I_n; z) = 0$, note that there are $3n$ roots and their sum is $9n$, so the centroid is at the point 3. Thus it is convenient to put $w = z - 3$, giving

$$P(I_n; z) = (w^3 + 2w + 1)^n + G_n(w),$$

where $G_n(w)$ is a polynomial of degree $2n + 1$.

The zeros of $w^3 + 2w + 1$ are (approximately)

$$-0.4534, \quad 0.2267 + 1.4677i, \quad 0.2267 - 1.4677i,$$

which lie in the disc $|w| \leq 1.4852$. It follows from Rouché's Theorem that all the zeros of $(w^3 + 2w + 1)^n + G_n(w)$ lie in the disc $|w| \leq R$, provided that $R > 1.4852$ and $|w^3 + 2w + 1|^n \geq |G_n(w)|$ on the circle $|w| = R$. Since the degree of $G_n(w)$ is $2n + 1$, it is clear that a suitable value of R can be found: for example $R = 3$ suffices for all sufficiently large n. In the light of the remarks at the end of the previous section, it is worth remarking that this implies that all roots of $P(I_n; z) = 0$ have non-negative real parts.

Further information follows from the theorem of Beraha, Kahane and Weiss [1] mentioned in the Introduction to this paper. Stated fully, the result says that the limit points of the zeros of a sequence of polynomials, of the form

$$P_n(z) = \sum_{i=1}^{s} m_i(z)\lambda_i(z)^n,$$

are the points ζ lying on the curves where two of the terms $\lambda_i(\zeta)$ are of equal modulus and dominate the other terms (together with some isolated points, which need not concern us).

In the case of the cyclic octahedra we have obtained the eigenvalues:

$$\lambda_A = w^3 + 2w + 1, \quad \lambda_B = -2(w-1)^2, \quad \lambda_C = w^2 + w + 1.$$

$$\lambda_D = 3w - 5, \quad \lambda_E = w + 1, \quad \lambda_F = -2w + 1, \quad \lambda_G = -2, \quad \lambda_H = 1.$$

In fact, one of the three eigenvalues $\lambda_A, \lambda_B, \lambda_D$ always dominates the other five. This means that the limiting behaviour of the roots is determined by these three.

Denote by Γ_{AB} the curve defined by the equation $|\lambda_A| = |\lambda_B|$, and so on. Then Γ_{AB} and Γ_{BD} are simple closed curves intersecting in two points

$$t, \bar{t} = 0.9971.. \pm 1.6284..i.$$

Γ_{AD} is another simple closed curve, which necessarily contains t and $\bar{t}$.

The portions of these curves that satisfy the domination condition are the arc of Γ_{AD} that joins t and $\bar{t}$ and lies entirely in the half-plane $Re\ w > 0$, and the arcs of Γ_{AB} and Γ_{BD} that join t and $\bar{t}$ and do not lie entirely in the half-plane $Re\ w > 0$. Note that these arcs all lie in the half-plane $Re\ z > 0$.

These arcs divide the complex plane into three regions: a crescent-shaped region containing $w = 0$, in which λ_D dominates; another crescent-shaped region contiguous with the first, in which λ_B dominates, and the remainder of the complex plane, in which λ_A dominates. Apart from some isolated points, such as $z = 0$ $(w = -3)$, the limit points of the chromatic roots of the graphs I_n lie on the parts of $\Gamma_{AB}, \Gamma_{AD}, \Gamma_{BD}$ that bound these regions.

7. Third application: bracelets

For this application we take the base graph B to be a complete graph K_b, where b is any positive integer, and the linking set to be

$$L = \{11, 22, 33, \ldots, bb\}.$$

With these choices, the graph $\mathcal{C}_n(K_b, L)$ is a *bracelet*, which we denote here by $B_n(b)$. In this case the bracelet is 'untwisted', but if L is replaced by a different matching we obtain a *twisted bracelet*. There is a simple correspondence [4] between the leading terms of the chromatic polynomials in the two cases.

Clearly, Condition C is satisfied and for each $X \subseteq V$, the set L_X contains only one injection, the inclusion map $X \to V$. Thus the sieve formula for $T[\alpha]$ reduces to

$$T[\alpha] \;=\; \sum_{X \subseteq V} (-1)^{|X|}\ [X|\alpha_X],$$

where α_X is the restriction of α to X.

