communications in mathematica

and in computer chemistry

no. 46, October 2002 MATCDY (46) 215 – 233 (2002) ISSN 0340 - 6253

Redfield's Contributions to Enumeration

E. Keith Lloyd

Faculty of Mathematical Studies
University of Southampton
SOUTHAMPTON, SO17 1BJ
United Kingdom
ekl@maths.soton.ac.uk

1. Introduction

One of the first mathematicians to consider the problem of enumerating chemical isomers was Arthur Cayley¹ (1821-1895) (see, for example [2]). In the 1930s, his ideas were followed up by George Pólya (1887-1985) whose work culminated with a lengthy paper published in 1937 [11]; this was quickly recognised as a major contribution to the subject. Pólya's paper is based largely on a single theorem, his "Hauptsatz", and it was to be many years before the mathematical world became aware that Pólya was not the first person to discover the technique in that theorem. Whilst not explicitly stating the theorem, J. Howard Redfield had used it in a paper in 1927 [14]. This was the only paper

¹ In several places in the chemistry literature (see [15] for example), he is incorrectly referred to as Sir Arthur Cayley. This may be due to confusion with Sir George Cayley (1772-1857), the pioneer of aerodynamics.

by Redfield published in his lifetime, but it was not the end of his mathematical researches, for he went on to develop a theory of what he termed extended characters. But just as Pólya wrote his paper unaware of Redfield's work, so Redfield was not aware that his extended characters had also been discovered previously: they are in the second edition of Burnside's book [1], but Burnside called them marks. Redfield continued his researches during the 1930s and, in 1940, he submitted a second paper to the American Journal of Mathematics. Unfortunately this paper was rejected and it was not to appear in print until 1984 [17]. Other unpublished material has also been found in Redfield's "Nachlass". The two Redfield papers anticipated many of the major developments in the theory of enumeration made from the 1930s to the 1960s.

This is not the place to discuss why Redfield's first paper remained unread, nor whether his second paper should have been rejected. Suffice it to say that if their contents had been known and appreciated at the time, then the history of enumeration in the Twentieth Century would have been very different. In the present paper some of the main ideas in Redfield's work are discussed and it is concluded that sometimes it is simpler to dispense with Redfield's frame group. Chemical applications of Redfield's techniques are not given here, but some can be found in [7] and [8] and in the references therein.

2. Who was Redfield?

John Howard Redfield, Jnr, (1879-1944) was born in Philadelphia. He attended the Penn Charter School (motto: "Good instruction is better than riches"), where he received a good classical education. Then, over a rather protracted period, interspersed with periods of work, he obtained qualifications from a number of reputable colleges and universities in a variety of subjects:

- 1899 B.S. (mechanalia), Haverford College;
- 1902 B.S. (civil engineering), Massachusetts Institute of Technology;
- 1908 Certificat d'études Françaises, Université de Paris;
- 1910 M.A. (Romance languages) Harvard;
- 1914 Ph.D. Harvard.

His Ph.D. thesis was entitled "The earlier Latin-Romance Loan Words in Basque and their Bearing on the History of Basque and the Neighbouring Romance Languages". Part

of it consists of long lists of words and it is of interest to note that his grand-father, another John Howard Redfield, also produced long lists in his field of interest (see, for example, [13]).

Although the younger Redfield had several short term lecturing appointments, variously in languages and in mathematics, for much of his working life he earned his living as a civil engineer. For a few months in 1937, for example, he was structural designer of steel and reinforced concrete for a technical high school building at Wilmington, Delaware. Further biographical details of Redfield may be found in [6].

3. The 1927 Paper

Amongst the few mathematical books which Redfield owned were Love's two volumes on Elasticity [9]. This material would have been relevant to his professional work, but his interest in enumeration seems to have come from studying work of MacMahon, including [10], though what prompted him to do that is unknown.

Kerber [5], in this issue of *Match*, discusses the principal ideas of enumeration under group action in the present day language and notation of permutation groups. Except where stated otherwise, all references in this paper to Kerber are to [5]. The basic tool of the theory of enumeration under finite group action is what Kerber terms the Cauchy-Frobenius Lemma, but it is also referred to as Burnside's Lemma or, more neutrally, as the Orbit-Counting Lemma.

