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Calculating symmetric group split-standard transformation coefficients using the block selective method: a proof

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Abstract
The *split basis* for the symmetric group S_n is adapted to S_n and to the product subgroup $S_{n-a} \times S_a$. The entries in the matrix that transforms between the split-basis representation and the standard Young–Yamanouchi (YY) basis, the split-standard transformation coefficients, are closely related to a-particle coefficients of fractional parentage. Recently the *block selective conjecture* was proposed for calculating the coefficients. The conjecture implies that the transformation matrix is directly related to the representation matrix, in the YY basis, of a cycle permutation. We present a proof of this conjecture.

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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 coefficient (Haase and Butler 1984a, 1984b). In particular, the $6j$ of the unitary groups can be expressed as a sum over a product of coefficients of fractional parentage (cfp) of symmetric groups.

Cfp describe the coupling of a-particle states to $(n-a)$-particle states to give n-particle states. For the symmetric group they can alternatively be viewed as relating matrix representations in the standard or Young–Yamanouchi (YY) basis (Yamanouchi 1937, Young 1977) to matrix representations in the *split basis* (Elliott *et al* 1953, McAven and Butler 1999). As Kramer *et al* (1981) point out, cfp and split-standard transformation coefficients (SSTC) are closely related. Split bases are adapted to a direct product subgroup of S_n of the form $S_a \times S_b$ where S_a and S_b are independently symmetry adapted as standard bases.

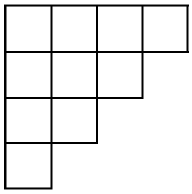

Figure 1. The Ferrers diagram associated with the irrep [4 3 2 1] of S_{10}.

In the latter context an algorithm was recently (McAven and Butler 1999) proposed for calculating the cfp of the symmetric group. This block selective conjecture centres around the argument that the transformation matrix of SSTC is directly related to the representation matrix, in the YY basis, of a cycle permutation. We prove this conjecture.

The block selective method is of significance for several reasons. First, it is direct in the sense of not relying on numerical methods such as diagonalization. Second, the relationship (the coefficients) between split and standard bases is made more apparent through the identification mentioned in the last paragraph. Third, only one representation matrix in S_n needs to be calculated. Fourth, the block selective method provides a process for making universal, but not algebraic, choices of multiplicity separation and phases. Finally, although it does not explicitly do so, the block selective method may provide means to give some physical interpretation to the Young tableaux (McAven and Schlesinger 2001).

The general problem of calculating SSTC and cfp has been treated before (Kramer 1968, Kramer *et al* 1981, Kaplan 1975, Horie 1964, Suryanrayana and Kondala Rao 1982, Chen *et al* 1983). Earlier publications have given solutions for special cases, or described complete methods which lack the directness or multiplicity and phase separations of the method proved herein described. This problem can be considered to be a special case of transforming between any two $S(n)$ bases of the form $S_{n_1} \times S_{n_2} \times \cdots \times S_{n_k}$ and $S_{m_1} \times S_{m_2} \times \cdots \times S_{m_l}$ for $n_1+n_2+\cdots+n_k = m_1+m_2+\cdots+m_l = n$, where all the S_i are YY adapted. Solutions for such transformations could be obtained by repeated use of the block selective method (McAven and Butler 1999).

2. Notation

We follow the usual convention and label the irreducible representations (irreps) of S_n by partitions of S_n. We can do this because the number of inequivalent irreps and conjugacy classes of S_n are equal and the latter are labelled by partitions.

A partition $[\lambda]$ of n into i parts may be written as $[\lambda_1, \lambda_2, \dots, \lambda_i]$ such that $\sum_{j=1}^{i} \lambda_j = n$ and so the λ_j are weakly decreasing ($\lambda_j \geqslant \lambda_{j+1}, \forall j$).

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 jth row and with the kth row below the $(k-1)$th row, we obtain a Ferrers or Young diagram. As an example, in figure 1, we give the Ferrers diagram associated with the irrep [4 3 2 1] of S_{10}.

We shall consider two different bases, the standard or YY basis and the split basis. In the former, one labels the basis vectors or eigenstates by Young tableaux, different fillings of the Ferrers diagram with the numbers 1 to n increasing across rows and down columns. The number of Young tableaux and labels is equal to the dimension of the irrep and we enumerate the basis vectors of an irrep ν by an integer m running from 1 to the dimension of ν. Loosely, the Young tableaux describe the symmetry relations between the $(i-1)$-particle state and the

1	3	4	7
2	5	10	
6	9		
8			

Figure 2. A typical Young tableaux for the irrep [4 3 2 1] of S_{10}.

ith particle for all $2 \leqslant i \leqslant n$. They are equivalent to labelling the basis vectors by irreps (Ferrers diagrams) for each $S_i, i \leqslant 1 \leqslant n$. It is not known how to physically interpret the standard basis labels however, in the sense that the tableaux are not known to specifically relate to any observables or conserved quantities, such as orbital or spin angular momentum. The particular advantage of the basis is that there are no multiplicity labels, that is, each Young tableaux is distinct. A typical Young tableaux for the irrep [4 3 2 1] of S_{10} is given in figure 2.

