

Home Search Collections Journals About Contact us My IOPscience

Split-standard transformation coefficients: the block-selective conjecture

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 1999 J. Phys. A: Math. Gen. 32 7509 (http://iopscience.iop.org/0305-4470/32/43/306)

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

Download details: IP Address: 171.66.16.111 The article was downloaded on 02/06/2010 at 07:48

Please note that terms and conditions apply.

Split–standard transformation coefficients: the block-selective conjecture

Luke F McAven[†] and Philip H Butler[‡]

 † Department of Physics, Nanjing University, Nanjing 210008, People's Republic of China
 ‡ Department of Physics and Astronomy, University of Canterbury, Private Bag 4800, Christchurch, New Zealand

E-mail: l.mcaven@phys.canterbury.ac.nz

Received 23 December 1998

Abstract. The *split basis* for the symmetric group S_n is adapted to S_n and to the product subgroup $S_{n-a} \times S_a$. We consider matrices transforming between split bases and the standard Young–Yamanouchi basis of the symmetric group S_n . We present a conjecture for directly relating those transformation matrices to a representation matrix, in the Young–Yamanouchi basis, of a cycle permutation. This *block-selective* conjecture agrees with previously obtained solutions for the transformation matrices up to, and including, S_6 . In particular, the conjecture provides a correct solution for the early occurrences of multiplicities in the product $S_{n-a} \times S_a$. To motivate the main result of this paper we first present transformations between permuted symmetric groups.

1. Introduction

The coupling (3jm) and recoupling (6j) coefficients of unitary groups are often useful for simplifying many-body calculations in physics and chemistry. Schur–Weyl duality relates the unitary group coefficients to different types of symmetric group coefficients (Elliott *et al* 1953, Kramer 1968, Vanagas 1971, Haase and Butler 1984a, b). In particular, the unitary group 6jare related to subduction coefficients of S_n . The S_n subduction coefficients transform between one basis adapted to S_n , to $S_a \times S_b$, and then to $S_a \times S_e \times S_d$; and a second basis, adapted to S_n , to $S_c \times S_d$, and to $S_a \times S_e \times S_d$, where a + b = a + e + d = c + d = n.

The subduction coefficients can be expressed in terms of transformation coefficients between the standard Young–Yamanouchi basis and a second basis adapted to a direct product subgroup of the form $S_a \times S_b$. Elliott *et al* (1953) introduced this particular type of non-standard basis. We call it a *split basis*, and denote it as the S_n – $S_{a,b}$ basis.

Since Elliott *et al* (1953) many techniques have been given for calculating split–standard transformation coefficients. The investigation of these coefficients is incomplete. Several issues are of particular interest.

Firstly, there are some numerical methods for calculating the coefficients. However, they require non-direct operations such as diagonalization or recursion (Horie 1964, Kaplan 1961, Kaplan 1975, Chen *et al* 1983, Pan and Chen 1993). Such methods may begin with well understood representation matrices, but non-direct operations on those matrices insure the link between the bases is purely numerical. No insight into the structure of the transformations can be obtained.

0305-4470/99/437509+14\$30.00 © 1999 IOP Publishing Ltd

7510 *L F McAven and P H Butler*

Secondly, closed algebraic formulae exist for some cases (Horie *et al* 1964, Hamel *et al* 1996), for example when the Ferrers diagram labelling an irrep has two or fewer columns (Suryanarayana and Rao 1982). Tools exist for deriving algebraic solutions independent of n. One such technique is the linear equation method (McAven *et al* 1998, Pan *et al* 1993). However, the linear equation approach restricts one to deriving algebraic solutions for particular a and b. Transformations between the S_n basis and the $S_n-S_{n-2,2}$ basis were obtained some time ago (Kaplan 1961, Kaplan 1975). Recently, the linear equation method (Pan *et al* 1993) was used to calculate the transformations between the S_n basis and the $S_n-S_{n-3,3}$ basis (McAven *et al* 1998). They present case by case general solutions which are independent of n but depend on the relative values of a and b. Although useful, the linear equation method is therefore unlikely to give a general algebraic formula for all n, a and b.

Thirdly, the transformation coefficients up to and for S_6 have been calculated and published. The irrep [3 2 1] of S_6 occurs twice in the decomposition of the square of the irrep [2 1] of S_3 . Thus there is a multiplicity freedom in the transformation matrix between the S_6 basis and the S_6 - $S_{3,3}$ basis. Different choices have been made (Chen *et al* 1983, Pan *et al* 1993). A recent investigation of the S_n basis to S_n - $S_{n-3,3}$ basis transformation (McAven *et al* 1998) presents considerations which can be applied to obtain a simple form for the multiplicity separation. However, only this simplest multiplicity class has been investigated (McAven *et al* 1998). The multiplicity resolution remains a significant problem for developing a combinatorial prescription for split–standard transformation coefficients; how should the multiplicity separation be chosen, if it can be, without explicit dependence on *n*, *a* or *b*?

We have a technique which addresses a number of the issues mentioned above. We call this the *block-selective conjecture*. There are several significant features.

Firstly, the conjecture is direct in the sense that the numerical methods are not. The blockselective conjecture begins with the standard basis representation of a well prescribed cycle permutation. The Littlewood–Richardson rule is used to select blocks out of the matrix. The resulting matrix is then normalized.

Secondly, the relationship between the split and standard bases is made more apparent, as the ratios of entries in the transformation matrix are the ratios of entries in the appropriate permutation matrix.

Thirdly, only one representation matrix in the S_n basis needs to be calculated, compared with many required for the construction of the complete sets of commuting operators used in Chen *et al* (1983). Using recent methods (Rettrup *et al* 1996, Wu *et al* 1994) any permutation can be expressed as the product of two matrices, one for the irrep and the other for the permutation. Thus our method requires much less calculation than that of Chen *et al* (1983).