3.1 The Orbit-Counting Lemma The number of orbits of a finite group G acting on a finite set X is equal to the average number of fixed points:

$$\frac{1}{|G|} \sum_{g \in G} |X_g|,$$

where $X_g = \{x \in X | gx = x\}$ is the fixed point set of g.

Redfield introduced a polynomial which he called the *group-reduction function*; the same polynomial was introduced by Pólya and it is usually known by the name which he gave it: the *cycle index*. The polynomial leads to a generating function version of the

orbit-counting lemma. The new lemma is essentially a special case of the weighted version of the orbit-counting lemma discussed by Kerber, but in much of Pólya's work, the set Y is an infinite set, but subject to the restriction that for each $f \in Y^X$ and each $y \in Y$, the inverse image $f^{-1}(y)$ is a finite set. In such cases, the generating functions are usually power series rather than polynomials, but as this paper concentrates on Redfield's work, the reader is referred to Pólya and Read [12] for examples of the use of power series in the theory.

If a finite group G acts on a finite set X, then the action of each $g \in G$ splits X into disjoint cycles. For enumeration purposes, it is only the numbers of cycles of the various lengths (sizes) which are important, and not which set element is in which cycle.

3.2 Definition Let G be a finite group acting on a finite set X. The *cycle monomial* of the element $g \in G$ is defined to be the product

$$\prod_{i=1}^{|X|} S_i^{a_i(g)}$$

in the variables $s_1, s_2, ...$, where $a_i(g)$ is the number of *i*-cycles (cycles of length *i*) induced in X by g.

3.3 Definition The *cycle index* $Z(G, X; s_1, s_2,...)$ of a finite group G acting on a finite set X is the average of the cycle monomials of the group elements. Hence,

$$Z(G, X; s_1, s_2,...) = \frac{1}{|G|} \sum_{g \in G} \prod_{i=1}^{|X|} s_i^{a_i(g)}$$
.

(When convenient the left hand side will be abbreviated to $Z(G; s_1, s_2, ...)$.)

The polynomial in Kerber's Corollary 4.4 can be obtained by making the substitution

$$s_i = \sum_{v \in Y} y^i$$

in the cycle index. The notation s_i used here follows Redfield and he chose it since, in the above substitution, s_i is interpreted as the power sum symmetric function in the elements $y \in Y$.

3.5 Example How many ways are there to place four identical blue and two identical yellow balls at the vertices of a tetratagonal bipyramid?

The solid in question (see Fig. 1) can be obtained from the regular octahedron by moving vertically the top and bottom vertices the same distance away from (or closer to) the centre of the solid. Hence the tetragonal bipyramid has fewer symmetries than the octahedron. Hans Dolhaine has kindly pointed out to the author that this type of tetragonal distortion of icosahedral geometry does occur for some co-ordination complexes such as tetra-ammine cobalt dichloride Co(NH₃)₄Cl₂.



Fig, 1 A tetragonal bipyramid

As an abstract group, the rotation group of the tetragonal bipyramid is the dihedral group D_4 . The cycle index $Z(G, A; s_1, s_2,...)$ for the action of D_4 on a square A with vertices numbered 1, 2, 3, 4 cyclically is

$$Z(G, A; s_1, s_2,...) = \frac{1}{8} \{s_1^4 + 2s_4 - 3s_2^2 - 2s_1^2 s_2\}.$$

Each of the rotations (including the identity) extends to a rotation of the bipyramid with both 0 and 5 as fixed points. The four reflexions of the square correspond to rotations of the bipyramid in which vertices 0 and 5 interchange. Hence the cycle index for the action on the six vertices of a bipyramid B is

3.6
$$Z(D_4, B; s_1, s_2, ..., s_6) = \frac{1}{8} \{s_1^6 + 2s_1^2 s_4 + 2s_2^3 + 3s_1^2 s_2^2\}.$$

Here the weight w(t) of a ball can be defined informally as the initial letter of its colour, so.