Using this formula, the entire chromatic polynomial for $B_n(3)$ has been calculated [3,6]:

$$\begin{aligned} P(B_n(3);z) \;=\; & (z^3-6z^2+14z-13)^n \\ & + (z-1)\Big((-z^2+7z-13)^n + 2(-z^2+4z-4)^n\Big) \\ & + z(z-3)/2\Big((z-5)^n + 2(z-2)^n\Big) \\ & + (z-1)(z-2)/2\Big((z-1)^n + 2(z-4)^n\Big) \\ & + (z^3-6z^2+8z-1)(-1)^n. \end{aligned}$$

The form of the result confirms that the terms occur in 'levels', the terms at level i being of the form

$$\big(\text{Polynomial of degree } i\big) \times \big(\text{Polynomial of degree } 3-i\big)^n.$$

Here we shall describe a general method that can, in principle, be used to calculate the terms at all levels, for any b. The terms at levels $0, 1$, and 2 will be given explicitly.

Let S be a subset of the set of colours $\{1,2,\ldots,k\}$. The key result (Theorem 2) concerns the action of T on functions of the form $[Y|\beta]$, where $\beta(Y)=S$. We shall show that $T[Y|\beta]$ is a linear combination of terms of the form $[Z|\gamma]$, for all of which $\gamma(Z)$ is a subset of S. This implies that the invariant subspace $\langle[Y|\beta]\rangle_T$ is just the subspace $\mathcal{U}(S)$ of $\mathcal{V}_k$ spanned by all terms in which the set of colours assigned is a subset of $S=\beta(Y)$.

We shall also obtain a formula (Theorem 3) that gives the coefficients of the terms that appear in $T[Y|\beta]$. This formula is remarkably simple, despite the complicated arguments that are needed to justify it.

Suppose that S is given, and Y,β are such that $\beta(Y)\subseteq S$. As usual, we begin with the calculation

$$\begin{aligned} T[Y|\beta] &= T\Big(\sum_{\alpha_Y=\beta}[\alpha]\Big) \\ &= \sum_{\alpha_Y=\beta} T[\alpha] \\ &= \sum_{\alpha_Y=\beta}\sum_{X\subseteq V}(-1)^{|X|}\,[X|\alpha_X] \\ &= \sum_{X\subseteq V}(-1)^{|X|}\,\phi(X,Y,\beta), \end{aligned}$$

where

$$\phi(X, Y, \beta) = \sum_{\alpha_Y = \beta} [X|\alpha_X].$$

The aim is to find a 'formula' for $\phi(X, Y, \beta)$ that can be used to determine $T[Y|\beta]$. This requires some preparation.

If δ is an injection from X to $\{1, 2, \ldots, k\}$ such that δ and β agree on $X \cap Y$, then there is a function $\delta * \beta$ from $X \cup Y$ to $\{1, 2, \ldots, k\}$ defined by

$$(\delta * \beta)(v) = \begin{cases} \delta(v) & \text{if } v \in X; \\ \beta(v) & \text{if } v \in Y. \end{cases}$$

Note that $\delta * \beta$ may not exist, and if it does exist, it may not be an injection (because it is possible that, for some $x \in X \setminus (X \cap Y)$ and $y \in Y \setminus (X \cap Y)$, $\delta(x) = \beta(y)$). We define

$$G(\beta) = \{\theta \in P_k \mid \theta_X * \beta \text{ exists and is an injection}\}.$$

Recall that for any complex number z and non-negative integer n the 'falling factorial' $(z)_n$ is defined by

$$(z)_0 = 1, \qquad (z)_n = z(z-1)_{n-1} \quad (n \geq 1).$$

In other words, $(z)_n = z(z-1)\cdots(z-n+1)$.

