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Inversion of the fractional parentage matrix

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Abstract. The Racah fractional parentage coefficients used in atomic structure calculations contribute to a part of an ordinary unitary matrix transformation. In the present paper we describe three different approaches for completing this matrix using (i) projection operator techniques, (ii) the factorisation lemma of Racah and (iii) the spin-free formalism already used in theoretical studies of nuclear structures. We hope to give a deeper insight into the fractional parentage expansion and to its inverse transformation.

1. Introduction

In atomic structure calculations, the fractional parentage expansion (Racah 1943)

$$\Phi(l^N\alpha SL)=\sum_{\alpha'S'L'}(l^{N-1}\alpha'S'L'lSL|\}l^N\alpha SL)\Phi(l^{N-1}\alpha'S'L',l_N,SL) \qquad (1)$$

is used to expand the antisymmetric wavefunction of N equivalent electrons in terms of fractional parentage where the subscript N specifies that the Nth electron has been removed from the antisymmetrised part of the wavefunction. This transformation is widely used for evaluating matrix elements of one- and two-particle operators (Fano 1965). In his well known paper, Racah (1943) pointed out that the transformation matrix $(l^{N-1}\alpha'S'L'lSL|\}l^N\alpha SL)$ is not an ordinary unitary matrix but only a rectangular matrix which is part of a unitary one since its columns do not exhaust all states of l^{N-1} but only those which are allowed in l^N, i.e. those which belong to the antisymmetric representation $[1^N]$ of the symmetric (permutation) group S_N (Condon and Odabasi 1980). To complete this matrix, we have to consider all the coupling schemes of the N-particle wavefunction giving rise to the SL symmetry, whatever the permutation symmetry is. We can generalise expansion (1) as

$$\Phi(l^N\alpha SL\Gamma_i)=\sum_j U_{ij}\Phi(l^{N-1}\alpha_jS_jL_j\Gamma_j,l_N,SL) \qquad (2)$$

where Γ_i and Γ_j specify the representation of the symmetric groups S_N and S_{N-1} respectively. The fractional parentage coefficients of Racah (equation (1)) are simply the matrix elements U_{ij} with $\Gamma_i=[1^N]$ and $\Gamma_j=[1^{N-1}]$. The transformation matrix $\mathbf{U}$ is now complete and can be taken to be a real orthogonal unitary matrix ($\mathbf{U}^{-1}=\mathbf{U}$). We can then write the inverse transformation as

$$\Phi(l^{N-1}\alpha_jS_jL_j\Gamma_j,l_N,SL)=\sum_i U_{ij}\Phi(l^N\alpha SL\Gamma_i). \qquad (3)$$

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Such inverse relations have been already discussed by Jahn and Van Wieringen (1951) in the orthogonal transformation of orbital fractional parentage coefficients for nuclear shells.

In the present paper we describe three different approaches for calculating the matrix elements U_{ij} of the transformations (2) and (3) for $l^N\alpha SL = \mathrm{p}^3\,{}^2\mathrm{P}$.

2. The projection operator techniques

For the three-particle system p^3, we can consider the following six coupling schemes:

$$\mathrm{p}^2[{}^{1,3}\mathrm{D},\ {}^{1,3}\mathrm{P},\ {}^{1,3}\mathrm{S}]\mathrm{p}\ {}^2\mathrm{P} \tag{4}$$

spanned by the 18 Hartree products $h_1 = \mathrm{p}_{+1}(1)\mathrm{p}_0(2)\bar{\mathrm{p}}_0(3)$, $h_2 = \mathrm{p}_0(1)\bar{\mathrm{p}}_{+1}(2)\mathrm{p}_0(3), \ldots, h_{18} = \mathrm{p}_{-1}(1)\mathrm{p}_{+1}(2)\bar{\mathrm{p}}_{+1}(3)$; $\{h_q, q = 1, 18\}$ allowed for $(M_S, M_L) = (\frac{1}{2}, 1)$ and given in table 1. The A_{ij} matrix elements of

$$\Phi(\mathrm{p}^2[S_iL_i]\mathrm{p}\ {}^2\mathrm{P}) = \sum_{q=1}^{18} A_{iq}h_q \tag{5}$$

can be calculated using vector-coupling techniques and are shown in table 2(*a*).

By using projection operator techniques (Cotton 1971) we can find six ${}^2\mathrm{P}$ symmetry-adapted functions belonging to the irreducible representations [3], $[1^3]$ and [21] of

Table 1. The notation is $0\bar{0}+ = \mathrm{p}_0\bar{\mathrm{p}}_0\mathrm{p}_{+1}$, etc.