Finally, the block-selective conjecture can be used to make a universal, although not algebraic, choice of multiplicity separation. The method is independent of n, a or b. Similarly, the conjecture makes consistent phase choices.

The problems in obtaining a general algebraic solution, particularly with multiplicity separation issues, suggest that a more realistic aim is a combinatorial recipe for any split–standard transformation coefficient.

The paper is structured as follows. In section 2 we provide some background. We refer the reader to McAven *et al* (1998), and references therein, for background information on the standard and split bases and the ordering of basis tableaux in those bases. We discuss, in particular, the well known association between basis tableaux and sets of partitions, for standard and split bases.

In Hamel *et al* (1996) a dual basis, constructed by removing lower labelled boxes first (rather than highest labelled boxes first, as in the standard basis), is related to the standard basis. In section 3 we generalize that result. We find the transformation between the standard

basis and a basis described by the removal of any single box at each level $i, 1 \le i \le n$. The appropriate transformation matrix is shown to simply be a (permuted) representation matrix, in the standard basis, of a permutation.

Section 4 naturally extends those results to the reordering of split bases. Thus, we consider the transformation from the S_n - $S_{a,b}$ basis to the S_n - $S_{b,a}$ basis. Rather than just considering the rearrangement of one box at a time, we are able to consider any number of boxes being moved around. The transformation matrix is shown to be a (permuted) representation matrix of a cycle permutation in a split basis. More general permutations describe transformations to bases with boxes removed in different orders.

Compared to the aim of obtaining the split-standard transformation coefficients, those results may seem to be of limited use. However, they serve the purpose of motivating our conjecture for calculating split-standard transformation coefficients. We introduce the conjecture in section 5. The block-selective conjecture also uses representations of cycle permutations as a basic structure for the transformation matrix. However, the cycle permutation is now in the well understood standard basis, rather than in a split basis. We discuss the conjecture, before considering in section 5.1 some considerations relating to multiplicity separations.

We summarize and discuss our results in section 6.

2. Background

Much of the necessary background has previously been given in McAven *et al* (1998). In particular, see McAven *et al* (1998) for the definitions of *jeu de tacquin*, and for the first-letter ordering of split and standard bases. We will restate critical points as we introduce other background material. The labelling of basis vectors using Young tableaux is well known. However, the permuted basis transformations to be discussed in sections 3 and 4 depend so vitally on the relationships between labels, Young tableaux and basis vectors that a brief discussion on those relationships is useful here.

Let us then describe the labelling of the basis vectors for irreps in the standard basis. The number of conjugacy classes of a group is equal to the number of inequivalent irreps. Since partitions of *n* can be used to label the classes of S_n , they are also used to label irreps of S_n . A partition $[\lambda]$ of *n* into *i* parts may be written as $[\lambda_1, \lambda_2, ..., \lambda_i]$ such that $\sum_{j=1}^i \lambda_j = n$ and the λ_j are weakly decreasing $(\lambda_j \ge \lambda_{j+1}, \forall j)$.

A useful way to manipulate the irreps through the partition labels is to use diagrams and tableaux. By forming a left-justified array with λ_j boxes on the *j*th row and with the *k*th row below the (k - 1)th row, we obtain a Ferrers or Young diagram. Having identified the irreps of S_n we can discuss the basis vectors which span the irreps. One way of labelling the basis vectors is to look at their behaviour under the chain of subgroups,

$$S_n \supset S_{n-1} \supset S_{n-2} \cdots \supset S_2. \tag{2.1}$$

To understand the resulting labelling let us examine the reduction of irreps from S_n to S_{n-1} . The irreps of the group S_{n-1} may also be labelled by partitions. However, the S_n and S_{n-1} partitions must differ only in one part, smaller by one in the S_{n-1} partition. This is equivalent to retaining Ferrers diagrams on n-1 boxes obtained by removing one outer box from the Ferrers diagram for the S_n irrep. Recording the S_n irrep (partition) and the S_{n-1} irrep we have a basis for the irreps in a $S_n \supset S_{n-1}$ group–subgroup chain. This does not uniquely label the basis vectors, since the S_{n-1} irreps will generally be of dimension greater than one. Only S_2 and S_1 have all one-dimensional irreps. So if we extend the chain as in equation (2.1) we obtain a set of irreps (partitions) which do uniquely label each basis vector. We give an example in figure 1.



Figure 1. The set of irreps (partitions) associated with each of the basis vectors of the irrep [3 2].

The sequence of diagrams is an awkward way of labelling the basis vectors. But the Ferrers diagram in a labelling sequence differs in only one box between steps. So we can associate each sequence with a numbered Ferrers diagram, where the box which is removed going from S_i to S_{i-1} is filled with *i*. Thus the procedure of generating the labelling of the basis vectors is equivalent to filling the Ferrers diagram with the numbers $1, \ldots, n$, such that each number appears exactly once and values strictly increase across rows and down columns. Those filled diagrams are called Young tableaux and for a given partition (Ferrers diagram) the number of Young tableaux corresponds to the dimension of the irrep. At the bottom of figure 1 we give Young tableaux for the basis vectors labelled by the sequences given.

But one need not use the basis adapted to the chain of subgroups in equation (2.1), indeed one need not have a basis with any adaption scheme. In general the differently adapted bases are called non-standard bases. The particular non-standard representations we are interested in were first discussed by Elliott *et al* (1953). They were interested, along with Jahn *et al* (1954), Kaplan (1961) and others, in constructing functions with a definite permutation symmetry, from functions for subsystems each of which has its own permutation symmetry. Elliott *et al* (1953) introduced a basis in which the S_n basis functions are adapted to S_n and to the direct product subgroup $S_a \times S_b$, where a + b = n. Each factor group, the S_a basis and the S_b basis, is standard basis adapted. Because there are many non-standard bases, we introduce a distinctive new term, *split basis*, to emphasize this type. We denote such a split basis as an $S_n-S_{a,b}$ basis. In the trivial case, namely when b = 1, the $S_n-S_{n-1,1}$ basis is the S_n basis.