Lemma 1 Suppose that X and Y are subsets of V, where $|X \cup Y| = p$ and $|V| = b$, and let β be an injection from Y into $\{1, 2, \ldots, k\}$. Then

$$\phi(X, Y, \beta) = (k-p)_{b-p} \sum_{\theta \in G(\beta)} [\theta].$$

Proof Using the definitions of $\phi(X, Y, \beta)$ and $[X|\alpha_X]$ we have

$$\begin{aligned} \phi(X, Y, \beta) &= \sum_{\alpha_Y = \beta} [X|\alpha_X] \\ &= \sum_{\alpha_Y = \beta} \sum_{\theta_X = \alpha_X} [\theta]. \end{aligned}$$

In order to reverse the order of summation it is convenient to write this as a sum taken over pairs (α, θ):

$$\phi(X, Y, \beta) = \sum_{(\alpha, \theta) \in A(\beta)} [\theta],$$

where

$$A(\beta) = \{(\alpha, \theta) \mid \alpha_X = \theta_X \text{ and } \alpha_Y = \beta\}.$$

Treating this a repeated sum we have

$$\sum_{(\alpha,\theta)\in A(\beta)} [\theta] = \sum_{\theta} [\theta] \sum_{(\alpha,\theta)\in A(\beta)} 1 = \sum_{\theta} [\theta]\, m(\theta,\beta),$$

where $m(\theta,\beta)$ is the number of α such that $\alpha_X = \theta_X$ and $\alpha_Y = \beta$.
Suppose first that θ is in the set $G(\beta)$ defined above. Then $\theta_X * \beta$ exists and is an injection on $X \cup Y$, and $m(\theta,\beta)$ is the number of ways of extending this injection to an injection defined on the whole of V. This number is just

$$(k-p)(k-p-1)\dots(k-b+1) = (k-p)_{b-p}.$$

On the other hand, if θ is not in the set $G(\beta)$, there can be no injection α satisfying the conditions, and $m(\theta,\beta) = 0$. □

We now investigate the general formula for $\phi(X,Y,\beta)$. If Z is a subset of X containing $X \cap Y$ define

$$\Pi(Z) = \{\pi \mid \pi : Z \to Y \text{ is an injection and } \pi_{X\cap Y} = id\}.$$

Note that $\Pi(X \cap Y)$ contains only the inclusion function $X \cap Y \to Y$.

Lemma 2 With $\Pi(Z)$ as above, and the other notation as in Lemma 1,

$$\phi(X,Y,\beta) \ = t(X,Y) \sum_{X\cap Y\subseteq Z\subseteq X} (-1)^{|Z|}\tau(Z),$$

where

$$t(X,Y) = (-1)^{|X\cap Y|}(k-p)_{b-p}, \qquad \tau(Z) = \sum_{\pi\in\Pi(Z)} [Z \mid \beta\pi].$$

Proof Given the result of Lemma 1, it remains to evaluate $\sum[\theta]$ taken over the set $G(\beta)$.
Recall that $G(\beta)$ consists of those θ in P_k for which (i) $\theta_X * \beta$ is defined, and (ii) $\theta_X * \beta$ is an injection on $X \cup Y$. The set of all θ satisfying condition (i) consists of those for which $\theta_{X\cap Y} = \beta_{X\cap Y}$, and the sum of $[\theta]$ taken over this set is, by definition,

$$[X \cap Y | \beta_{X\cap Y}].$$

We apply the sieve principle to obtain the relationship between this sum and the sum taken over all θ for which both conditions hold. It is convenient to put $Z = (X \cap Y) \cup D$, so that summing over Z such that $X \cap Y \subseteq Z \subseteq X$ corresponds to summing over all subsets D of $X \setminus (X \cap Y)$.

So we write the sum over $G(\beta)$ as

$$\sum_{D \subseteq X \setminus (X \cap Y)} (-1)^{|D|} F(D, \beta),$$

where $F(D, \beta)$ is the sum taken over θ that satisfy condition (i), but fail to satisfy condition (ii) on the set D. The second statement means that for each $v \in D$ there is some $\pi(v)$ in Y such that $\theta(v) = \beta(\pi(v))$. Clearly, this defines an injection π from D to $Y \setminus (X \cap Y)$. We can extend π to an injection from $(X \cap Y) \cup D$ to Y, by defining it to be the identity on $X \cap Y$, and since condition (i) holds this means that $\theta_{(X \cap Y) \cup D} = \beta\pi$. In other words

$$F(D, \beta) = \sum_{\pi \in \Pi(X \cap Y) \cup D} [(X \cap Y) \cup D \mid \beta\pi] = \tau((X \cap Y) \cup D).$$

Putting $Z = (X \cap Y) \cup D$ we have the result. □

The results obtained in Lemmas 1 and 2 provide the required formula for $T[Y|\beta]$.

