IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Combinatorial enumeration and group representations

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1982 J. Phys. A: Math. Gen. 15 3395

(http://iopscience.iop.org/0305-4470/15/11/016)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 129.252.86.83
The article was downloaded on 30/05/2010 at 15:01

Please note that terms and conditions apply.

J. Phys. A: Math. Gen. 15 (1982) 3395–3404. Printed in Great Britain

Combinatorial enumeration and group representations

D J Newman
Department of Physics, University of Hong Kong, Hong Kong

Received 21 May 1982

Abstract. It is shown that, in addition to the number of distinct equivalence classes, the representation characters of a 'labelling' can also be derived using standard combinatorial methods. These characters provide additional information on the structure of the equivalence classes which is relevant in physical applications.

1. Introduction

It is often necessary to enumerate the number of distinct configurations of a system embedded in a symmetrical framework, such as a lattice, described by a group G. In mathematical terms, it is necessary to determine the number of equivalence classes (or 'orbits') generated by G. The answer to this problem will, of course, depend on the symmetry of the system itself, as well as that of the framework in which it is embedded.

Enumeration problems of this type can be solved by applying the standard combinatorial theorems of Pólya and de Bruijn (Berge 1971). Pólya's theorem applies to the case of different labellings (or colourings) of components of a symmetric framework, such as points in a lattice, while de Bruijn's theorem selects systems in which the equivalence classes are also closed for a certain label permutation.

One limitation of the combinatorial approach is that it determines only the *number* of equivalence classes and provides no information on the number of system configurations contained in each class or the structure of the configurations. Another limitation is that the standard approach deals only with 'classical' objects (such as atoms) and not quantum mechanical objects (such as electrons), but we shall investigate this problem elsewhere. The aim of this work is to show that more information can be extracted from the standard combinatorial methods of analysis by exploiting the relationship between this approach and the (for physicists) more familiar techniques of group representation theory.

One application of this approach, used as an introductory example in § 2, is the labelling of symmetry coordinates describing displacements of shells of atoms surrounding a substituted ion in a crystal (e.g. see Newman 1981). Other examples occur in the description of the states of, and interactions between, electrons on lattices. The discussion of the a^2b^2 labelling given in §§ 3 and 4 is closely related to the description

0305-4470/82/113395+10\$02.00 © 1982 The Institute of Physics

of Coulomb interactions. It is intended to pursue these applications in subsequent publications in the process of developing a comprehensive theory of many-electron states in finite lattices.

2. Permutation representations for shells of atoms

It is convenient, in labelling and determining symmetry coordinates for displacements in a finite lattice of atoms, to study the permutations of atomic positions in the first instance (e.g. see Fieck 1977, Cousins 1978, Newman 1981). The characters of permutation representations are usually determined by counting the number of atoms left in fixed positions under the symmetry group operations of the finite lattice (or larger structure containing the lattice). They are therefore always positive.

Consider the labelling (or colouring) problem in which a single atom in a shell (Newman 1981) is distinguished from the remainder. The symmetry group then generates an equivalence class consisting of r labellings, where r is the number of atoms in the shell. The permutations of the members of this equivalence class under the group operations generate the same set of characters as those determined by counting fixed atoms under group operations. We shall show, in § 3, that standard combinatorial procedures can be adapted to calculate the characters corresponding to any given labelling. This provides an alternative procedure to counting fixed atoms.

A third method of finding the permutation representation characters is to determine the symmetry group which leaves one member of the equivalence class invariant. This must be a subgroup of the atomic framework group. Hence 'correlation' relations (such as those given in figure 2 of Newman (1981)) can be used to determine which irreducible representations of the atomic framework group correspond to the invariant representation of this subgroup. These representations are just the equivalence class representations referred to above. It is interesting to note that Littlewood (1958, ch IX) describes the subgroups of the symmetric groups in just this way: i.e. by giving the compound characters corresponding to the irreducible representations of the symmetric group induced by the invariant representation of the subgroup.