$$w(\text{blue ball}) = b,$$

 $w(\text{yellow ball}) = y.$

More precisely, the weights lie in a polynomial ring generated by elements b and y with rational coefficients. Substituting $s_i = b^i + y^i$ in the cycle index gives a polynomial

$$P(b,y) = Z(D_4, B; s_i \to b^i + y^i)$$

$$= \frac{1}{8} \{ (b+y)^6 + 2(b+y)^2 (b^4 + y^4) + 2(b^2 + y^2)^3 + 3(b+y)^2 (b^2 + y^2)^2 \}$$

$$= b^6 + 2b^5 v + 4b^4 v^2 + 4b^3 v^3 + 4b^2 v^4 + 2bv^5 + v^6.$$

The coefficient 4 of the term $4b^4y^2$ is the solution to the question asked: there are four different ways to place four blue and two yellow balls at the corners of a regular tetragonal bipyramid.

The above solution has produced more information than was sought. For any non-negative integers p and q, the coefficient of $b^p y^q$ is the number of ways of placing p blue balls and q yellow balls at the vertices of the tetragonal bipyramid. Of course, if just one term in the expansion is required then there is no need to calculate P(b, y) in full - the labour can be reduced by expanding only those factors which will contribute to the desired term.

Much of Redfield's 1927 paper considers an alternative method of solution which does produce just the single number sought, but it involves the use of more than one cycle index. For the present example, two cycle indices are needed and the second one is that of the symmetry group of the four blue and two yellow balls. This is just the direct product $S_4 \times S_2$ of the symmetric group S_4 acting on the blue balls with the symmetric group S_2 on the yellow balls. The cycle indices of S_4 and S_2 are

$$Z(S_4; s_1, s_2, s_3, s_4) = \frac{1}{24} \{s_1^4 + 6s_1^2 s_2 + 8s_1 s_3 + 3s_2^2 + 6s_4\}$$

and

$$Z(S_2; s_1, s_2) = \frac{1}{2} \{s_1^2 + s_2\}.$$

Since the cycle index of a direct product is the product of the cycle indices, the cycle index of $S_4 \times S_2$ is

3.7
$$Z(S_4 \times S_2; s_1, s_2, s_3, s_4) = \frac{1}{24} \{s_1^4 + 6s_1^2 s_2 + 8s_1 s_3 + 3s_2^2 + 6s_4\} \times \frac{1}{2} \{s_1^2 + s_2\}$$

$$= \frac{1}{48} \left\{ s_1^6 + 7s_1^4 s_2 + 8s_1^3 s_3 + 9s_1^2 s_2^2 + 6s_1^2 s_4 + 8s_1 s_2 s_3 + 3s_2^3 + 6s_2 s_4 \right\}$$

Redfield introduced a composition of (binary operation on) polynomials which nowadays is usually denoted by *. It is defined as follows:

· for two identical monomials

$$s_1^{a_1}s_2^{a_2}...s_r^{a_r} * s_1^{a_1}s_2^{a_2}...s_r^{a_r} = 1^{a_1}a_1!2^{a_2}a_2!...r^{a_r}a_r!s_1^{a_1}s_2^{a_2}...s_r^{a_r};$$

- the composition of two non-identical monomials is zero;
- the composition * is distributive over addition of monomials, so the composition of two polynomials can be multiplied out as if * were ordinary multiplication.

Applying these rules to the cycle indices 3.6 and 3.7 gives:

$$\begin{split} &\frac{1}{8}\{s_1^6 + 2s_1^2s_4 + 2s_2^3 + 3s_1^2s_2^2\} \\ &* \frac{1}{48}\{s_1^6 + 7s_1^4s_2 + 8s_1^3s_3 + 9s_1^2s_2^2 + 6s_1^2s_4 + 8s_1s_2s_3 + 3s_2^3 + 6s_2s_4\} \\ &= \frac{1}{88448}\{1^66!s_1^6 + 12(1^22!4^1!!)s_1^2s_4 + 6(2^33!)s_2^3 + 27(1^22!2^22!)s_1^2s_2^2\} \,. \end{split}$$

Finally, the answer to the question posed is the sum of the coefficients in this polynomial. This is

$$\{720 + 96 + 288 + 432\}/384 + 4$$

in agreement with the answer obtained earlier.