Lemma 3 The action of T is given by

$$T[Y|\beta] \ = \ \sum_{X \subseteq V} (-1)^{|X \setminus (X \cap Y)|} (k - |X \cup Y|)_{b - |X \cup Y|} \sum_{X \cap Y \subseteq Z \subseteq X} (-1)^{|Z|} \tau(Z),$$

where

$$\tau(Z) \ = \ \sum_{\pi \in \Pi(Z)} [Z|\beta\pi].$$

□

We shall now establish the existence of invariant subspaces $\mathcal{U}(S)$ (Theorem 2), and an explicit matrix representation for the action of T on $\mathcal{U}(S)$ (Theorem 3).

Theorem 2 Let S be a subset of the colours $\{1, 2, \ldots, k\}$, and let $\mathcal{U}(S)$ be the subspace of $\mathcal{V}_k$ spanned by all functions $[Z|\gamma]$ with $\gamma(Z) \subseteq S$. Then $\mathcal{U}(S)$ is invariant under the action of T.

Proof Let Y, β be such that $\beta(Y) \subseteq S$. According to Lemma 3, $T[Y|\beta]$ is a linear combination of terms of the form $[Z|\beta\pi]$. Here π is an injection $Z \to Y$, and so $\beta\pi(Z) \subseteq S$. In other words, all the terms have the property that the set of assigned colours is a subset of S. It follows that $\mathcal{U}(S)$ is the invariant subspace $\langle [Y|\beta] \rangle_T$. □

Lemma 4 Suppose that Y and β are given, and that A and α are such that

$$\alpha(A) \subseteq \beta(Y), \qquad \alpha_{A\cap Y} = \beta_{A\cap Y}.$$

Then $[A|\alpha]$ appears as a term in $\phi(X, Y, \beta)$ if and only if X is a subset of V satisfying

$$A \subseteq X \subseteq V \setminus Y',$$

where $Y' = Y \setminus (A \cap Y)$.

Proof It follows from Lemma 2 that the terms $[A|\alpha]$ appearing in $\phi(X, Y, \beta)$ are precisely those for which

$$[A|\alpha] = [Z|\beta\pi], \quad \text{where } X \cup Y \subseteq Z \subseteq X, \text{ and } \pi \in \Pi(Z).$$

The given conditions on α ensure that $\alpha = \beta\pi$ for some $\pi \in \Pi(A)$, so the effective condition is that $X \cup Y \subseteq A \subseteq X$. Rearranging this as a condition on X we obtain the stated result. □

Now that we have established which terms occur in $T[Y|\beta]$, it remains only to find the coefficients.

For each integer $n \geq 0$ and any complex number z, the following formula defines a monic polynomial of degree n:

$$C(n, z) \;=\; \sum_{r=0}^{n} (-1)^r \binom{n}{r} (z - r)_{n-r}.$$

In particular, the polynomials $C(n, z)$ for $0 \leq i \leq 4$ are:

$$C(0, z) = 1, \quad C(1, z) = z - 1, \quad C(2, z) = z^2 - 3z + 3,$$

$$C(3, z) = z^3 - 6z^2 + 14z - 13, \quad C(4, z) = z^4 - 10z^3 + 41z^2 - 84z + 73.$$

The relevance of these polynomials stems from the fact that $C(b, k)$ is the number of k-colourings τ of K_b such that (σ, τ) is compatible with L, for any given σ. In other words, it is the number of τ that are 'derangements' of σ: $\sigma(v) \neq \tau(v)$ for all $v \in \{1, 2, \ldots, b\}$. From this observation it follows that

$$P(B_2(b); k) = (k)_b C(b, k).$$

For simplicity of notation, we fix the integers b and $k \geq b$, and define

$$c_i = c_i(b, k) = C(b - i, k - i) \quad (0 \leq i \leq b).$$

Theorem 3 Let A and Y be subsets of $V = \{1, 2, \ldots, b\}$, and let α, β be injections from A and Y respectively to $\{1, 2, \ldots, k\}$, such that $\alpha(A) \subseteq \beta(Y)$ and $\alpha_{A\cap Y} = \beta_{A\cap Y}$. Then the coefficient of $[A|\alpha]$ in $T[Y|\beta]$ is