One can label the basis vectors of the split basis by a pair of tableaux, one with *a* boxes and the other with *b* boxes. These tableaux determine the representation matrices of the adjacent transpositions in the split bases using the method described above for the standard basis tableaux. The first tableau is used if the adjacent transposition is in S_a ; the second tableau is used if the adjacent transposition is in S_b . The transposition between the factor subgroups (n - b, n - b + 1), the bridging permutation, cannot be calculated in this manner, but can be found by using the split–standard transformation. It is of particular interest to us that multiplicities can arise in the split basis (McAven *et al* 1998).

3. Permuting bases

The dual basis of Hamel *et al* (1996) corresponds to removing the lowest S_1 factor at each level, as opposed to the standard basis in which the highest S_1 factor is removed at each level. In this section we generalize the result of Hamel *et al* (1996) to bases described in terms of the removal of any S_1 factor at each level. We interpret this as dealing with a standard basis on a rearranged list of labels. We show that the transformation matrix we require is a representation matrix of an S_n permutation in the standard basis.

Our procedure follows the derivation by Hamermesh (1962) of the representation matrices in the standard basis. In his derivation, Hamermesh works recursively, assuming the representation matrices for the first n - 1 elements are known and deriving the matrix for the transposition (n - 1, n). Here we consider choosing the set of n - 1 elements to differ from the set of n elements by an element other than that labelled n. We label the element excluded by p, thus 'removing the box labelled p first'. Then, given $\sigma \in S_n$ that leaves p invariant, there exists some permutation $\pi \in S_n$ such that for all such σ , the permutation $\pi \sigma \pi^{-1}$ leaves the object labelled n invariant. We can then proceed as Hamermesh did for the S_n basis but with the permutation $\pi^{-1}\sigma\pi$ in our modified basis occupying the same role σ did in the S_n basis.

It remains now to describe π . Clearly π needs to carry *n* to *p*, *p* to *p* + 1, *p* + 1 to *p* + 2, and so on until *n* - 1 to *n*, while leaving the other elements fixed. Hence,

$$\pi = \begin{pmatrix} 1 & 2 & \dots & p-1 & p & p+1 & \dots & n-1 & n \\ 1 & 2 & \dots & p-1 & p+1 & p+2 & \dots & n & p \end{pmatrix}.$$
 (3.1)

Having removed any factor at the S_n level, we can just as easily consider removing any box at the S_{n-1} , and the S_{n-2} level, and so on. In particular, we can consider a variation on the split $S_n - S_{1,n-1}$ basis, where the S_{n-1} basis is adapted, not to the standard basis, but to the group-subgroup chain $S_1 \times S_{b-1} \supset S_1 \times S_1 \times S_{b-2} \supset \cdots \supset S_1 \times S_1 \times \cdots \times S_1$, such that each factor is removed from the left. This describes the dual basis of Hamel *et al* (1996). Denoting a subgroup adapted to the dual basis $S_{\bar{a}}$ we can write the dual basis as $S_n - S_{1,\overline{n-1}}$, or simply as the $S_{\bar{n}}$ basis. Setting *p* equal to one at each level in the basis chain produces the π of Hamel *et al* (1996):

$$\pi = \begin{pmatrix} 1 & 2 & \dots & n-1 & n \\ n & n-1 & \dots & 2 & 1 \end{pmatrix}.$$
 (3.2)

In Hamel *et al* (1996) $M^{\lambda}(\pi)$ was denoted by Q. We use $M^{\lambda}(\sigma)$ to label the matrix, in the representation λ , for the permutation σ .

Another way of understanding this result is to look back to the discussion in section 2 and examine how the basis vectors are labelled. If we remove the boxes in the Young tableaux in a different order we will, in general, obtain a different partition chain relating to a different Young tableau for the same irrep. So we have the same irrep, just with all the labels mixed up. We still have a Ferrers diagram for each integer $i \leq n$.

Although those transformations are somewhat limited in value we can use them to calculate some of the transformation matrices given by Chen *et al* (1983). For example, the transformation between the S_5 basis and the $S_5-S_{1,4}$ basis for the irrep [3 2] (Chen *et al* 1983, table II.5) can be shown to be like the representation matrix of the permutation $\begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 5 & 1 & 2 & 3 & 4 \end{pmatrix}$. We say 'like' since there are differences in the signs of some rows due to different phase choices. If our method is used for calculating such transformation matrices, the phase freedom in the transformation matrices disappears. The choices have been made in the representation matrices of the standard basis.

7514



Figure 2. The Young tableaux associated with the irrep [3 2], ordered according to the last letter.



Figure 3. The pair tableaux used to label the basis vectors, for the irrep [3 2], in the S_5 - $S_{3,2}$ basis. They are ordered according to the prescription of McAven *et al* (1998).

1 2	1 2	1 2	1 2	12
3 4 5	3 4	3 5	3 4	3 5
	5	4	5	4

Figure 4. The pair tableaux used to label the basis vectors, for the irrep [3 2], in the S_5 - $S_{2,3}$ basis. They are ordered according to the prescription of McAven *et al* (1998).

Another difference is in the orders of the rows and columns. In figures 1 and 2 we see that the first-letter ordering, used by us, and the last-letter ordering, used by Chen *et al* (1983), differ only in the order of the third and fourth basis vectors. So, to recognize the relationship between the transformation matrix and the permutation representation matrix we need to exchange the third and fourth rows, and the third and fourth columns of one of them.