We can make the above considerations more concrete by means of a simple example: six atoms at the vertices of an octahedron. For the sake of simplicity we shall neglect inversion and reflection symmetries. It is easy to see (using the usual notation) that C_4 and C_2 operations leave the two atoms on the symmetry axis in fixed positions, while C_3 and C_2' operations move all atoms. In terms of the usual class sequence (E, $8C_3$, $3C_2$, $6C_2'$, $6C_4$) we obtain the characters (6, 0, 2, 0, 2) corresponding to the representation A_1+E+T_1. The combinatoric method of obtaining this result is described in § 3.

The third approach mentioned above begins with the observation that a six-fold octahedral system in which one atom is distinguished has symmetry C_4. Use of the correlation tables (such as those given by Butler 1981) then shows directly that the A representation of C_4 generates the octahedral group representation A_1+E+T_1.

Two useful relationships between combinatorial methods and group representation methods have emerged in this section:

(i) Every equivalence class corresponds to a representation with positive characters.

(ii) Every equivalence class corresponds to a specific subgroup of the overall symmetry of the framework.

These relationships form a background to the techniques developed in the following discussion.

3. Combinatorial methods and group characters

Pólya (1937; Berge 1971) introduced a very powerful method for determining the number of distinct equivalence classes corresponding to the labelling (or colouring) of elements in a framework. For our present purposes it is appropriate to suppose that the framework is a rigid array of similar atoms with symmetry group G. Each framework is characterised by a *cycle index*

$$P=\sum_{\lambda} n_{\lambda} \prod_{r} p_r^{\lambda_r} \Big/ \sum_{\lambda} n_{\lambda} \tag{3.1}$$

where n_λ is the multiplicity of class λ, and p_r represents a permutation cycle of length r. The exponent λ_r corresponds to the number of times a cycle of length r appears in the operators of class λ. $\Sigma_\lambda n_\lambda = |G|$, the number of elements in the group G.

It should be noted that P is determined by the way in which the elements in the framework transform under G, not just the group itself. For example, in the case of the octahedral system introduced in § 2,

$$P=\tfrac{1}{24}(p_1^6+8p_3^2+3p_1^2p_2^2+6p_2^3+6p_1^2p_4) \tag{3.2}$$

so that $\Sigma_r r\lambda_r = 6$ for each term. The corresponding expression for eight atoms at the corners of a cube has $\Sigma_r r\lambda_r = 8$.

In order to determine the number of equivalence classes for a labelled framework we substitute the following labelling specification for the p_k:

$$p_k = 1 + \mathrm{a}^k + \mathrm{b}^k + \ldots$$

where a, b etc represent the different labels. The coefficient of $\mathrm{a}^\alpha \mathrm{b}^\beta \ldots$ in P then gives the number of equivalence classes in which α atoms are labelled a, β atoms are labelled b, etc.

The example introduced in § 2 corresponds to determining the coefficients of a in P with the substitution $p_k = 1 + \mathrm{a}^k$. This gives the result

$$P = \begin{array}{llllll} & (p_1^6) & (3p_1^2p_2^2) & & (6p_1^2p_4) & \\ \tfrac{1}{24}(& 1\times 6+ & \;\;3\times 2 & + & \;\;6\times 2) & =1 \end{array} \tag{3.3}$$

showing that the systems in which a single atom of the octahedral framework is labelled a form an equivalence class. More useful information can be obtained from this calculation however. It will be noticed that the coefficients in equation (3.3) corresponding to each cycle structure (or class) define the same character set (6, 0, 2, 0, 2) as was obtained by two alternative methods in § 2. This simple extension of the usual combinatoric calculation thus provides a third method of obtaining the irreducible representations corresponding to a permutation representation.