The two methods of solution correspond to two different formulations of the problem. In the first method a distribution of balls at the vertices is regarded as a function $f: X \to Y$ where X is the set of six vertices and $Y = \{b, y\}$ is a set of two coloured balls. The single group G acts on the set X. In the second method, a distribution is regarded as a one-one correspondence between the set of six vertices and the collection (or multiset) of four blue and two yellow balls. There are two groups, one acting on the vertices and the other on the balls. Thus in the second formulation, the vertices and balls play symmetrical roles and the ideas can be extended to one-one-...-one correspondences. In

the 1927 paper Redfield considers q sets which he calls *ranges*, each of which has a group G_b , called a *range group*, acting on it (i = 1, 2, ..., q).

The above example is not one given by Redfield; he illustrates the method by finding the number of ways of placing four black and four white balls at the vertices of a cube. The answer to this problem is seven, but the method gives only the number of cubes and no information on how to construct them. With so few, however, it is not hard to think out what they are and Redfield draws them. He then notes that each of the seven has its own symmetry (or stabiliser) group and he seeks a method for breaking down the counting according to the individual symmetry groups. In the 1920s, he was only partially successful in solving this problem. If the possible symmetry groups are $H_1, H_2, ..., H_r$ and there are ξ_i arrangements with symmetry group H_i , then he proved that the various cycle indices satisfy

3.8
$$Z(G_1)^* Z(G_2)^* ... * Z(G_q) = \sum_{i=1}^r \xi_i Z(H_i),$$

where G_1 , G_2 , ..., G_q are the range groups. But to solve the problem posed by Redfield requires finding the ζ_i when the range groups G_i are given. This cannot be done in general, since different H_i may have identical cycle indices and, furthermore, the cycle indices of the H_i are not always linearly independent. Redfield gave two possible decompositions for his example of the cube:

$$\begin{split} &\frac{1}{24} \{70s_1^8 + 54s_2^4 - 32s_3^2s_1^2 - 12s_4^2\} \\ &= \frac{1}{12} \{s_1^8 + 3s_2^4 + 8s_3^2s_1^2\} + \frac{1}{4} \{s_1^8 + s_2^4 + 2s_4^2\} + \frac{1}{4} \{s_1^8 + 3s_2^4\} \\ &+ \frac{1}{3} \{s_1^8 + 2s_2^2s_1^2\} + 2[\frac{1}{2} \{s_1^8 + s_2^4\}] + s_1^8 \\ &= \frac{1}{4} \{s_1^8 + s_2^4 + 2s_4^2\} + 2[\frac{1}{3} \{s_1^8 + 2s_3^2s_1^2\}] - 4[\frac{1}{2} \{s_1^8 - s_2^4\}]. \end{split}$$

The first decomposition is the correct one, but this cannot be deduced from the algebra alone. The fact is that the cycle index is the wrong tool to do enumeration according to symmetry groups as Redfield was later to realise.

4. Redfield's Researches in the 1930s (Marks of Permutation Groups)

From a typescript dated 1935 [15], we know that by that date Redfield knew how to solve the problem of enumeration by symmetry group, but he had not yet proved that the method always works. Not long afterwards, he had obtained a proof, but, in a typescript produced for a lecture which he gave at Pennsylvania State University in 1937, he stated "... none of these proofs has yet been brought to a degree of elegance which would permit me to give any intelligible account of them in the time available". The 1937 typescript has now been published [16]. Instead of the cycle index, Redfield used what he termed extended characters, but Burnside [1] had introduced them under the name of marks. It was not until 1940 that Redfield submitted a paper containing his solution, but it was rejected at that time and was to remain unpublished until 1984 [17].

Much of Redfield's 1927 paper can be reformulated in terms of group characters and this was done by Foulkes [3]. In addition, he showed in that paper that marks can be used to solve the problem of enumerating by symmetry group, but he was, of course, unaware that Redfield had already done this in the 1930s.

In the 1940 paper, Redfield again considers one-one-...-one correspondences between q sets of objects each with a range group G_i (i = 1, 2, ..., q) acting on it. But now every range group is a subgroup of a supergroup F which he termed the *frame group*. The frame group was absent from the 1927 paper but, with hindsight, Redfield points out that it can be introduced there as a symmetric group; it would be S_8 in the case of his cube problem.