$h_1 = +\bar{0}0$	$h_2 = 0\bar{+}0$	$h_3 = \bar{+}00$	$h_4 = \bar{0}+0$	$h_5 = +\bar{-}+$	$h_6 = -\bar{+}+$
$h_7 = \bar{+}-+$	$h_8 = \bar{-}++$	$h_9 = 0\bar{0}+$	$h_{10} = 00\bar{+}$	$h_{11} = 0+\bar{0}$	$h_{12} = +\bar{+}-$
$h_{13} = +-\bar{+}$	$h_{14} = ++\bar{-}$	$h_{15} = \bar{0}0+$	$h_{16} = +0\bar{0}$	$h_{17} = \bar{+}+-$	$h_{18} = -+\bar{+}$

Table 2. Matrix elements for **A** and **B** (normalisation factor$=1/\sqrt{N}$).

(*a*) matrix **A**

	q																		
S_iL_i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	*N*
$[{}^3\mathrm{D}]$	3	3	3	3	−1	−1	−1	−1	−2	4	−6	−6	2	12	−2	−6	−6	2	360
$[{}^1\mathrm{D}]$	−3	−3	3	3	1	1	−1	−1	2			6			−2		−6		120
$[{}^3\mathrm{P}]$	−1	1	−1	1	1	−1	1	−1			−2		−2			2		2	24
$[{}^1\mathrm{P}]$	1	−1	−1	1	−1	1	1	−1											8
$[{}^3\mathrm{S}]$					−1	−1	−1	−1	1	−2			2		1			2	18
$[{}^1\mathrm{S}]$					1	1	−1	−1	−1						1				6

(*b*) matrix **B**

	q																		
Γ_i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	*N*
$[1^3]$	1			−1		1	−1		−1		1	−1	1		1	−1	1	−1	12
[3]	1	−2	−2	1	−2	1	1	−2	1	−2	1	1	1	−2	1	1	1	1	36
$[21]^{\mathrm{I}}_{\mathrm{a}}$	2	−1	−1	2	−1	2	2	−1	−1	2	−1	−1	−1	2	−1	−1	−1	−1	36
$[21]^{\mathrm{I}}_{\mathrm{b}}$		1	−1		1			−1	−1		−1	−1	−1		1	1	1	1	12
$[21]^{\mathrm{II}}_{\mathrm{a}}$	1	1	1	1	−2	−2	−2	−2	1	−2	−2	−2	4	4	1	−2	−2	4	90
$[21]^{\mathrm{II}}_{\mathrm{b}}$	−1	−1	1	1	2	2	−2	−2	−1			2			1		−2		30

the symmetric group S_3 (Condon and Odabasi 1980). This can be done by the application of the standard Young operators associated with the standard Young tableaux of S_3 (Chisholm 1976)

$$\hat{Y}_1=\begin{array}{|c|c|c|}\hline 1&2&3\\\hline\end{array}\qquad \hat{Y}_2=\begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\hline\end{array}\qquad \hat{Y}_3=\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}\qquad \hat{Y}_4=\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array} \tag{6}$$

on the ^{2}P functions of equation (5).

For instance, we may generate the function which forms a basis for the $[1^3]$ representation of S_3 from the sixth line of table 2(a):

$$\hat{Y}_1(\mathrm{p}^2[^1\mathrm{S}]\mathrm{p}\,^2\mathrm{P})=1/\sqrt{12}(h_1-h_4+h_6-h_7-h_9+h_{11}-h_{12}+h_{13}+h_{15}-h_{16}+h_{17}-h_{18}). \tag{7}$$

Using the same generator $\mathrm{p}^2[^1\mathrm{S}]\mathrm{p}\,^2\mathrm{P}$ we can get two basis functions for the [21] representation:

$$\begin{aligned}\hat{Y}_3(\mathrm{p}^2[^1\mathrm{S}]\mathrm{p}\,^2\mathrm{P})&=1/\sqrt{14}(h_1+h_4-h_5-h_8-h_{11}-h_{12}+h_{13}+2h_{14}-h_{16}-h_{17}+h_{18})\\ \hat{Y}_4(\mathrm{p}^2[^1\mathrm{S}]\mathrm{p}\,^2\mathrm{P})&=1/\sqrt{14}(-h_1+2h_5+h_6-h_7-h_8-h_9+h_{12}-h_{13}-h_{14}+h_{15}+h_{16}).\end{aligned} \tag{8}$$