In order to develop this idea we now introduce a running example in which the vertices of an octahedron are labelled a or b. In particular, we shall be interested in the number of equivalence classes for the $\mathrm{a}^2\mathrm{b}^2$ labelling which is given by the coefficient of $\mathrm{a}^2\mathrm{b}^2$ in P when $p_k = 1 + \mathrm{a}^k + \mathrm{b}^k$. This problem is related to counting the number of different possible Coulomb interactions. According to equation (3.2) the coefficient of a^2b^2 given by

$$\begin{array}{llll} & (p_1^6) & (3p_1^2p_2^2) & (6p_2^6) \\ \frac{1}{24}(& 1\times 90+ & 3\times 6 & +\ 6\times 6) = \frac{144}{24} = 6. \end{array} \tag{3.4}$$

This result gives no clue as to the *form* of the different systems which generate the equivalence classes or the number of systems in a given class. Nevertheless, it provides information which is of use in obtaining diagrams corresponding to each class, as it determines the number of distinct forms of diagram to look for. (These are shown in figure 1 for the present example.)

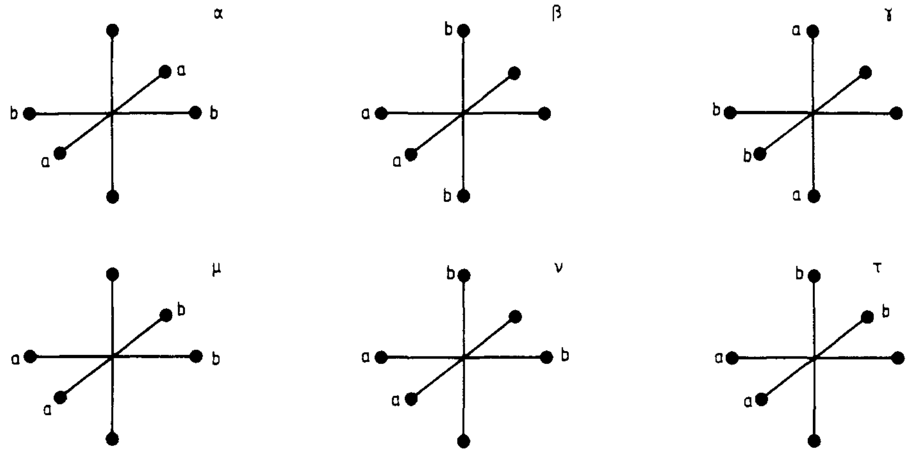

Figure 1. Members of the six equivalence classes for the a^2b^2 labelling of the vertices of an octahedron.

The calculation shown in equation (3.4) in fact provides the complete set of characters (90, 0, 6, 6, 0) for the a^2b^2 labelling. These can in turn be related to the decomposition of the labelling into irreducible representations which, however, do not themselves correspond to equivalence classes. We shall discuss the analysis of labellings into equivalence classes in § 4.

An extension of Pólya's method by de Bruijn (1964; Berge 1971) allows for the possibility that further symmetries are required between distinct labellings. For example, we may only be interested in those equivalence classes which are preserved under the interchange $a \leftrightarrow b$ in the above example. Inspection of figure 1 shows that this is true for α, μ, ν and τ but not β and γ.

de Bruijn's method involves the calculation of the coefficient of a^2b^2 in P with the substitution

$$p_k = 1 + 2a^{k/2}b^{k/2} \qquad (k \text{ even}),$$

$$p_k = 1 \qquad (k \text{ odd}).$$

This gives (for our example):

$$\begin{array}{llll} & (3p_1^2p_2^2) & (6p_2^3) & (6p_1^2p_4) \\ \frac{1}{24}(& 3\times 4 & +\ 6\times 12+ & 6\times 2) = 4 \end{array} \tag{3.5}$$

confirming that two of the diagrams in figure 1 are eliminated by the additional restriction of closure under a$\leftrightarrow$b interchange. Again we note that information is being lost in the above calculation, for we have determined the character set $(0, 0, 4, 12, 2)$ in (3.5).