4. Split basis transformations

In this section we address the problem of transforming between two split bases which differ only in that the two factors in the direct product subgroup are swapped. That is, we will transform between the S_n - $S_{a,b}$ basis and the S_n - $S_{b,a}$ basis.

Consider the matrix $M_{a,b}^{\lambda}(\pi^{a,b})$, being the matrix for the permutation $\pi^{a,b}$ represented in the S_n - $S_{a,b}$ basis, where

$$\pi^{a,b} = \begin{pmatrix} 1 & 2 & \dots & b & b+1 & \dots & n-1 & n \\ a+1 & a+2 & \dots & n & 1 & 2\dots & a-1 & a \end{pmatrix}.$$
 (4.1)

This matrix carries the representation matrices in the S_n - $S_{a,b}$ basis to the representation matrices in the S_n - $S_{b,a}$ basis by the relation

$$PM_{a,b}^{\lambda}(\pi^{a,b})M_{a,b}^{\lambda}(\sigma)(PM_{a,b}^{\lambda}(\pi^{a,b}))^{-1} = M_{b,a}^{\lambda}(\sigma)$$
(4.2)

where P is a permutation matrix used to reorder the basis vectors so that the basis vectors for the representation matrices are all ordered according to our standard prescriptions. We will give the procedure for obtaining P later in this section.



Figure 5. The matrix representations of the generators of S_5 , for the irrep [3 2]. In the $S_5-S_{3,2}$ basis (left column) and the $S_5-S_{2,3}$ basis (right column).

Before discussing this result in more detail, we consider an example, the $S_5-S_{3,2}$ basis and the $S_5-S_{2,3}$ basis. The tableaux pairs labelling those bases are in figures 3 and 4 respectively, each ordered according to the prescription in McAven *et al* (1998).

We cannot calculate the representation matrices for the bridging permutations directly, we need to use the split–standard transformation matrices of Chen *et al* (1983) to obtain them. We give the matrix representations in figure 5.

The appropriate permutation π for transforming from the $S_5 - S_{2,3}$ basis to the $S_5 - S_{3,2}$ basis is $\pi^{2,3} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 3 & 4 & 5 & 1 & 2 \end{pmatrix}$. The inverse is used to transform back. The two representation matrices used in the transformations are then, for $M^{[3\ 2]}(\pi^{2,3})$ and $M^{[3\ 2]}(\pi^{3,2})$ respectively, $\begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{\sqrt{3}} & 0 & 0 \\ \frac{-2\sqrt{2}}{3} & \frac{1}{6} & \frac{1}{2\sqrt{3}} & 0 & 0 \\ 0 & 0 & 0 & \frac{-1}{2} & \frac{-1\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & \frac{-1}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & \frac{-1}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{-1\sqrt{3}}{\sqrt{3}} & \frac{-1}{2} \end{pmatrix}$ and $\begin{pmatrix} \frac{1}{3} & \frac{2\sqrt{2}}{3} & 0 & 0 \\ -\frac{1\sqrt{2}}{3} & \frac{1}{6} & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{1\sqrt{2}}{\sqrt{3}} & \frac{1}{2\sqrt{3}} & \frac{-1}{2} & 0 & 0 \\ 0 & 0 & 0 & -\frac{1\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$.

The appropriate permutation matrix for the transformations is

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$
 (4.4)

To prove the general result, we turn to developments of Chen and Gao (1982). Chen *et al* (1983) follow Chen and Gao (1982) in introducing complete sets of commuting operators (CSCOs). We give some details about the CSCOs here, more can be found in Chen and Gao (1982) or Chen (1989).

(4.3)

Consider the operator, which Chen et al (1983) call a two-cycle class operator,

$$C(l) = \sum_{1 \le i < j}^{l} (i, j).$$
(4.5)

For example, C(4) = (12) + (13) + (14) + (23) + (24) + (34). Chen and Gao (1982) showed that the set of these two-cycle class operators C(n), C(n - 1), ..., C(2), of the permutation groups S_n , S_{n-1} , ..., S_2 , constitute a complete set of commuting operators. We denote this set $\{C_n(i)\}$, noting that *i* runs from 2 to *n*.

Chen *et al* (1983) refer to this complete set of commuting operators as the second kind of CSCO, or CSCO-II. The simultaneous eigenvectors of those operators constitute vectors the Young–Yamanouchi basis of S_n . The correspondence with operators in the groups S_i , $2 \le i \le n$, is in accordance with the sequence of Ferrers diagrams used to label basis vectors of symmetric group irreps, or alternately the Young tableaux (section 2). Similarly, CSCO-IIs can be defined for the S_a and S_b groups appearing in the direct product subgroup in the split basis. Explicitly, the CSCO-II of S_a is,

$$\{C_a(i)\} = \{C(a), C(a-1), C(a-2), \dots, C(2)\}$$
(4.6)

where each C(l) is as in equation (4.5). The CSCO-II of S_b is,

$$\{C'_{b}(i)\} = \{C'(b), C'(b-1), C'(b-2), \dots, C'(2)\}$$
(4.7)

where we add a prime to the two-cycle class operators, since the operators differ slightly to those in (4.6),

$$C'(l) = \sum_{a+1 \le i < j}^{a+l} (i, j).$$
(4.8)

Chen and Gao (1982) point out that it is more convenient for computer computation to collect all the sets of operators in a CSCO into one operator. Thus, instead of $\{C(a)\}$ and (C'(b)) we consider

$$M_1^{a,b} = \sum_{l=2}^b k_l C(l)$$
 and $M_2^{a,b} = \sum_{l=2}^b k_l C'(l).$ (4.9)

The coefficients k_l and k'_l can be freely chosen (as long as the eigenvalues are non-degenerate), so that the CSCOs span classes of operators. Chen *et al* (1983) choose $k_i = i + 7$. We have similar CSCO-IIs for the S_n - $S_{b,a}$ basis, obtained from (4.9) by swapping the symbols *a* and *b*.