Redfield's method for enumerating arrangements is to use the mark table of the frame group. Both Burnside and Redfield wrote mark tables as lower triangular matrices, so they are transposed about the main diagonal compared with the way in which Kerber

writes them. When written in lower triangular form each number in the first column of the mark table is the number of cosets of the corresponding subgroup in the whole group.

4.1 Definition The row $\mathbf{m}(H_i)$ of a lower triangular mark table corresponding to subgroup H_i is called the *mark vector* of H_i .

The analogue of the composition * of cycle indices is the co-ordinate by co-ordinate product (denoted here by •) of mark vectors, and the analogue of equation 3.8 is:

4.2
$$\mathbf{m}(G_1) \bullet \mathbf{m}(G_2) \bullet \dots \bullet \quad (G_q) = \sum_{i=1}^r \xi_i \quad (H_i),$$

where the marks are those of the subgroups of the frame group F.

In his 1940 paper, Redfield illustrates his theory by superposing icosahedra each of which has certain faces marked in some way. Specifically he marks an antipodal pair of faces of the first icosahedron with the letter A, an antipodal pair of the second icosahedron with B, etc. The frame group is the icosahedral group (the rotation group of the icosahedron), and this is isomorphic to the alternating group A_3 . Each range group is the rotation group of an icosahedron with two antipodal faces marked in the same way and this group has order six. Redfield does calculations for the superposition of two and of three icosahedra. Not surprisingly with three icosahedra, most superpositions have identity symmetry.

The frame group can be any supergroup containing all the range groups, but it is desirable to take it as small as possible. The bigger the group, the more subgroups it will have and the bigger the mark table will be. For many examples, the frame group is so large that finding its mark table is difficult or impossible. Nevertheless, when the mark table of the frame group is known, then Redfield's use of it has an elegant simplicity about it and the method will be illustrated with a larger example than Redfield gave. The frame group will be the symmetric group S_5 , which has twice the order of A_5 and nineteen conjugacy classes of subgroups instead of nine. A transversal $\{U_i\}$ of the conjugacy classes of the subgroups of S_5 , together with the mark table is given by Kerber [4]. These are reproduced below, but with the mark table in lower triangular form. As is now customary, zeros above the main diagonal are omitted and other zeros are denoted by dots.

4.3 Problem Enumerate according to their symmetry groups, the structures obtained by placing three blue and two yellow balls at the vertices of a square-based pyramid (see Fig. 2).



Fig. 2 A square-based pyramid

```
120
U_1 = \langle 1 \rangle
U_2 = \langle (34) \rangle
U_3 = \langle (01)(34) \rangle
                                          60
U_4 = \langle (021) \rangle
U_5 = \langle (04123) \rangle
U_6 = \langle (02), (34) \rangle
U_7 = \langle (0413) \rangle
U_8 = \langle (01)(34), (04)(13) \rangle
U_9 = \langle (021), (34) \rangle
U_{10} = \langle (021), (01) \rangle
U_{11} = \langle (021), (01)(34) \rangle
U_{12} = \langle (04123), (12)(34) \rangle
U_{13} = \langle (0413), (34) \rangle
U_{14} = \langle (021), (02), (34) \rangle
U_{15} = \langle (041), (043) \rangle
U_{16} = \langle (1423), (0312) \rangle
                                                                       . 2
U_{17} = \langle (0413), (0143) \rangle
                                                            2
U_{18} = \langle (04123), (01243) \rangle
                                           2
                                                       2 2 2 . . 2
                                                                                                 2 2
                                                       1111111111111111111
                                          1
U_{19} = S_5
```

Any rotation of the square-based pyramid fixes vertex 0 and cyclically permutes the other four vertices, so the rotation group of the pyramid is the cyclic group C_4 , which has 30 cosets in S_5 . There are three classes of subgroups with 30 cosets, but it is clear from the generating elements, that U_7 is the only one which is cyclic. So the mark vector for the rotation group of the bipyramid is

$$\mathbf{m}(U_7) = (30, 0, 2, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0).$$