In physical applications we are likely to take a rather different attitude towards the enumeration of equivalence classes from that taken by de Bruijn. The a$\leftrightarrow$b interchange symmetry would arise from physical considerations and hence would be interpreted as producing a single equivalence class $\beta+\gamma$ from the separate classes β, γ rather than eliminating both of them. This approach also enables us to find an interpretation of the de Bruijn characters.

An algebraic expression of the above interpretation is to say that we seek the equivalence classes under the direct product group $\mathbf{O}\otimes\mathbf{H}$, where $\mathbf{H}=\{\mathrm{E}, h\}$ and h is the a$\leftrightarrow$b interchange operator. $\mathbf{H}$ can be treated in an analogous fashion to the assignment of parity in point groups which contain the inversion operator. That is to say we construct a direct product of the character tables for $\mathbf{O}$ and $\mathbf{H}$. Then the de Bruijn characters correspond to the classes (h, $8h\mathrm{C}_3$, $3h\mathrm{C}_2$, $6h\mathrm{C}_2'$, $6h\mathrm{C}_4$) in sequence. Putting the two sets of characters together we obtain the number of equivalence classes for $\mathbf{O}\otimes\mathbf{H}$ as follows:

$$\begin{array}{lllllll} (p_1^6) & (3p_1^2p_2^2) & (6p_2^3) & (3hp_1^2p_2^2) & (6hp_2^3) & (6hp_1^2p_4) & \\ \frac{1}{48}(1\times 90+ & 3\times 6 & +6\times 6+ & 3\times 4 & +6\times 12+ & 6\times 2) & =5. \end{array} \tag{3.6}$$

This shows that two of the original equivalence classes have been condensed into one. The methods of analysing characters discussed in § 4 will enable us to be rather more explicit.

4. Equivalence class representations

It was shown in § 2 that each system in an equivalence class determines a unique subgroup of the framework group, and that the characters of the equivalence class representation can be generated by means of its correlation with the invariant representation of this subgroup. Using this method it is easy to determine a unique representation for any subgroup of a framework group. As an example, they are given for all subgroups of the octahedral groups O and $\mathrm{O_h}$ in tables 1 and 2 respectively. In these tables (geometrically) isomorphic but non-conjugate subgroups are distinguished, for example $\mathrm{D_2}$ and $\mathrm{D_2'}$, where $\mathrm{D_2}$ contains three $\mathrm{C_2}$ operators and $\mathrm{D_2'}$ contains two $\mathrm{C_2'}$ operators and only one $\mathrm{C_2}$ operator.

It should be noted that every equivalence class group contains the invariant representation of the framework group once, and once only. This follows from the method of generation outlined above. In the usual application of Pólya's theorem the characters are used to determine the number of occurrences of the invariant representation in the labelling representation, and the result is interpreted as the number of equivalence classes.

In § 3 we noticed that some information was lost in the standard procedure of determining the number of distinct equivalence classes using the theorems of Pólya and de Bruijn and that, in fact, the complete characters of the representations induced by the labelling can be derived. Characters derived from Pólya's theorem for the a, b labelling of the six vertices of an octahedron are given in table 3 for the group O. It

Table 1. Equivalence class representations and characters for the octahedral group O.

Subgroup	E	$8C_3$	$3C_2$	$6C_2'$	$6C_4$	Irreducible components
O	1	1	1	1	1	A_1
T	2	2	2	0	0	A_1+A_2
D_4	3	0	3	1	1	A_1+E
D_3	4	1	0	2	0	A_1+T_2
C_3	8	2	0	0	0	$A_1+A_2+T_1+T_2$
C_4	6	0	2	0	2	A_1+E+T_1
D_2	6	0	6	0	0	A_1+A_2+2E
D_2'	6	0	2	2	0	A_1+E+T_2
C_2	12	0	4	0	0	$A_1+A_2+2E+T_1+T_2$
C_2'	12	0	0	2	0	$A_1+E+T_1+2T_2$
C_1	24	0	0	0	0	$A_1+A_2+2E+3T_1+3T_2$

(Classes: E, $8C_3$, $3C_2$, $6C_2'$, $6C_4$)

will be seen that these characters alone are sufficient to specify uniquely the symmetry of the members of all equivalence classes in all cases except one. We cannot, of course, expect to obtain a unique reduction to equivalence class representations in general (in an analogous way to the reduction to irreducible representations) because there are eleven distinct equivalence class representations for the group O, and only five classes.