In a basis the CSCO-IIs associated with that basis are diagonal. Thus, if we could map the CSCO-IIs of the S_n - $S_{a,b}$ basis into the CSCO-IIs of the S_n - $S_{b,a}$ basis, we would have a mapping between the two bases. But simply relabelling the elements is enough to do this. Consider our example from earlier in this section. For the S_5 - $S_{2,3}$ basis and the S_5 - $S_{3,2}$ basis,

$$\begin{split} & M_1^{2,3} = k_2(1\,2) \\ & M_2^{2,3} = k_2'(3\,4) + k_3'[(3\,4) + (3\,5) + (4\,5)] \\ & M_2^{3,2} = k_2'(4\,5) \\ & M_1^{3,2} = k_2(1\,2) + k_3[(1\,2) + (1\,3) + (2\,3)]. \end{split}$$

Relabelling the elements in the CSCOs of the $S_5-S_{2,3}$ basis according to the permutation $\pi^{2,3} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 3 & 4 & 5 & 1 & 2 \end{pmatrix}$, we obtain the same form for the CSCOs as in the $S_5-S_{3,2}$ basis. The variation of k_l and k'_l generates the same class of operators, so that the permutation carries one class of operators to the other. Hence an operator that performs the transformation from the $S_5-S_{2,3}$ basis to the $S_5-S_{3,2}$ basis is the matrix $Q^{2,3} = M^{\lambda}(\pi^{2,3})P$. The matrix P ensures the basis vectors are correctly ordered. The permutation π depends on the bases we are transforming between, but is independent of the representation.

Since adjacent transpositions are self invertible, it is clear that the permutation π is not unique. For this example, we need only insure that one of the $S_{2,3}$ labels 1 and 2 becomes one of the $S_{3,2}$ labels 4 and 5, and the other of those two $S_{2,3}$ labels becomes the other $S_{3,2}$ label. Thus, 1 to 5 and 2 to 4 is a valid alternative. Similarly, the label 3 of $S_{2,3}$ could go to 2 of $S_{3,2}$, 4 of $S_{2,3}$ to 1 of $S_{3,2}$, leaving the label 5 of $S_{2,3}$ to go to 3 of $S_{3,2}$. So how can this freedom be explained? In the $S_5-S_{2,3}$ basis the adjacent transpositions (1 2) and (3 4) must be diagonal, since they are elements in a CSCO-II of that basis. (See, for this example, the representation matrices of (1 2) and (3 4) in the $S_5-S_{2,3}$ basis in figure 5.) Being orthogonal, they must also have ± 1 in each diagonal position. Thus, they can at most change the signs of rows of the matrix representation of π in the $S_5-S_{2,3}$ basis.

Returning to the general forms of the CSCO-IIs, from (4.9),

$$M_{1}^{a,b} = k_{2}(1\ 2) + k_{3}[(1\ 2) + (1\ 3) + (2\ 3)] + \dots + k_{a}[(1\ 2) + (1\ 3) + (2\ 3) \dots (a-2,a) + (a-1,a)]$$

$$M_{2}^{a,b} = k_{2}'(a+1,a+2) + k_{3}'[(a+1,a+2) + (a+1,a+3) + (a+2,a+3)] + \dots + k_{b}[(a+1,a+2) + (a+1,a+3) + \dots + (n-2,n) + (n-1,n)]$$

$$(4.11)$$

$$M_1^{b,a} = k_2(1\ 2) + k_3[(1\ 2) + (1\ 3) + (2\ 3)] + \dots + k_b[(1\ 2) + (1\ 3) + (2\ 3) \dots (b-2,b) + (b-1,b)]$$
(4.13)

$$M_2^{b,a} = k'_2(b+1, b+2) + k'_3[(b+1, b+2) + (b+1, b+3) + (b+2, b+3)] + \dots + k_a[(b+1, b+2) + (b+1, b+3) + \dots + (n-2, n) + (n-1, n)]$$
(4.14)

we can see that the permutation given in equation (4.1) performs the transformation.

The permutation P which acts to reorder the basis vectors is calculated from the basis vectors. The action of π on the basis vectors is to renumber the labels in the boxes of the pair of tableaux. The lower numbered boxes are then in the second tableau of the pair. But it is standard to have the lower numbered boxes in the first tableau of the pair. So we swap the first and second parts of all the basis tableaux pairs. But now the new basis ordering will not, in general, be standard. The permutation P is required to standardise the ordering in the new basis. For the example considered, P swaps the third and fourth basis vectors.

The result for single boxes given in section 3 is a special case of the result of this section, which applies to many boxes. However, bases can also be defined with respect to product subgroups of S_n with three or more factors, for example $S_n-S_a \times S_b \times S_c$. Another adaption for a basis is to have split bases at several levels. For example, a basis could be adapted to S_n , $S_a \times S_b$, n = a + b, and $S_c \times S_d$, a = c + d. All those bases can be rearranged using permutations derived from this CSCO analysis.

Before investigating the calculation of the split–standard transformation coefficients, we make one final point. Since one can transform between split bases via the standard basis, a relationship between the split–standard transformation matrices and the reordering matrices can be obtained. This relationship can be written

$$T_{a,b}^{\lambda}(T_{b,a}^{\lambda})^{t} \equiv M_{b,a}^{\lambda}(\pi^{b,a}) \tag{4.15}$$

with the two split–standard transformation matrices on the left, and the split–split matrix on the right. We leave out the ordering permutation matrices.

5. The block-selective conjecture

The block-selective conjecture calculates split–standard transformation coefficients. The conjecture builds on the results of the previous sections.