The symmetry group of the balls is $S_3 \times S_2$ which, since it has order 12, has 10 cosets in S_5 . There are two classes of subgroups with 10 cosets, but again it is clear from the generating elements that U_{14} is an $S_3 \times S_2$ but that U_{15} is not. Hence the required mark vector for the group acting on the balls is

$$\mathbf{m}(U_{14}) = (10, 4, 2, 1, 0, 2, 0, 0, 1, 1, 1, 0, 0, 1, 0, 0, 0, 0, 0).$$

The co-ordinate by co-ordinate product of the two vectors is

To solve the problem, it remains to express this vector as a linear combination of the rows of the mark table. In other words, the vector $\xi = (\xi_1, \, \xi_2, \, ..., \, \xi_{19})$ must be found which satisfies

$$\mathbf{m}(U_7) \bullet \mathbf{m}(U_{14}) = \xi \mathbf{M}$$

where M is the mark table matrix. Hence

$$\xi = \{ \mathbf{m}(U_7) \bullet \mathbf{m}(U_{14}) \} \mathbf{B}$$

where the Burnside matrix $\mathbf{B} = \mathbf{M}^{-1}$. But since \mathbf{M} is triangular, rather than inverting \mathbf{M} , it is much easier to note that the final non-zero entry in the matrix is the 4 in the 3rd coordinate, and this can only be obtained from $\mathbf{m}(U_3)$. Subtracting $\mathbf{m}(U_3)$ from $\mathbf{m}(U_7) \bullet \mathbf{m}(U_{14})$ gives

and this vector is just twice the first row of the table. Hence

$$\mathbf{m}(U_7) \bullet \mathbf{m}(U_{14}) = \mathbf{m}(U_3) + 2\mathbf{m}(U_1).$$

The interpretation of this equation is that there are three ways to distribute three blue and two yellow balls at the vertices of a square based pyramid. One of these arrangements has a group conjugate to U_3 as its symmetry group whilst the other two have only identity symmetry (see Fig. 3, bottom row).

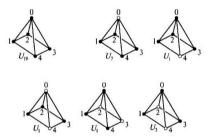


Fig. 3 Distributions of blue • and yellow • balls on a square-based pyramid.

It is just as easy to find the number of ways of distributing four blue and one yellow balls. The symmetry group $S_4 \times S_1$ has order 24, so it has 5 cosets in S_5 , therefore it must be conjugate to group U_{17} . Now

$$\mathbf{m}(U_7) \bullet \mathbf{m}(U_{17}) = (150, 0, 2, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

= $\mathbf{m}(U_7) + \mathbf{m}(U_1)$.

This time there are only two arrangements, one with U_7 symmetry and the other with identity symmetry (see Fig. 3, top row). Finally, there is, of course, only one way to place five blue balls on the pyramid (also shown in Fig. 3 top row) and this corresponds to the simple result that

$$\mathbf{m}(U_7) \bullet \mathbf{m}(U_{19}) = \mathbf{m}(U_7).$$

None of the distributions of the balls is chiral, so if the problem is reworked using the full symmetry group (including reflexions) of the square-based pyramid instead of the rotation group, then the same numbers of pyramids will be obtained but all the individual symmetry groups double in size. The mark vector $\mathbf{m}(U_{13})$ replaces the vector $\mathbf{m}(U_{7})$ in the products above and the reader may care to work out the corresponding linear combinations.

5. Post Redfield: Dispensing with the Frame Group

As already mentioned, Redfield's use of marks is constrained by the need to know the mark table of the frame group. When there are only two range groups G_1 and G_2 , however, it is sometimes possible to dispense with the frame group F. For problems of distributing balls at vertices (or ligands on sites of a co-ordination complex), the group G_2 is a direct product of symmetric groups. In such cases, reverting to the first formulation discussed in §3 dispenses with both the range group G_2 and the frame group F. It is then possible to use the mark table of G_1 for the enumeration. Furthermore, weight functions can also be incorporated into the enumeration (see Kerber's Corollary 7.3). This will be illustrated by revisiting example 3.5, but now the enumeration will be done according to symmetry groups as well as by weight. The mark table used will not be that of S_6 (which has 56 conjugacy classes of subgroups) but that of D_4 (which has only 8 such classes).