We now return to the example of a^2b^2 labelling, which was introduced in § 3. We shall use curly brackets to denote representations corresponding to the enclosed symbols. Inspection of tables 1 and 3 shows that we may write $\{a^2b^2\}$ as a sum over possible equivalence class representations as follows:

$$\{a^2b^2\}=A\{D_2\}+B\{D_2'\}+C\{C_2\}+D\{C_2'\}+E\{C_1\}.$$

Using the characters given in table 1, three equations can be obtained:

$$90=6A+6B+6C+12D+24E, \tag{4.1}$$

$$6=6A+2B+4C, \tag{4.2}$$

$$6=2B+2D, \tag{4.3}$$

where all unknowns are positive integers or zero. Equation (4.2) allows the solutions

$$\begin{aligned} &\text{(i)} && A=1, && B=C=0, && \\ &\text{(ii)} && A=0, && B=3, && C=0, \\ &\text{(iii)} && A=0, && B=1, && C=1. \end{aligned} \tag{4.4}$$

Putting these values into equations (4.1) and (4.3) it is easy to show that all three solutions lead to possible values of D and E as follows:

$$\begin{aligned} &\text{(i)} && D=3, && E=2, \\ &\text{(ii)} && D=0, && E=3, \\ &\text{(iii)} && D=2, && E=2. \end{aligned} \tag{4.5}$$

Although we cannot distinguish between these three solutions algebraically, figure 1α alone shows it is possible to construct a D_2 symmetry class, so that (i) is the unique

Table 2. Equivalence class of subgroup representations of the group O_h.