Two other basis functions for the [21] representation can be generated from the application of $\hat{Y}_3$ and $\hat{Y}_4$ on $\mathrm{p}^2[^3\mathrm{P}]\mathrm{p}\,^2\mathrm{P}$ (third line of table 2(a)). The projected functions are not orthogonal and a final Schmidt orthogonalisation procedure is required to obtain orthogonal symmetry-adapted ^{2}P functions:

$$\Phi(\mathrm{p}^3\,^2\mathrm{P}[\Gamma_i])=\sum_{q=1}^{18} B_{iq}h_q \tag{9}$$

where Γ_i specifies a subspecies of an irreducible representation of the group S_3. Let us introduce the labels I and II for the two states of mixed symmetry [21] and a and b for their respective subspecies. The B_{ij} matrix elements of equation (9) are given in table 2(b).

From (9) and (5) we can now determine the coefficients of the transformation required:

$$\Phi(\mathrm{p}^3\,^2\mathrm{P}[\Gamma_i])=\sum_{j=1}^{6} U_{ij}\Phi(\mathrm{p}^2[S_jL_j]\mathrm{p}\,^2\mathrm{P}) \tag{10}$$

by solving for each Γ_i the set of 18 equations in six unknowns:

$$\mathbf{UA}=\mathbf{B}. \tag{11}$$

We obtain the following matrix transformation:

$$\begin{pmatrix}\mathrm{p}^3\,^2\mathrm{P}\,[1^3]\\ [3]\\ [21]^{\mathrm{I}}_{\mathrm{a}}\\ [21]^{\mathrm{I}}_{\mathrm{b}}\\ [21]^{\mathrm{II}}_{\mathrm{a}}\\ [21]^{\mathrm{II}}_{\mathrm{b}}\end{pmatrix}=\begin{pmatrix}-1/\sqrt{2} & -\sqrt{\frac{5}{18}} & \sqrt{2}/3 & 0 & 0 & 0\\ 0 & 0 & 0 & 1/\sqrt{2} & -\sqrt{\frac{5}{18}} & \sqrt{2}/3\\ 0 & 0 & 0 & 1/\sqrt{2} & \sqrt{\frac{5}{18}} & -\sqrt{2}/3\\ 1/\sqrt{2} & -\sqrt{\frac{5}{18}} & \sqrt{2}/3 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & \frac{2}{3} & \sqrt{5}/3\\ 0 & \frac{2}{3} & \sqrt{5}/3 & 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\mathrm{p}^2[^3\mathrm{P}]\mathrm{p}\,^2\mathrm{P}\\ [^1\mathrm{D}]\\ [^1\mathrm{S}]\\ [^1\mathrm{P}]\\ [^3\mathrm{D}]\\ [^3\mathrm{S}]\end{pmatrix}. \tag{12}$$

The coefficients of the first line are the well known coefficients of fractional parentage expressing the $\mathrm{p}^3\,^2\mathrm{P}$ antisymmetric $[1^3]$ function in terms of the three $\mathrm{p}^2[LS]\mathrm{p}\,^2\mathrm{P}$

functions, antisymmetric for the two first particles $[1^2]$. The transformation matrix **U** is now complete and is a real orthogonal unitary matrix.

3. Using the factorisation lemma of Racah

It is possible to predict the irreducible representations (IR) of S_3 to which the six ^2P belong by using the branching rules for the reduction $U(6)\to SU(2)\times U(3)\to SU(2)\times SO(3)$. This is done by Condon and Odabasi (table 1^7) for the n-particle state function p^n, limiting to the antisymmetric partitions. We can complete this table (see table 3) by considering the other Young diagram shapes corresponding to the IR [3] and [21] and the IR [2] of U(6) for p^3 and p^2 respectively. We can now see from this table that amongst the six ^2P found in §2, one arises from $[111]=[1^3]$ of U(6) (antisymmetric), another from [3] (symmetric) while the last four are the components of two [21] representations, (mixed symmetry) which are each doubly degenerate.