(4.12)

The problem we want to solve is to find the matrix, $T_{a,b}^{\lambda}$, which satisfies

$$M_{a\,b}^{\lambda}(\sigma) = T_{a\,b}^{\lambda} M^{\lambda}(\sigma) (T_{a\,b}^{\lambda})^{t}$$
(5.1)

for all permutations σ of n = a + b elements. We continue to use $M^{\lambda}(\sigma)$ as the standard basis matrix irrep of the permutation σ in the irrep λ .

Let us first describe our conjecture in a formal manner.

- (1) List the standard basis tableaux in first-letter order. Call the list L.
- (2) Construct $Q = M^{\lambda}(\pi^{a,b})$ (Hamermesh 1962, Rettrup *et al* 1996, Wu *et al* 1994), where

$$\pi^{a,b} = \begin{pmatrix} 1 & 2 & \dots & b & b+1 & \dots & n-1 & n \\ a+1 & a+2 & \dots & n & 1 & \dots & a-1 & a \end{pmatrix}.$$
 (5.2)

- (3) Generate the list L' of split basis pair tableaux by the following procedure. For each tableaux in L:
 - (a) remove the boxes containing the last *a* labels, giving a tableau T_1 of *b* boxes;
 - (b) remove the boxes containing the first *b* labels using *jeu* (section 2), giving a tableau T_2 of *a* boxes;
 - (c) apply the permutation $\pi^{a,b}$ of (5.2) to the labels in the pair tableaux T_1, T_2 ;
 - (d) the lower labels are now in T_2 so reorder the pair tableaux to label the basis vectors T_2 , T_1 . This is the same action as we took in section 4.
- (4) Order L' according to the standard prescription for split bases (McAven *et al* 1998). Record in *P* the permutation required to reorder L'.
- (5) Let T = PQ.
- (6) If the first tableau in the *i*th pair tableaux of L' is not equal to the sub-tableau of the first *a* boxes in the *j*th tableaux of *L* then set $T_{ij} = 0$.
- (7) Normalize rows of T which have no multiplicity associated with them.
- (8) Apply the Gram–Schmidt orthogonalization procedure to any set of rows of T differing only in multiplicity.
- (9) The resulting matrix describes the transformation $T_{a,b}^{\lambda}$.

We have used the conjecture to generate all the transformation coefficients of Chen *et al* (1983), to within phases. This includes $T_{3,3}^{[3\ 2\ 1]}$, for which there is a product multiplicity (McAven *et al* 1998). Preliminary speculations on this method (McAven and Butler 1998) did not include this multiplicity result. We shall now consider an example, [3 2] in the $S_5-S_{2,3}$ basis.

Consider the irrep [3 2], and the transformation from the standard to the S_5 - $S_{2,3}$ basis. The basis vectors for the standard and split bases are given in figures 1 and 2, respectively. The permutation associated with our algorithm is

$$\pi^{2,3} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 3 & 4 & 5 & 1 & 2 \end{pmatrix}.$$
 (5.3)

The representation matrix of this permutation in the standard basis is

$$Q = M^{2,3}(\pi^{2,3}) = \begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{\sqrt{3}} & 0 & 0\\ \frac{-1}{3\sqrt{2}} & \frac{-1}{3} & \frac{1}{2\sqrt{3}} & \frac{\sqrt{3}}{2} & 0\\ \frac{-1}{\sqrt{6}} & \frac{-1}{\sqrt{3}} & \frac{1}{2} & \frac{-1}{2} & 0\\ \frac{-1}{\sqrt{6}} & \frac{1}{2\sqrt{3}} & 0 & 0 & \frac{\sqrt{3}}{2}\\ \frac{-1}{\sqrt{2}} & \frac{1}{2} & 0 & 0 & \frac{-1}{2} \end{pmatrix}.$$
 (5.4)



Figure 6. The relationship between split and standard tableaux for the [3 2] example, prescribed by the block-selective conjecture. The first two rows are from steps (3a) and (3b) respectively. The second two rows are given by the action of steps (3c) and (3d) on the first two rows.

The results of step (3) are in figure 6. Comparing figures 4 and 6, we find (step (4))

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$
 (5.5)

After applying P and the selection rule of step (6) we obtain

$$T = \begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{\sqrt{3}} & 0 & 0\\ \frac{-1}{\sqrt{6}} & \frac{-1}{\sqrt{3}} & \frac{1}{2} & 0 & 0\\ \frac{-1}{\sqrt{2}} & \frac{1}{2} & 0 & 0 & 0\\ 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0\\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} \end{pmatrix}$$
(5.6)

which is then normalized. As in section 3 the third and fourth columns must be exchanged to compare our result with Chen *et al* (1983). The split basis order is consistent with that used by Chen *et al* (1983), so the rows may be left.

This example is simple, but the compactness should not, however, mislead the reader into thinking larger examples are any more difficult. We state in sections 1 and 6 reasons why this conjectured method is more efficient and elegant than techniques previously proposed for calculating those coefficients. Examining a larger case would require the handling of larger matrices but otherwise, apart from the use of step (8) for multiplicity cases, would add nothing.

Let us return to the general algorithm. The critical stage is identifying the permutation matrix in the standard basis with the transformation matrix. This identification is motivated by the CSCOs considered in the previous section. The permutation $\pi^{a,b}$ is the same as that given in equation (4.1). The matrix representation of $\pi^{a,b}$ in the S_n - $S_{a,b}$ basis was used to transform from the S_n - $S_{a,b}$ basis to the S_n - $S_{b,a}$ basis. In the block-selective conjecture the permutation carries the standard basis to a permuted basis. In the example above the permuted basis corresponds to

$$S_5 \supset S_4 \times S_1(2)$$

$$\supset S_3 \times S_1(1) \times S_1(2) \supset S_2 \times S_1(5) \times S_1(1) \times S_1(2) \supset S_1(3) \times S_1(4) \times S_1(5) \times S_1(1) \times S_1(2).$$

$$(5.7)$$

In section 4 we mentioned that if all the operators in the CSCO-II associated with a basis are diagonal, then we are in that basis. The *P* of the algorithm reorders standard basis vector order to split basis vector order, and can be ignored in the analysis of the CSCOs. Both the split and standard bases have the diagonal C(n) CSCO, and the permutation in equation (5.2) will preserve this. The CSCO-II associated with the first factor group S_a is already diagonal in the standard basis, and must remain so after applying the transformation matrix. The other problem is to diagonalize the CSCO-II associated with the second factor group, S_b .