$$(-1)^{|A\cap Y|}\ c_{|A\cup Y|}.$$

Proof According to Lemma 2, the coefficient of a term $[A|\alpha]$ that occurs in $\phi(X, Y, \beta)$ is $t(X, Y)(-1)^{|A|}$. If α satisfies the given conditions then, by Lemma 3, $[A|\alpha]$ occurs in $\phi(X, Y, \beta)$ if and only if X is such that $A \subseteq X \subseteq V \setminus Y'$. Since

$$T[Y|\beta] = \sum_{X\subseteq V} (-1)^{|X|}\phi(X, Y, \beta),$$

it follows that the coefficient of $[A|\alpha]$ in $T[Y|\beta]$ is

$$\sum_{A\subseteq X\subseteq V\setminus Y'} (-1)^{|X|} t(X, Y)(-1)^{|A|}.$$

Writing $X = A \cup R$, with $A \cap R = \emptyset$, the condition $A \subseteq X \subseteq V \setminus Y'$ is equivalent to the condition that R is a subset of $V \setminus (A \cup Y)$. Furthermore,

$$|X| = |A| + |R|, \quad |X \cap Y| = |A \cap Y|, \quad |X \cup Y| = |A \cup Y| + |R|.$$

Hence

$$\begin{aligned} t(X, Y) &= (-1)^{|X\cap Y|}(k - |X \cup Y|)_{b-|X\cup Y|} \\ &= (-1)^{|A\cap Y|}(k - |A \cup Y| - |R|)_{b-|A\cup Y|-|R|}, \end{aligned}$$

and the required coefficient is

$$\begin{aligned} &\sum_{R\subseteq V\setminus(A\cup Y)} (-1)^{|A|+|R|} t(X, Y)(-1)^{|A|} \\ &= (-1)^{|A\cap Y|} \sum_{R\subseteq V\setminus(A\cup Y)} (-1)^{|R|}(k - |A \cup Y| - |R|)_{b-|A\cup Y|-|R|} \\ &= (-1)^{|A\cap Y|} \sum_{r=0}^{b-|A\cup Y|} (-1)^r \binom{b - |A \cup Y|}{r} (k - |A \cup Y| - r)_{b-|A\cup Y|-r} \\ &= (-1)^{|A\cap Y|}\ C(b - |A \cup Y|,\ k - |A \cup Y|). \end{aligned}$$

□

The general formula given in Theorem 3 can be used (in principle) to determine the spectral decomposition of the action of T on the invariant subspaces $\mathcal{U}(S)$. Fortunately, the smallest values of $|S|$ give the most important eigenvalues. The calculation has been done in full when $|S| = 0, 1$, and 2, that is, for 'levels' $0, 1$, and 2.

The equation $Tu = c_0 u$ follows from Theorem 3, and so the level 0 invariant subspace $\mathcal{U}(\emptyset)$, or $\langle u \rangle_T$, is just $\langle u \rangle$. This checks with the fact that c_0 is the number of k-colourings β of K_b such that (α, β) is a compatible pair, for any given α, in other words, it is the number of 1's in each row of the matrix T. As noted in the previous section, standard arguments lead to the conclusion that the eigenvalue c_0 has multiplicity 1.

At level 1, we fix a colour h and consider $\mathcal{U}(h)$. We shall show that, for any given $v \in V$,

$$\mathcal{U}(h) = \langle [v|h] \rangle_T = \langle u, [1|h], [2|h], \ldots, [b|h] \rangle.$$

The terms that appear in $T[v|h]$ are the $[A|\alpha]$ for which $A = \emptyset$, $A = \{v\}$ and $A = \{w\}$, for all $w \neq v$. Clearly, there is a unique α in each case. Theorem 3 tells us that the complete formula is

$$T[v|h] = c_1\Big(u - [v|h]\Big) + c_2\Big(\sum_{w \neq v} [w|h]\Big).$$

We observe that if $k < b$ the situation is vacuous (since the set of k-colourings of K_b is empty). If $k = b$ the set of functions

$$u, [1|h], [2|h], \ldots, [b|h],$$

is linearly dependent (u is the sum of the other functions, since every b-colouring of K_b assigns colour h to exactly one vertex). However, if $k > b$ there are k-colourings of K_b that do not use the colour h, so u is linearly independent of the other functions, and the set is a basis for $\mathcal{U}(h)$. We shall assume henceforth that this condition holds.