Classes:	E	$8C_3$	$3C_2$	$6C_2'$	$6C_4$	i	$8iC_3$	$3iC_2$	$6iC_2'$	$6iC_4$	Irreducible components
O_h	1	1	1	1	1	1	1	1	1	1	A_{1g}
O	2	2	2	2	2	0	0	0	0	0	$A_{1g}+A_{1u}$
T_d	2	2	2	0	0	0	0	0	2	2	$A_{1g}+A_{2u}$
T_h	2	2	2	0	0	2	2	2	0	0	$A_{1g}+A_{2g}$
T	4	4	4	0	0	0	0	0	0	0	$A_{1g}+A_{2g}+A_{1u}+A_{2u}$
D_{4h}	3	0	3	1	1	3	0	3	1	1	$A_{1g}+E_g$
D_4	6	0	6	2	2	0	0	0	0	0	$A_{1g}+E_g+A_{1u}+E_u$
D_{3d}	4	1	0	2	0	4	1	0	2	0	$A_{1g}+T_{2g}$
D_3	8	2	0	4	0	0	0	0	0	0	$A_{1g}+T_{2g}+A_{1u}+T_{1u}$
D_{2h}	6	0	6	0	0	6	0	6	0	0	$A_{1g}+A_{2g}+2E_g$
D_2	12	0	12	0	0	0	0	0	0	0	$A_{1g}+A_{2g}+2E_g+A_{1u}+A_{2u}+2E_u$
C_{4h}	6	0	2	0	2	6	0	2	0	2	$A_{1g}+E_g+T_{1g}$
C_4	12	0	4	0	4	0	0	0	0	0	$A_{1g}+E_g+T_{1g}+A_{1u}+E_u+T_{1u}$
D_{2h}'	6	0	2	2	0	6	0	2	2	0	$A_{1g}+E_g+T_{2g}$
D_2'	12	0	4	4	0	0	0	0	0	0	$A_{1g}+E_g+T_{2g}+A_{1u}+E_u+T_{2u}$
D_{2d}	6	0	6	0	0	0	0	0	2	2	$A_{1g}+A_{2u}+E_u+E_g$
D_{2d}'	6	0	2	0	2	0	0	4	0	2	$A_{1g}+E_g+T_{2u}$
C_{4v}	6	0	2	0	2	0	0	4	2	0	$A_{1g}+E_g+T_{1u}$
S_6	8	2	0	0	0	8	2	0	0	0	$A_{1g}+A_{2g}+T_{1g}+T_{2g}$
C_3	16	4	0	0	0	0	0	0	0	0	$A_{1g}+A_{2g}+T_{1g}+T_{2g}+A_{1u}+A_{2u}+T_{1u}+T_{2u}$
C_{3v}	8	2	0	0	0	0	0	0	4	0	$A_{1g}+A_{2u}+T_{1u}+T_{2g}$
C_{2h}	12	0	4	0	0	12	0	4	0	0	$A_{1g}+A_{2g}+2E_g+T_{1g}+T_{2g}$
C_2	24	0	8	0	0	0	0	0	0	0	$A_{1g}+2E_g+T_{1u}+A_{2g}+T_{2u}+T_{1g}+A_{1u}+2E_u+T_{2g}+A_{2u}$
C_{2h}'	12	0	0	2	0	12	0	0	2	0	$A_{1g}+E_g+2T_{2g}+T_{1g}$
C_2'	24	0	0	4	0	0	0	0	0	0	$A_{1g}+E_g+2T_{2g}+T_{1u}+2T_{2u}+T_{1g}+A_{1u}+E_u$
C_{2v}''	12	0	0	2	0	0	0	4	2	0	$A_{1g}+E_g+T_{2g}+T_{1u}+T_{2u}$
C_{2v}'	12	0	4	0	0	0	0	0	4	0	$A_{1g}+A_{2u}+E_g+E_u+T_{1u}+T_{2g}$
C_{2v}	12	0	4	0	0	0	0	8	0	0	$A_{1g}+2E_g+T_{1u}+A_{2g}+T_{2u}$
S_4	12	0	4	0	0	0	0	0	0	4	$A_{1g}+A_{2u}+E_g+E_u+T_{1g}+T_{2u}$
C_s, C_{1h}	24	0	0	0	0	0	0	8	0	0	$A_{1g}+A_{2g}+2E_g+T_{1g}+T_{2g}+2T_{1u}+2T_{2u}$
C_{1h}'	24	0	0	0	0	0	0	0	4	0	$A_{1g}+E_g+2T_{2g}+T_{1g}+A_{2u}+E_{1u}+2T_{1u}+T_{2u}$
S_2	24	0	0	0	0	24	0	0	0	0	$A_{1g}+A_{2g}+2E_g+3T_{1g}+3T_{2g}$
C_1	48	0	0	0	0	0	0	0	0	0	$A_{1g}+A_{2g}+2E_g+3T_{1g}+3T_{2g}+A_{1u}+A_{2u}+2E_u+3T_{1u}+3T_{2u}$

Table 3. Octahedral group O representations generated by a, b labelling of the six vertices of an octahedron.

Labelling	(1^6) E	$8(3^2)$ $8C_3$	$3(1^2 2^2)$ $3C_2$	$6(2^3)$ $6C_2'$	$6(1^2 4)$ $6C_4$	Equivalence classes
$a, b, a^5b, ab^5, a^5, b^5$	4	0	2	0	2	C_4
$a^2, b^2, a^4b^2, a^2b^4, a^4, b^4$	15	0	3	3	1	D_4+C_2'
ab, a^4b, ab^4	30	0	2	0	2	C_1+C_4
a^3, b^3, a^3b^3	20	2	4	0	0	C_3+C_2
$a^2b, b^2a, a^2b^3, a^3b^2, a^3b, ab^3$	60	0	4	0	0	$2C_1+C_2$
a^2b^2	90	0	6	6	0	see text
a^6, b^6	1	1	1	1	1	O
Equivalence classes g the subgroup $[6]+[2^3]$ of S_6						
a^2b^2	30	0	6	0	0	D_2+C_1
	60	0	0	6	0	$3C_2'+C_1$
	60	0	4	0	0	$2C_1+C_2$