The symmetry group of the tetragonal bipyramid is the dihedral group D_4 , but since it is easier to write vectors of polynomials as column vectors rather than as row vectors, the mark table for D_4 and its inverse will now be written, in the style favoured by Kerber, as upper triangular matrices.

The cycle monomial of a group element $g \in G$ acting on a set X was defined in 3.2. In the theory of marks, the emphasis shifts to considering actions of entire subgroups rather than individual elements. It is appropriate, therefore, to introduce for groups an analogue of the cycle monomial.

5.1 Definition If G is a finite group acting on a finite set X, then the *orbit monomial* of the action is

where $a_i(G)$ is the number of *i*-orbits (orbits of size *i*) in the action.

The mark table of a group G is independent of the way in which G acts, but the orbit monomials are not. Kerber gives a transversal of the conjugacy classes of the subgroups of D_4 , together with the mark table. The subgroups in his list act on a square with vertices numbered 1, 2, 3, 4 in cyclic order. The square is two-dimensional and four of the elements in this action are reflexions. In the action on the tetragonal bipyramid, however, the corresponding elements are rotations in which vertices 0 and 5 are interchanged.

In §3, the substitution 3.4 was made into the cycle monomials in the cycle index; the same substitution will now be made into the orbit monomials. Details of the actions of D_4 on a square and on a tetragonal bipyramid are given in Tables 1 and 2 respectively.

Table 1 The Dihedral Group D4 acting on a Square

Column 1: the generators for subgroups acting on the square.

Column 2: the orbit monomials for the action on the square.

Column 3: the mark table of D_4 .

Table 2 The dihedral Group D4 acting on a Tetragonal Bipyramid

Column 1: the generators for subgroups acting on the bipyramid.

Column 2: the orbit monomials for the action on the bipyramid.

Column 3: generating functions for the orbits obtained by making substitution 3.4 into the orbit monomials.

$$\begin{array}{lll} U_1 = & \langle 1 \rangle & s_1^6 & \left[(b+y)^6 \\ U_2 = & \langle (13)(24) \rangle & s_1^2 s_2^2 \\ U_3 = & \langle (14)(23)(05) \rangle & s_2^3 & (b^2 + y^2)^2 \\ U_4 = & \langle (13)(05) \rangle & s_1^2 s_2^2 & (b^2 + y^2)^3 \\ U_5 = & \langle (14)(23), ((12)(34) \rangle & s_1^2 s_4 & (b^2 + y^2)(b^2 + y^2)^2 \\ U_6 = & \langle (13)(05), (24)(05) \rangle & s_2^2 & (b^2 + y^2)(b^4 + y^4) \\ U_7 = & \langle (1234) \rangle & s_1^2 s_4 & (b^2 + y^2)(b^4 + y^4) \\ U_8 = & \langle (1234), (24)(05) \rangle = D_4 & s_2 s_4 & (b^2 + y^2)(b^4 + y^4) \end{array}$$

One could solve the present problem without inverting the mark table, but since the vectors involved contain polynomials rather than integer entries, it is not quite so easy to do so. Instead Kerber's Corollary 7.3 can be used. That states that to enumerate arrangements according to symmetry group and weight, the Burnside matrix (inverse of the mark table) is applied to the vector of generating functions for the orbits. For the present example, the calculation gives

The summands b^5y , $2b^3y^3$, by^5 in row 4 of the column vector on the right hand side mean, respectively, that amongst the distributions with U_4 symmetry, there is one with 5 blue and 1 yellow balls, two with 3 balls of each colour and 1 with 1 blue and 5 yellow balls. The zero in row 5 means that none of the distributions has U_5 symmetry.

If only the numbers of distributions are required, then the solutions can be obtained by setting b = 1 = y. The corresponding calculation is

$$\begin{bmatrix}
1 & -1 & -2 & -2 & 2 & 2 & . & . \\
2 & . & . & -2 & -2 & -2 & 4 \\
4 & . & -4 & . & . & . \\
4 & . & -4 & . & . & . \\
4 & . & -4 & . & . & -4 \\
4 & . & -4 & . & . & 4
\end{bmatrix}
\begin{bmatrix}
64 \\
16 \\
8 \\
16 \\
4 \\
0 \\
2 \\
2 \\
4
\end{bmatrix}$$

Alternatively, in this case, the solutions can be obtained as in §4 without inverting the mark table.