The matrix representation of the permutation $\pi^{a,b}$ in equation (5.2) diagonalizes the CSCO-II of S_b . But it also makes the CSCO-II of S_a generally non-diagonal. The permuted basis is not generally diagonal in $C'_b(a)$, or for the example relating to the basis in (5.7), the permuted basis is not diagonal in the CSCO-II $C'_3(2)$. This problem for S_a is overcome by the block-selective rule of step (6), without upsetting S_b . The block selection rule ensures that the product of the split basis pair tableaux contains the standard basis tableaux. The rule is not represented as a matrix product, so we cannot consider the transformation to be via the permuted basis. Rather the split–standard transformation is to a basis 'near' the permuted basis.

The permutation structure of this method emphasises the strong link between the matrix elements of permutations and the ratios of split-standard transformation coefficients. Each row of the transformation matrix is taken from a row of the representation matrix of $\pi^{a,b}$ in the standard basis, or alternately from a row of the transformation to the permuted basis. Consider labelling the standard basis vectors by u_i , the permuted basis vectors by v_i and the split basis vectors by w_i . Then the relationships between the permuted and standard basis vectors, and between the split and standard basis vectors can be respectively expressed as

$$v_i = \sum_j C_{ij} u_j$$
 and $w_i = \sum_j T_{ij} u_j$. (5.8)

Then the block selection conjecture tells us that the following two relationships hold whenever the product of the two split basis vectors can give the standard basis vector:

$$\frac{C_{ij}}{C_{ij'}} = \frac{T_{P(i)j}}{T_{P(i)j'}} \qquad \frac{C_{ij}}{C_{i'j}} = \frac{T_{iP^{-1}(j)}}{T_{i'P^{-1}(j)}}.$$
(5.9)

We have two results which, if proved, would confirm the block-selective conjecture. Firstly, that the CSCO-II for the split basis be diagonalized by the transformation matrix in the conjecture. Secondly, that the ratios in equation (5.9) hold.

Finally, note that one may simplify step (3b) in calculations performed by hand by removing all the boxes at once. For programming purposes though it is necessary to identify the original position of the box containing 1 and there is in general no advantage.

5.1. The block-selective conjecture and multiplicities

It is especially significant that the conjecture suggests solutions for multiplicity cases. However, step (8) of the algorithm, application of the Gram–Schmidt procedure, is not unique in giving a correct multiplicity separation. We shall evaluate here the simplest case, one of the two blocks of [3 2 1] in the S_6 – $S_{3,3}$ basis, and discuss the freedom allowed in going from the block of the representation matrix to a valid separation.

7520

Parameters	[3 2 1] Blocks		[4 2 1] Blocks		
	One	Two	One	Two	Three
x	$\frac{1}{36\sqrt{14}}$	$-\frac{\sqrt{5}}{36\sqrt{6}}$	$-\frac{\sqrt{2}}{21\sqrt{185}}$	$-\frac{1}{28\sqrt{30}}$	$-\frac{1}{14\sqrt{30}}$
у	$-\frac{1}{162\sqrt{14}}$	$-\frac{1}{162\sqrt{30}}$	$\frac{1}{112\sqrt{370}}$	$-\frac{\sqrt{5}}{2016\sqrt{6}}$	$\frac{1}{504\sqrt{30}}$
r	$-\frac{2}{9}$	$-\frac{2}{45}$	$-\frac{3}{32}$	$\frac{5}{72}$	$-\frac{1}{36}$
θ	+1	+1	-1	-1	+1
ϕ	+1	-1	-1	+1	-1
ψ	-1	+1	-1	+1	+1

Table 1. The multiplicity two solutions for the irreps [3 2 1] and [4 2 1] in terms of the parameters of McAven *et al* (1998).

The relevant block of the representation matrix prior to step (8) is,

$$\begin{pmatrix} \frac{\sqrt{3}}{16} & \frac{3}{8} & \frac{3}{16} & \frac{\sqrt{15}}{8} & -\frac{\sqrt{15}}{16} & -\frac{3\sqrt{5}}{16} \\ \frac{\sqrt{5}}{8} & -\frac{\sqrt{15}}{16} & \frac{\sqrt{15}}{8} & -\frac{5}{16} & 0 & 0 \\ \frac{3}{8} & \frac{5\sqrt{3}}{16} & -\frac{\sqrt{3}}{8} & -\frac{3\sqrt{5}}{16} & 0 & 0 \\ -\frac{\sqrt{15}}{16} & 0 & \frac{\sqrt{5}}{16} & 0 & \frac{5\sqrt{3}}{16} & -\frac{5}{16} \end{pmatrix}.$$
(5.10)