correct solution to our problem, and

$$\{a^2b^2\}=\{D_2\}+3\{C_2'\}+2\{C_1\}.$$

This approach is still not entirely satisfactory. Although it provides a much more detailed check on the enumeration of equivalence class diagrams than that obtained in the usual method of applying Pólya's theorem, it still does not provide an explicit set of instructions for constructing such diagrams. Yet, in principle, there is sufficient information in the algebraic structure to enable this to be done.

Any labelling of n objects generates a single equivalence class with respect to the symmetric group S_n. Hence, if we can find an intermediate group X in the chain $S_6 \supset X \supset O$, it may provide a unique separation of the a^2b^2 labelling class in S_6. These equivalence classes may then, in turn, provide a unique separation into the equivalence classes of the group O. In fact Littlewood (1958, p 274) lists a subgroup of order 120, denoted by the S_6 characters $[6]+[2^3]$, which has just this property.

In S_6, the a^2b^2 labelling is invariant under the group E, (12), (34), (56), (12)(34), (12)(56), (34)(56) and (12)(34)(56). The subgroup $[6]+[2^3]$ does not contain the elements with cycle structure $1^4 2$, so that the only possible non-trivial symmetries of the a^2b^2 labelling are the four-element group E, (12)(34), (12)(56), (34)(56) and the two-element groups E, (12)(34)(56) and E, (12)(34), etc. These define equivalence classes with $120/4=30$ and $120/2=60$ components respectively. Hence the 90-component equivalence class corresponding to the a^2b^2 labelling must break down into one class of each dimension or three of dimension 30. The characters for each class are shown at the bottom of table 3, where the *unique* separation into $[6]+[2^3]$ equivalence classes and the consequent *unique* separation of these into O equivalence classes is also shown.

The de Bruijn characters for the direct product of the point symmetry and $a \leftrightarrow b$ label interchange groups are given in table 4. In the cases of ab and a^3b^3 labelling the equivalence classes given in table 3 are not affected. However, as was shown in § 3, the a^2b^2 labelling has one less equivalence class with $a \leftrightarrow b$, interchange symmetry. This implies that two of the original equivalence classes, which interchange under $a \leftrightarrow b$, have been joined into a single class. (Inspection of figure 1 shows these to be the equivalence classses β and γ.)

Table 4. Characters for the additional classes of the direct product group $O\otimes(E, h)$.

	h	$8hC_3$	$3hC_2$	$6hC_2'$	$6hC_4$	Representations
$O\|T$	0	0	0	2	2	$A_1+\tilde{A}_2$
$D_3\|C_3$	0	0	0	4	0	$A_1+\tilde{A}_2+\tilde{T}_1+T_2$
$D_4\|C_4$	0	0	4	2	0	$A_1+E+\tilde{T}_1$
$D_4\|D_2$	0	0	0	2	2	$A_1+\tilde{A}_2+E+\tilde{E}$
$D_4\|D_2'$	0	0	4	0	2	$A_1+E+\tilde{T}_2$
$D_2\|C_2$	0	0	8	0	0	$A_1+A_2+2E+\tilde{T}_1+\tilde{T}_2$
$D_2'\|C_2$	0	0	0	4	0	$A_1+\tilde{A}_2+E+\tilde{E}+\tilde{T}_1+T_2$
$D_2'\|C_2'$	0	0	4	2	0	$A_1+E+\tilde{T}_1+T_2+\tilde{T}_2$
$C_2'\|C_1$	0	0	0	4	0	$A_1+\tilde{A}_2+E+\tilde{E}+2T_2+\tilde{T}_2+2\tilde{T}_1+T_1$
$C_2\|C_1$	0	0	8	0	0	$A_1+A_2+2E+T_1+T_2+2\tilde{T}_1+2\tilde{T}_2$
ab	0	0	4	6	0	$C_2'\|C_1+D_4\|C_4$
a^2b^2	0	0	4	12	2	$2C_2'\|C_1+D_2'\|C_2'+(C_2'\tilde{C}_2')+D_4\|D_2$
a^3b^3	0	0	0	8	0	$D_2'\|C_2+D_3\|C_3$