Another basis is the *split basis*, first introduced by Elliott *et al* (1953). The basis vectors in this basis are labelled by the irrep of S_n, by Young tableaux of S_a and S_b where $n = a + b$, and by a product multiplicity τ arising in the generation of the S_n irrep from the S_a and S_b irreps.

We are interested in transforming between the two bases. The coefficients which perform the transformation are SSTC. We shall denote the matrix of SSTC which transforms a representation in the standard basis into a representation in the split basis by $T^{a,b}$. When we write a matrix of SSTC we follow Chen *et al* (1983) in labelling the rows by the split-basis labels and the columns by the standard basis vectors.

To represent more concisely the SSTC we introduce the notation

$$[mm_2] = \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \middle| [\nu], \tau \begin{matrix} [\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \right\rangle. \tag{2.1}$$

We do this since we will only need to consider SSTC differing in the m- and m_2-labels.

3. The block selective conjecture

The block selective conjecture is formally presented in McAven and Butler (1999), we shall only summarize the main parts here.

- Identification of the transformation matrix with the representation matrix, in the standard basis, of a permutation

$$\pi^{a,b} = \begin{pmatrix} 1 & 2 & \cdots & b & b+1 & \cdots & n-1 & n \\ a+1 & a+2 & \cdots & n & 1 & \cdots & a-1 & a \end{pmatrix}. \tag{3.1}$$

- Reordering of the split-basis labels.
- Application of the block selection rule on the tableaux product.
- Row normalization to ensure that the transformation matrix is unitary.

The issues of multiplicity and phase slightly complicate the algorithm but we shall examine those later.

We are going to prove the conjecture by proving the associated ratio relationship, the first part of equation (5.9) of McAven and Butler (1999)[3]. This asserts the equality of a ratio of entries from the block selective matrix to a ratio of entries from the transformation matrix:

[3] Note that the second of the ratio relationships given therein cannot also be true. This is because we use orthonormality on either the rows or columns.

$$\frac{\langle v_1|\pi^{a,b}|Pv_2\rangle}{\langle v_1'|\pi^{a,b}|Pv_2\rangle} = \frac{\langle v_1|T^{a,b}|v_2\rangle}{\langle v_1'|T^{a,b}|v_2\rangle}. \tag{3.2}$$

This equality only holds when neither of the SSTC is zero due to the block selection rule. The v_1, v_2, and v_1' are arbitrary basis vectors specifying the positions in the SSTC and permutation matrix. The block selection rule looks at the pair of tableaux labelling the split basis and determines whether they can combine to give the standard basis tableau. This is allowed if the sub-tableau of the standard tableau of equal size as the first split tableau in the reordered and renumbered split list is equal to that first split tableau. P is a permutation matrix required to consistently reorder the basis vectors so that they are in the standard order that we use. The prescription for generating P is given in McAven and Butler (1999) (step 4 of the formal conjecture on p 7518). The ratio of two entries (SSTC) in the same row of the transformation matrix is equal to the ratio of two entries in the same row of the representation matrix of the permutation in equation (3.1).

4. A proof of two halves

We are going to prove the conjecture by proving the associated ratio relationship as given in equation (3.2).

To do this, we set up two systems of equations for the matrix elements involved, one set for the representation matrix entries and another for the transformation matrix entries (the SSTC). We address the latter first.

The starting point is equation (14) of Chen *et al* (1983). In that paper the equation is written as

$$\left\langle \begin{matrix}[\nu]\\ m'\end{matrix} \,\middle|\, [\nu],\tau \begin{matrix}[\nu_1][\nu_2]\\ m_1m_2'\end{matrix}\right\rangle = \frac{1}{D^{[\nu_2]}_{m_2'm_2}(T_2)} \sum_m \left[D^{[\nu]}_{m'm}(T_2') - D^{[\nu_2]}_{m_2m_2}(T_2)\delta_{mm'}\right] \times \left\langle \begin{matrix}[\nu]\\ m\end{matrix} \,\middle|\, [\nu],\tau \begin{matrix}[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle \tag{4.1}$$