If one uses step (8) then the particular solution obtained is

$$\begin{pmatrix} \frac{1}{2\sqrt{14}} & \frac{\sqrt{3}}{\sqrt{14}} & \frac{\sqrt{3}}{2\sqrt{14}} & \frac{\sqrt{5}}{2\sqrt{14}} & -\frac{\sqrt{5}}{2\sqrt{14}} & -\frac{\sqrt{15}}{2\sqrt{14}} \\ -\frac{3\sqrt{5}}{4\sqrt{14}} & \frac{\sqrt{15}}{4\sqrt{14}} & -\frac{3\sqrt{15}}{4\sqrt{14}} & \frac{5}{4\sqrt{14}} & \frac{1}{4\sqrt{14}} & \frac{\sqrt{3}}{4\sqrt{14}} \\ \frac{\sqrt{3}}{\sqrt{14}} & \frac{5}{2\sqrt{14}} & -\frac{1}{\sqrt{14}} & -\frac{3\sqrt{15}}{4\sqrt{14}} & 0 & 0 \\ \frac{\sqrt{15}}{4\sqrt{14}} & -\frac{\sqrt{5}}{4\sqrt{14}} & -\frac{\sqrt{5}}{4\sqrt{14}} & \frac{\sqrt{3}}{4\sqrt{14}} & -\frac{7\sqrt{3}}{4\sqrt{14}} & \frac{7}{4\sqrt{14}} \end{pmatrix}.$$
(5.11)

This corresponds to choosing $x = 1/(36\sqrt{14})$, $y = -/(162\sqrt{14})$, $\theta = +1$, $\psi = +1$ and $\phi = -1$ in the solutions (equation (4.10) of McAven *et al* (1998)).

The coefficients in equation (5.10) already satisfy almost all of the equations used by McAven *et al* (1998). Only normality and orthogonality are not satisfied. Row scaling, as in step (7), is enough to obtain normality but orthogonality looks more difficult. However, adding rows differing only in multiplicity effects just the orthogonality and normality equations. Thus while the Gram–Schmidt procedure only normalizes the first row, one can, in general, take the new first row to be a linear combination of the first and second rows. To retain the correct relations between the first and third rows, and between the second and fourth rows, it is necessary to mix first and second rows, and mix third and fourth rows, in the same proportions. The Gram–Schmidt procedure avoids the need to search for a solution.

To complete column normality one must consider the extra row above and below the block in (5.11) (McAven *et al* 1998). There is also an additional relation between the phases in McAven *et al* (1998) necessary for column normality to be satisfied, $\theta \psi = -\phi$. The complicated nature of the equations obscures this detail.

We have further tested our conjecture on the other multiplicity block of [3 2 1], and on the three multiplicity two blocks arising in the decomposition of [4 2 1] to $S_4 \times S_3$. We give those solutions in table 1 in terms of the parameters in McAven *et al* (1998). It is interesting that in each case one of the blocks gives the maximum number of zeros. The second block for the S_6 – $S_{3,3}$ basis contains two rows with two zeros. The third block for the S_7 – $S_{4,3}$ basis contains two rows with two zeros also.

6. Summary

We have considered transformations between permuted bases, split bases and standard bases of the symmetric group S_n . We have presented the block-selective conjecture, with which we have calculated split–standard transformation coefficients for groups up to and including S_6 . This conjecture provides multiplicity separations, correct for all S_6 transformations and for those S_7 cases we have checked. The block-selective conjecture gives a separation without reference to *n* or the factor group sizes.

Furthermore, whereas Chen *et al* (1983) require diagonalizing a CSCO-II matrix in the standard basis, we have a direct method for changing a representation matrix of a permutation into the transformation matrix required. We thus avoid indirect numerical techniques such as diagonalization and recursion. The method for making the change is a simple selection rule based on the Littlewood–Richardson rule. The direct relation with the permutation representation matrix is most easily seen in that the ratios of entries in the permutation representation coefficients, where the transformation coefficients are both non-zero.

Although our conjecture is unproven, the ratio relationship and the need for the CSCO-II of the split basis to be diagonalized are both possible paths to proofs.

Acknowledgments

LFM acknowledges partial support by the Marsden Fund: contract no UOC704, and subsequent support by the Foundation for Research, Science and Technology (NZ): contract no WND801. PHB acknowledges the support of the Marsden Fund: contract no UOC704.

References

Butler P H 1981 Point Group Symmetry Applications: Methods and Tables (New York: Plenum) Chen J-Q 1989 Group Representation Theory for Physicists (Singapore: World Scientific) Chen J-Q and Gao M-J 1982 J. Math. Phys. 23 928-43 Chen J-Q, Collinson D F and Gao M-J 1983 J. Math. Phys. 24 2695-705 Elliott J P, Hope J and Jahn H A 1953 Phil. Trans. R. Soc. A 246 241 Hamel A M, McAven L F, Ross H J and Butler P H 1996 J. Phys. A: Math. Gen. 29 5935-44 Hamermesh M 1962 Group Theory and its Application to Physical Problems (Addison-Wesley Series in Physics) (Reading, MA: Addison-Wesley) Horie H 1964 J. Phys. Soc. Japan 19 1783-99 Jahn H A 1954 Phys. Rev. 96 989 Kaplan I G 1961 Zh. Eksp. Teor. Fiz. 41 560 -1962 Sov. Phys.-JETP 14 401-7 -1975 Symmetry of Many-Electron Systems (New York: Academic) McAven L F and Butler P H 1998 The block selective conjecture for calculating a class of symmetric group transformation coefficients Group 22: Proc. 22nd Int. Collog. on Group Theoretical Methods in Physics (Hobart, 1998) ed S P Corney et al (Cambridge, MA: International) McAven L F, Butler P H and Hamel A M 1998 J. Phys. A: Math. Gen. 31 8363-72 Pan F and Chen J-Q 1993 J. Phys. A: Math. Gen. 26 4299-310 Rettrup S and Pauncz R 1996 Int. J. Quantum Chem. 60 91 Suryanarayana Ch and Rao M K 1982 J. Phys. A: Math. Gen. 15 2013-6 Yamanouchi T 1937 Proc. Phys. Math. Soc. Japan 18 623

Young A 1977 The Collected Papers of Alfred Young (Toronto: University of Toronto)

Wu W and Zhang Q-E 1994 Int. J. Quantum Chem. 50 55