According to the formula given above, the action of T on $\mathcal{U}(h)$ with respect to the canonical basis is represented by the matrix

$$\begin{pmatrix} c_0 & c_1 & c_1 & . & . & . & c_1 \\ 0 & -c_1 & c_2 & . & . & . & c_2 \\ 0 & c_2 & -c_1 & . & . & . & c_2 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & c_2 & c_2 & . & . & . & -c_1 \end{pmatrix}.$$

The eigenvalues of this matrix are also eigenvalues of T. Clearly, they are c_0 and the eigenvalues of the $b \times b$ matrix M in the lower right-hand corner. In terms of the identity matrix I and the all-1 matrix J we have

$$M = c_2(J - I) - c_1 I.$$

The eigenvalues of a matrix of this form are well known: there are just two distinct ones, and they are:

$$\begin{aligned} (b-1)c_2 - c_1 &\quad \text{(multiplicity 1);} \\ -c_2 - c_1 &\quad \text{(multiplicity } b-1). \end{aligned}$$

The eigenfunctions can be obtained directly from the formula. First, let

$$\phi_h = [1|h] + [2|h] + \cdots + [b|h] - (b/k)u.$$

It is easy to check that $T\phi_h = ((b-1)c_2 - c_1)\phi_h$, so that ϕ_h spans a 1-dimensional space of eigenfunctions.

Next, for any vertices $v \neq w$ let

$$\psi_h^{vw} = [v|h] - [w|h].$$

Again, it is easy to check that $T\psi_h^{vw} = (-c_2 - c_1)\psi_h^{vw}$. So we have $b(b-1)/2$ eigenfunctions, one for each edge vw of K_b. These eigenfunctions span a space of dimension $b-1$, a basis for which is obtained by taking the functions corresponding to the edges of any spanning tree of K_b. For example, we may fix $w = b$, and take $v = 1, 2, \ldots, b-1$.

Up to this point we have been considering the action of T on the subspace $\mathcal{U}(h)$, for a given colour h. In fact, for each one of the k colours there is an eigenfunction ϕ_h, and the only linear relationship between them is that their sum is identically zero. Thus in the action of T on the whole space $\mathcal{V}_k$, the multiplicity of the eigenvalue $(b-1)c_2 - c_1$ is $(k-1)$. Similarly, the multiplicity of $-c_2 - c_1$ is $(b-1)(k-1)$.

In a similar way, but with more complicated details, we can compute the action of T on an invariant subspace $\mathcal{U}(S)$ with $|S| = 2$. The basic formula follows from Theorem 3:

$$\begin{aligned} T[1,2|h,i] \; &= c_2\Big(u - [1|h] - [2|i] + [1,2|h,i]\Big) \\ &\quad + \; c_3\Big(\sum_{w\neq 1,2} [w|h] + [w|i] - [1,w|h,i] - [w,2|h,i]\Big) \\ &\quad + \; c_4\Big(\sum_{w,w'\neq 1,2} [w,w'|h,i] + [w,w'|i,h]\Big). \end{aligned}$$

Note that for each set of two vertices $Y = \{w, w'\}$ there are two injections from Y to $\{h, i\}$ and thus two terms in the last sum. Equivalently, the space $\mathcal{U}(h,i)$ contains $b(b-1)$ functions of the form $[Y|\beta]$ with $\beta(Y) = \{h,i\}$, and thus we may expect that the action of T on it produces $b(b-1)$ new eigenvalues.

The space $\mathcal{U}(h,i)$ contains subspaces isomorphic to $\mathcal{U}(h)$ and $\mathcal{U}(i)$, and the action of T on these subspaces has already been determined. The rest of $\mathcal{U}(h,i)$ splits as a direct sum $\mathcal{U}^+ \oplus \mathcal{U}^-$, where the summands correspond to symmetric and skew-symmetric functions respectively. The action of T on each summand gives rise to eigenvalues with total multiplicity $\frac{1}{2}b(b-1)$. Thus we obtain the $b(b-1)$ 'new' eigenvalues, as expected.