Table 3. Classification of the p shell

	U(6)	SU(2)×U(3)	SU(2)×$SO_L(3)$
p^3	[111]	$^4[111]$	^4S
		$^2[21]$	$^2P,{}^2D$
	[3]	$^4[3]$	$^4F,{}^4P$
		$^2[21]$	$^2P,{}^2D$
	[21]	$^4[21]$	$^4P,{}^4D$
		$^2[3]$	$^2F,{}^2P$
		$^2[111]$	^2S
		$^2[21]$	$^2P,{}^2D$
p^2	[11]	$^3[11]$	^3P
		$^1[2]$	$^1S,{}^1D$
	[2]	$^1[11]$	^1P
		$^3[2]$	$^3S,{}^3D$

We can adopt a group-theoretical approach for calculating the complete fractional parentage transformation matrix using Racah's factorisation lemma for a chain of groups (Racah 1949). Indeed, repeated applications of Racah's theorem allows us to express a fractional parentage coefficient as an isoscalar product (Judd 1963), i.e.

$$
\begin{aligned}
&(l^{n-1}\bar{W}\bar{\xi}\bar{S}\bar{L}|\}l^nW\xi SL)\\
&\quad=(\bar{W}\bar{\xi}\bar{L}+l|W\xi L)([\bar{\lambda}]\bar{W}+[1](10\ldots0)|[\lambda]W)(l^{n-1}[\bar{\lambda}]+l|l^n[\lambda])\\
&\quad=\mathrm{Is}[U(4l+2)\to U(2)\times U(2l+1)]\mathrm{Is}[U(2l+1)\to R(2l+1)]\\
&\qquad\times\mathrm{Is}[R(2l+1)\to R(3)] \qquad (13)
\end{aligned}
$$

one isoscalar (Is) appearing for each step of the reduction $U(4l+2)\to U(2)\times U(2l+1)\to U(2)\times R(2l+1)\to U(2)\times R(3)$. For p electrons the last reduction is obviously avoided ($l=1$) while for f electrons a further factorisation must be performed. For the p shell, the isoscalar tables needed can be built by considering the different parentage schemes between the three- and two-particle functions for the two reductions $U(6)\to SU(2)\times U(3)$ (table 4(a)) and $SU(2)\times U(3)\to SU(2)\times SO(3)$ (table 6(a)). The

Table 4. Isoscalars for U(6) → SU(2) × U(3).

(*a*) $\langle p^3 | p^2 p \rangle$

U(6)		[11]		[2]	
	SU(2) × U(3)	^{3}[11]	^{1}[2]	^{1}[11]	^{3}[2]
[111]	^{2}[21]	$-1/\sqrt{2}$	$1/\sqrt{2}$		
	^{4}[111]	1	0		
[21]	^{2}[21]	$1/\sqrt{2}$	$1/\sqrt{2}$	$1/\sqrt{2}$	$-1/\sqrt{2}$
	^{4}[21]	1	0	0	1
	^{2}[3]	0	1	0	1
	^{2}[111]	1	0		0
[3]	^{2}[21]			$1/\sqrt{2}$	$-1/\sqrt{2}$
	^{4}[3]			0	1

(*b*) $\langle p^4 | p^3 p \rangle$

U(6)		[111]	
	SU(2) × U(3)	^{4}[111]	^{2}[21]
[1111]	^{5}[1111]	1	0
	^{1}[22]	0	1

coefficients required can be calculated from the orthonormality relation of isoscalars (Racah 1949, Judd 1963) and using the reciprocity relation proved by Racah (1949) and generalised by Jahn and Van Wieringen (1951). Since the general reciprocal relation connects the coefficients reducing a product representation involving the contragredient representation with those involving the original representation, the IR

Table 5.

	Representation of SU(M)	Equivalent representation of U(M)	Contragredient of SU(M)	Equivalent representation of U(M)
$M=6$	[11]	[11] [221111] [332222]	$[\overline{11}]$	[111] [222211] [333322]
	[111]	[111] [222111] [333222]	$[\overline{111}]$	[111] [222111] [333222]
$M=3$	[21]	[21] [321] [432]		
	[2]	[2] [311] [422]	$[\bar{2}]$	[22] [331] [442]
	[3]	[3] [411]	$[\bar{3}]$	[33] [441]

required and the corresponding contragredient IR of the special unitary group SU(M) as well as the equivalent representations of U(M) are given in table 5.