where $T_2' = (i, i+1) \in S_b(a+1\dots n)$ and $T_2 = (i-a, i-a+1) \in S_b(1, 2\dots n)$. Since T_2' is an adjacent permutation the m over which the sum runs can only take two values. The equation therefore becomes

$$\left\langle \begin{matrix}[\nu]\\ m'\end{matrix} \,\middle|\, [\nu],\tau \begin{matrix}[\nu_1][\nu_2]\\ m_1m_2'\end{matrix}\right\rangle = \frac{1}{D^{[\nu_2]}_{m_2'm_2}(T_2)} \times \left[\left(D^{[\nu]}_{m'm'}(T_2') - D^{[\nu_2]}_{m_2m_2}(T_2)\right)\left\langle \begin{matrix}[\nu]\\ m'\end{matrix} \,\middle|\, [\nu],\tau \begin{matrix}[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle + D^{[\nu]}_{m'm}(T_2')\left\langle \begin{matrix}[\nu]\\ m\end{matrix} \,\middle|\, [\nu],\tau \begin{matrix}[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle\right]. \tag{4.2}$$

Thus we have an equation relating three SSTC. If we vary the m' and m_2' on the left-hand side of the above equation, allowing them to also take the values m and m_2 respectively, we generate a system of four equations in four variables. The four variables are four SSTC. Since T_2 and T_2' are adjacent permutations, we can give explicit formulae for the entries in the representation matrices (the Ds).

Now let us use the notation of equation (2.1) to write down the four equations. In the tableaux labelled by m, the hook length from i to $i+1$ is σ and in the tableaux labelled by m_2, the hook length is μ. We use the following abbreviations:

$$\alpha = \frac{1}{\mu} + \frac{1}{\sigma} \qquad \beta = \frac{1}{\mu} - \frac{1}{\sigma}$$
$$f = \frac{|\mu|}{\sqrt{\mu^2 - 1}} \qquad g = \frac{\sqrt{\sigma^2 - 1}}{|\sigma|}. \tag{4.3}$$

Then the system of equations is

$$\begin{aligned}
[mm_2] &= f[-\alpha[mm_2'] + g[m'm_2']] \\
[mm_2'] &= f[\beta[mm_2] + g[m'm_2]] \\
[m'm_2] &= f[-\beta[m'm_2'] + g[mm_2']] \\
[m'm_2'] &= f[\alpha[m'm_2] + g[mm_2]].
\end{aligned} \tag{4.4}$$

Now we turn to the permutation matrix and the derivation of the second set of equations. We have the same m- and m'-tableaux corresponding to the standard basis as in the previous case. However, we also want two tableaux to label the rows, and we need them to have the same hook length μ as the m_2, m_2' pair. This can only be ensured by adopting a reordering scheme such as that in McAven and Butler (1999). We shall label the tableaux in the pair as n and n'.

We are interested in the four matrix elements of the permutation $\pi^{a,b}$ associated with the labels n, n' and m, m'. Consider for example the matrix element connecting tableaux n and m:

$$\langle n|\pi^{a,b}|m\rangle. \tag{4.5}$$

Those tableaux, or basis vectors, might be specifically chosen to examine a particular case of equation (3.2), with n and m corresponding directly to either x and Py or to x' and Py as the case may be. We want to consider the general case however and need not be more specific.

We can insert different identities on either side of the permutation

$$\langle n|(T_2T_2)\pi^{a,b}(T_2'T_2')|m\rangle \tag{4.6}$$

and then rebracket the operations

$$(\langle n|T_2)(T_2\pi^{a,b}T_2')(T_2'|m\rangle). \tag{4.7}$$

Since T_2 and T_2' are adjacent permutations we can again put in the explicit expression for the operation on the bras and kets, in terms of the hook lengths and the other tableaux n' and m'. For example,

$$\langle n|T_2 = \left(\langle n|\left(-\frac{1}{\mu}\right) + \langle n'|\left(\frac{\sqrt{\mu^2-1}}{|\mu|}\right)\right). \tag{4.8}$$

We need to have $(T_2\pi^{a,b}T_2') = \pi^{a,b}$, for all possible T_2, so that we get a system of equations in four variables, the four matrix elements. The first equation is

$$\begin{aligned}
\langle n|\pi|m\rangle = \langle n|\pi|m\rangle\left(\frac{1}{\sigma\mu}\right) - \langle n|\pi|m'\rangle\left(\frac{\sqrt{\sigma^2-1}}{\mu|\sigma|}\right) - \langle n'|\pi|m\rangle\left(\frac{\sqrt{\mu^2-1}}{\sigma|\mu|}\right) \\
+\langle n'|\pi|m'\rangle\left(\frac{\sqrt{\sigma^2-1}\sqrt{\mu^2-1}}{|\sigma||\mu|}\right).
\end{aligned} \tag{4.9}$$

5. The solution to the systems of equations

We use Maple (1996) to solve the two systems of equations, the first given in equation (4.4) and the second partially given in equation (4.9). The four variables in each system will be replaced by the common labels w, x, y, z. They represent the terms in equation (3.2). In the first system $w = [mm_2]$, $x = [mm_2']$, $y = [m'm_2]$, and $z = [m'm_2']$, while in the second $w = \langle n|\pi|m\rangle$, $x = \langle n'|\pi|m\rangle$, $y = \langle n|\pi|m'\rangle$, and $z = \langle n'|\pi|m'\rangle$.