The detailed calculations show that on $\mathcal{U}^+$ there are three distinct eigenvalues, for all $b \geq 4$,

$$\begin{array}{rl} c_2 - (2b-4)c_3 + (b-2)(b-3)c_4 & \text{multiplicity } 1; \\ c_2 - (b-4)c_3 - 2(b-3)c_4 & \text{multiplicity } b-1; \\ c_2 + 2c_3 + 2c_4 & \text{multiplicity } b(b-3)/2. \end{array}$$

When $b = 2$ only the first eigenvalue occurs, and it reduces to $c_2 = 1$. When $b = 3$ only the first two eigenvalues occur, and they reduce to $c_2 - 2c_3 = k-5$, and $c_2 + c_3 = k - 1$.

On $\mathcal{U}^-$ there are two distinct eigenvalues, for all $b \geq 3$,

$$\begin{array}{rl} c_2 - (b-2)c_3 & \text{multiplicity } b-1; \\ c_2 + 2c_3 & \text{multiplicity } (b-1)(b-2)/2. \end{array}$$

When $b = 2$ only the first occurs, reducing to $c_2 = 1$ (and thus coinciding with the $\mathcal{U}^+$-eigenvalue in this case).

Finally, it is necessary to allow for the fact that any 2-subset S of the k colours gives rise to these eigenvalues. In fact, for each $\mathcal{U}^+$-eigenvalue the multiplicity is multiplied by $\frac{1}{2}k(k-3)$ and for each $\mathcal{U}^-$-eigenvalue the multiplicity is multiplied by $\frac{1}{2}(k-1)(k-2)$.

Explicitly, the full set of eigenvalues at levels $0, 1, 2$, for all $b \geq 4$, is as follows.

Level 0

$$c_0 \quad \text{multiplicity } 1$$

Level 1

$$\begin{array}{rl} -c_1 + (b-1)c_2 & \text{multiplicity } k-1 \\ -c_1 - c_2 & \text{multiplicity } (k-1)(b-1) \end{array}$$

Level 2

$$\begin{array}{rl} c_2 - (2b-4)c_3 + (b-2)(b-3)c_4 & \text{multiplicity } k(k-3)/2 \\ c_2 - (b-4)c_3 - (2b-6)c_4 & \text{multiplicity } k(k-3)(b-1)/2 \\ c_2 + 2c_3 + 2c_4 & \text{multiplicity } k(k-3)b(b-3)/4 \\ c_2 - (b-2)c_3 & \text{multiplicity } (k-1)(k-2)(b-1)/2 \\ c_2 + 2c_3 & \text{multiplicity } (k-1)(k-2)(b-1)(b-2)/4 \end{array}$$

In these formulae, it must be remembered that each c_i is an expression involving b and k. Replacing k by a complex variable z, the eigenvalues listed determine the leading terms in the chromatic polynomial $P(B_n(b);z)$, and can be used to study the behaviour of its roots. The cases $b=2$ and $b=3$ have been covered fully in [7] and [6] respectively, and here we shall discuss briefly the general case $b \geq 4$.

Recall that the functions c_i are given by $c_i(b,z) = C(b-i, z-i)$, where C is defined by an explicit sum involving falling factorials. It follows from the definition that c_i satisfies the following recurrence (with respect to b):

$$c_i(b+1,z) = (z-b)c_i(b,z) - c_i(b,z-1) \quad (0 \leq i \leq b).$$

Using this recurrence in the case $i=0$, P.Reinfeld has shown that all real zeros ζ of $c_0(b,z)$ satisfy $|\zeta| \leq b$. The empirical evidence suggests that this holds also for the complex zeros. If that is so, the 'Rouché' argument, along the lines given at the end of Section 6, will establish the existence of constants R_b such that

$$\text{for all } n \geq 3, \quad P(B_n(b);\zeta) = 0 \quad \Longrightarrow \quad |\zeta| \leq R_b.$$

Note that the degree of $B_n(b)$ is $b+1$, so the general result of Sokal [10] yields the result with $R_b = 8(b+1)$.

More specific information about the zeros can be obtained from the theorem of Beraha, Kahane, and Weiss [1]. This will form the subject of another paper.

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