For the U(6) → SU(2) × U(3) reduction, the reciprocity relation can be expressed as

$$\frac{\langle \overline{[11]^1[2]} \,|\, \overline{[111]^2[21]} + [1]^2[1]\rangle}{\langle [111]^2[21] \,|\, [11]^1[2] + [1]^2[1]\rangle} = (-1)^x \left(\frac{g(^2[21])g([11])}{g(^1[2])g([111])}\right)^{1/2} = \pm\left(\frac{16\times 15}{6\times 20}\right)^{1/2} = \pm\sqrt{2} \qquad (14)$$

where x is an arbitrary phase factor and $[\bar{f}]$ is the contragredient representation of $[f]$ of SU(M). Using the equivalent representations of U(M), the reciprocity relation gives

$$\langle [111]^2[21] \,|\, [11]^1[2] + [1]^2[1]\rangle = (1/\sqrt{2})\langle [1111]^1[22] \,|\, [111]^2[21] + [1]^2[1]\rangle \qquad (15)$$

and the required isoscalars of $\langle p^3|p^2p\rangle$ can be directly deduced from that of $\langle p^4|p^3p\rangle$ (see table 4(b)), i.e.

$$\langle [111]^2[21] \,|\, [11]^1[2] + [1]^2[1]\rangle = 1/\sqrt{2}. \qquad (16)$$

The rest of table 4(a) can be obtained from the orthonormality relation:

$$\sum_{B_1} \langle AB|A_1B_1 + A_2B_2\rangle\langle A'B|A_1B_1 + A_2B_2\rangle = \delta_{A,A'} \qquad (17)$$

i.e.

$$\sum_{B_1} \langle [111]^2[21] \,|\, [11]B_1 + [1]^2[1]\rangle\langle A^2[21] \,|\, [11]B_1 + [1]^2[1]\rangle = \delta_{A,[111]} \qquad (18)$$

where A and B_1 denote the three-particle representations of U(6) and the two-particle representations of SU(2) × U(3), respectively.

Table 6. Isoscalars for U(3) → SO(3).

(a) $\langle p^3|p^2p\rangle$

U(3)		[11]	[2]	
	SO$_L$(3)	P	D	S
[111]	S	1		
[21]	D	1	1	0
	P	1	$-\sqrt{\frac{5}{9}}$	$\sqrt{\frac{4}{9}}$
[3]	F		1	0
	P		$\sqrt{\frac{4}{9}}$	$\sqrt{\frac{5}{9}}$

(b) $\langle p^7|p^6p\rangle$

U(3)		[33]	
	SO$_L$(3)	F	P
[331]	S	0	1

The same procedure can be applied for the second reduction step $SU(2)\times U(3)\rightarrow SU(2)\times SO(3)$ where the spin unitary group acts as a 'spectator' only. We have, for instance,

$$\frac{\langle[\bar{2}]S|[\bar{3}]P+[1]p\rangle}{\langle[3]P|[2]S+[1]p\rangle}=\left(\frac{g(P)g([2])}{g(S)g([3])}\right)^{1/2}=\left(\frac{3\times 6}{1\times 10}\right)^{1/2}=\sqrt{\tfrac{9}{5}}. \tag{19}$$

Using the equivalent representations of U(3) of the contragredient representations of SU(3) (see table 5), the reciprocity relation becomes

$$\langle[3]P|[2]S+[1]p\rangle=\sqrt{\tfrac{5}{9}}\langle[331]S|[33]P+[1]p\rangle$$
$$=\sqrt{\tfrac{5}{9}} \tag{20}$$

the parentage of the S state being obviously unique in the corresponding table $\langle p^7|p^6p\rangle$ (see table 6(*b*)). Again, the rest of table 6(*a*) can be easily constructed using the orthogonality relations.

Each coefficient of fractional parentage can now be expressed as a product of two isoscalars taken from tables 4(*a*) and 6(*a*) for the two successive reductions $U(6)\rightarrow SU(2)\times U(3)\rightarrow SU(2)\times SO(3)$. For instance, the matrix elements U_{11}, U_{25} and U_{55} of the transformation matrix of equation (12) can be written as

$$U_{11}=(p^2[11]^3[11]P|\}p^3[111]^2[21]P)$$
$$=\langle[111]^2[21]|[11]^3[11]+[1]^2[1]\rangle\langle^2[21]P|^3[11]P+^2[1]p\rangle$$
$$=(-1/\sqrt{2})(1)=-1/\sqrt{2} \tag{21}$$

$$U_{25}=(p^2[2]^3[2]D|\}p^3[3]^2[21]P)$$
$$=\langle[3]^2[21]|[2]^3[2]+[1]^2[1]\rangle\langle^2[21]P|^3[2]D+^2[1]p\rangle$$
$$=(1/\sqrt{2})(-\sqrt{\tfrac{5}{9}})=-\sqrt{\tfrac{5}{18}} \tag{22}$$

$$U_{55}=(p^2[2]^3[2]D|\}p^3[21]^2[3]P)$$
$$=\langle[21]^2[3]|[2]^3[2]+[1]^2[1]\rangle\langle^2[3]P|^3[2]D+^2[1]p\rangle$$
$$=(1)(\sqrt{\tfrac{4}{9}})=\tfrac{2}{3}. \tag{23}$$