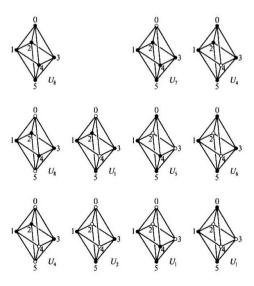


Fig. 4 Distributions of blue • and yellow o balls on a tetragonal bipyramid.

There are 18 distributions altogether, but each of the polynomials in the vectors above is symmetric in b and y. There are 11 distributions with p blue and q yellow balls with $p \ge q$. The 11 are illustrated in Fig. 4 with their symmetry groups indicated.

6. Conclusions

This paper has examined some of the enumeration techniques used by Redfield. In particular, his elegant use of mark tables has been explained, but this method is only practicable for fairly small groups, because of the difficulty of calculating mark tables. In certain cases, some of the groups can be eliminated and the mark table of a smaller group can be used.

References

- Burnside, W., Theory of Groups of Finite Order, Cambridge Univ. Press, London, 1897 (2nd edn. 1911, reprinted Dover, New York, 1955).
- [2] Cayley, A., On the analytical forms called trees, with application to the theory of chemical combinations, *Rep. Brit. Soc. Advance Sci.*, 45 (1875), 257-305 = *Math. Papers*, Vol. 9, 427-460.
- [3] Foulkes, H.O., On Redfield's group reduction functions, Canad. J. Math., 15 (1963), 272-284.
- [4] Kerber, A., Applied Finite Group Actions, Springer, Berlin, 1999.
- [5] Kerber, A., Enumeration under Finite Group Action, Basic Tools, Results and Methods, Match, No 46 (2002), 151-198.
- [6] Lloyd, E. Keith, J. Howard Redfield 1879-1944, J. Graph Theory, 8 (1984), 195-203.
- [7] Lloyd, E. Keith, Redfield's papers and their relevance to counting isomers and isomerizations, *Discrete Appl. Math.*, 19 (1988), 289-304; reprinted in: *Applications of Graphs in Chemistry and Physics*, (ewd. J.W. Kennedy and L.V. Quintas), North-Holland, Amsterdam, 1988, 289-304.
- [8] Lloyd, E. Keith, Marks of permutation groups and isomer enumeration, J. Math. Chem. 11 (1992), 207-222.

- [9] Love, A.E, A Treatise on the Mathematical Theory of Elasticity, Vols. I and II, Cambridge Univ. Press, Cambridge, 1892-3.
- [10] MacMahon, P.A., Combinatory Analysis, Vols. 1 and II, Cambridge Univ. Press, Cambridge, 1915-16.
- [11] Pólya, G., Kombinatorische Anzahlbestimmungen für Gruppen, Graphen und chemische Verbindungen, Acta Math., 68 (1937), 145-254.
- [12] Pólya, G. and Read, R.C., Combinatorial Enumeration of Groups, Graphs and Chemical Compounds, Springer, New York, 1987 [includes an English translation of [8]].
- [13] Redfield, J.H., [Snr], Catalogue of the known species, recent and fossil, of the family Marginellidæ, Amer. J. Conchol., 7 (1872), 215-269 Append.
- [14] Redfield, J. Howard, The theory of group-reduced distributions, Amer. J. Math., 49 (1927), 433-455.
- [15] Redfield, J. Howard, Further development of the theory of group-reduced distributions, unpublished typescript, 1935.
- [16] Redfield, J. Howard, Group theory applied to combinatory analysis, *Match* No 41 (2000), 7-27 [text written for a lecture given in 1937].
- [17] Redfield, J. Howard, Enumeration by frame group and range groups, J. Graph Theory, 8 (1984), 205-223 [originally submitted in 1940].
- [18] Rouvray, D.H., Uses of graph theory, Chemistry in Britain, 10 (1974), 11-18.