Subgroups of the direct product group $\mathbf{O}\otimes\mathbf{H}$ are of two types: those with zero and those with non-zero characters for the additional classes. All possible examples of the latter case are given in table 4. Group labels consist of two parts written $X|Y$, where X corresponds to the symmetry of the system with $hC\to C$, where $h\equiv a\leftrightarrow b$ and C is any rotation operation. Y gives the spatial symmetry subgroup of O for members of the equivalence class. All subgroups with zero additional characters correspond to adjoining two similar subgroups S of O, which we write as $(S\tilde{S})$. These groups correspond to a doubling of the size of the corresponding equivalence class. Note that the additional group labels provide a more precise description of the equivalence classes, quite apart from allowing the separation of those classes which are closed under $a\leftrightarrow b$ operations.

5. Discussion

We have shown that considerably more information can be obtained about the equivalence classes generated by the labelling of a symmetrical framework by using all the (character) information available. The problem of finding a *unique* breakdown of a labelling into equivalence classes sometimes requires the identification of suitable groups intermediate between S_n and the spatial symmetry. Some of these groups have already been identified by Littlewood (1958) and others, but a more thorough investigation of these groups and their properties will be necessary in order to develop the techniques introduced in this paper into a systematic method.

Appendix. Schur functions and Pólya's method

The method described in this paper involves generating the complete set of characters associated with a given labelling and then analysing them into equivalence class characters. The method involves the search for positive integer solutions to a set of linear simultaneous equations, where each class provides a separate equation. An equivalent method would be to express both the labelling representation and the equivalence classes as combinations of irreducible representations. Then the analysis would consist of finding the positive integer solutions for a set of equations, each of which corresponds to an irreducible representation.

The number of each type of irreducible representation in a labelling can, of course, be determined from the characters. Alternatively, we could combine the formulae for the characters in such a way as to give the number of irreducible representations directly. In fact, Pólya's original method does just this for the number of invariant representations by adding the products of characters with class size and then dividing by the order of the group. Similar formulae can be derived using the characters $\chi_\lambda^{(\mu)}$ for the irreducible representation μ and class λ. Let n_λ be the number elements in a class and p_λ have the same interpretation as in § 3. Each irreducible representation can then be associated with its own cycle index

$$P(\mu)=\sum_\lambda n_\lambda \chi_\lambda^{(\mu)} \prod p_r^{\lambda_r}/|G| \tag{A1}$$

which generalises equation (3.1).

It is particularly interesting to note that, in the case of the symmetric groups, this formula is identical to the expression for the Schur (or S) functions $\{\mu\}$ given by Littlewood (1958 equation (6.2; 14)). We have therefore discovered a physical application for a *generalised Schur function* which is generated by (A1) for any group of permutations G.

References

Berge C 1971 *Principles of Combinatorics* (New York: Academic)
de Bruijn N G 1967 *J. Comb. Theory* **2** 418–21
Butler P H 1981 *Point group symmetry applications and methods* (New York: Plenum)
Cousins C S G 1978 *J. Phys. C: Solid State Phys.* **11** 4867–900
Fieck G 1977 *Theor. Chim. Acta* **44** 279–91
Littlewood D E 1958 *The Theory of Group Characters* (Oxford: Clarendon)
Newman D J 1981 *J. Phys. A: Math. Gen.* **14** 3143–51
Pólya G 1937 *Acta Math.* **68** 145–254