It is found that the following set of solutions is common to both systems:

$$\begin{aligned} w &= \theta\frac{\phi y(\sigma+\mu) + z\sigma\sqrt{\mu^2-1}}{\mu\sqrt{\sigma^2-1}} & x &= \psi\frac{z(\sigma-\mu) - \phi y\sigma\sqrt{\mu^2-1}}{\mu\sqrt{\sigma^2-1}}. \\ y &= y & z &= z \end{aligned} \tag{5.1}$$

In the above, $\phi = \pm 1$, $\theta = \pm 1$, and $\psi = \pm 1$, with the additional restriction $\theta\psi\phi = -1$.

This shows that the entries of the permutation matrix can be used as entries in the transformation matrix. The full transformation matrices have the additional requirement of unitarity but the normalization factor is cancelled by the ratio in the relationship.

6. Multiplicities and phases

Thus far we have not mentioned the issues of phase and multiplicity. The argument applies, but with regard to multiplicity there is the additional constraint of orthogonality which must be addressed. Before orthonormalization the representation matrix of the permutation is otherwise acceptable as a SSTC matrix. Since the different row blocks in the 'multiplicity part' of the permutation representation matrix are associated with different solutions to the same linear system, we are entitled to use the Gram–Schmidt orthonormalization procedure to modify the transformation matrix to an acceptable orthogonal SSTC matrix.

A slight modification to the block selective algorithm proposed in McAven and Butler (1999) is advised as regards the phase issue. One is free to choose the phase of the rows with the same $\lambda_1 m_1 \lambda_2$. However, we suggest that one performs the trivial transformation (for the relevant representation λ) by calculating the appropriate permutation's representation matrix and recording the necessary phase to make it an identity matrix. These phases should then be applied to non-trivial transformations.

7. Summary

We have provided a proof of the block selective method proposed in McAven and Butler (1999). This method relates the matrix of SSTC transforming between the split and standard bases of the symmetric group directly to the representation matrix, in the YY basis, of a cycle permutation. We demonstrate by constructing systems of equations for a block of the permutation representation matrix, and for the corresponding block of SSTC, that ratios of entries from one matrix are equal to ratios of entries from the other:

$$\frac{\langle x|\pi^{a,b}|Py\rangle}{\langle x'|\pi^{a,b}|Py\rangle} = \frac{\langle x|T^{a,b}|y\rangle}{\langle x'|T^{a,b}|y\rangle}. \tag{7.1}$$

This relation is equivalent to the block selective method form as given in the first part of equation (5.9) of McAven and Butler (1999).

An algebraic proof may be obtainable through the use of double cosets. The work in Kramer *et al* (1981) and Sullivan ((1980) and references therein) on the use of double cosets for studying the Racah–Wigner calculus will be invaluable.

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References

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
Haase R and Butler P H 1984a *J. Phys. A: Math. Gen.* **17** 47–59
Haase R and Butler P H 1984b *J. Phys. A: Math. Gen.* **17** 61–74
Horie H 1964 *J. Phys. Soc. Japan* **19** 1783
Kaplan I 1975 *Symmetry of Many-Electron Systems* (New York: Academic)
Kramer P 1968 *Z. Phys.* **216** 68–83
Kramer P, John G and Schenzle D 1981 *Group Theory and the Interaction of Composite Nucleon Systems* (Braunschweig: Vieweg)
Maple V 1996 Release 4, power edition (University of Waterloo)
McAven L F and Butler P H 1999 *J. Phys. A: Math. Gen.* **32** 7509–22
McAven L F and Schlesinger M 2001 *J. Phys. A: Math. Gen.* **40** 8333–43
Sullivan J J 1980 *J. Math. Phys.* **21** 227–33
Suryanrayana Ch and Kondala Rao M 1982 *J. Phys. A: Math. Gen.* **15** 2013
Yamanouchi T 1937 *Proc. Phys. Math. Soc. Japan* **18** 623
Young A 1977 *The Collected Papers of Alfred Young* University of Toronto, Toronto