4. Using the spin-free formalism

This approach consists in calculating separately a spatial fractional parentage expansion:

$$\Phi^{[\lambda]}(r_nr_{n-1}\ldots r_n)(l^nL)=\sum_{L'}(l^{n-1}[\lambda']L';l|\}l^n[\lambda]L)$$
$$\times\Phi(l^{n-1}[\lambda']L'(r_{n-1}\ldots r_1);l;L) \tag{24}$$

and a spin fractional parentage expansion (Chisholm 1976):

$$\Gamma^{[\lambda]}(r_nr_{n-1}\ldots r_1)(\tfrac{1}{2}^nS)=\sum_{S'}(\tfrac{1}{2}^{n-1}[\lambda']S';\tfrac{1}{2}|\}\tfrac{1}{2}^n[\lambda]S)$$
$$\times\Gamma(\tfrac{1}{2}^{n-1}[\lambda']S'(r_{n-1}\ldots r_1);\tfrac{1}{2};S). \tag{25}$$

The spin and spatial functions can then be combined to give the required permutation symmetry:

$$\psi^{[\lambda]}_{(r)}[LS] = \sum_{r'=1}^{n_{\lambda'}} \sum_{r''=1}^{n_{\lambda''}} c_{r'r''} \Phi^{[\lambda']}_{(r')}(L)\Gamma^{[\lambda'']}_{(r'')}(S) \tag{26}$$

where the coefficients $c_{r'r''}$ are those of the symmetry-adapted functions of the reduced representation $[\lambda]$ appearing from $[\lambda']\otimes[\lambda'']$. The direct products of S_3 (see table 7) and the symmetry-adapted functions of the reduced representations of S_3 (see table 8) can be used to build the total function belonging to a given IR of S_3. Using the Young–Yamanouchi orthogonal representation of the permutation group, the orbital and spin fractional parentage coefficients were calculated independently by Jahn and Van Wieringen (1951) for the nuclear p shell, Jahn (1951) for the d shell and Flowers (1952) for the f shell. Their tables can be used directly in our atomic context by considering the entries referring to states with maximum T and T_ξ values in the charge–spin tables. The use of these tables is illustrated here for calculating some elements of the transformation matrix derived in §§ 2 and 3.

Taking the spatial coefficients of fractional parentage from table 3 of Jahn and Van Wieringen (1951):

$$\Phi(p^3(211)[21]P) = \sqrt{\tfrac{4}{9}}\,\Phi(p^2\,S, p, P) - \sqrt{\tfrac{5}{9}}\,\Phi(p^2\,D, p, P)$$

$$\Phi(p^3(121)[21]P) = \Phi(p^2\,P, p, P)$$

$$\Phi(p^3(111)[3]P) = \sqrt{\tfrac{5}{9}}\,\Phi(p^2\,S, p, P) + \sqrt{\tfrac{4}{9}}\,\Phi(p^2\,D, p, P) \tag{27}$$

and the spin coefficients of fractional parentage from table 6 of Jahn (1951):

$$\Gamma(\gamma^3(121)[21]^{42}\Gamma) = \Gamma(\gamma^2\,{}^{31}\Gamma, \gamma, {}^{42}\Gamma)$$

$$\Gamma(\gamma^3(211)[21]^{42}\Gamma) = \Gamma(\gamma^2\,{}^{33}\Gamma, \gamma, {}^{42}\Gamma) \tag{28}$$

Table 7. Direct products of S_3.

	[3]	[111]	[21]
[3]	[3]	[111]	[21]
[111]	[111]	[3]	[21]
[21]	[21]	[21]	[3]+[111]+[21]

Table 8. Reduction of product representations of S_3 (from table 4 of Jahn 1951).

$[21]\times[21]=[3]+[21]+[111]$	$[21]\times[111]=[21]$	$[21]\times[3]=[21]$
$[3](111)=\frac{1}{\sqrt{2}}\{(211)_1(211)_2+(121)_1(121)_2\}$		
$[21](211)=-\frac{1}{\sqrt{2}}\{(211)_1(211)_2-(121)_1(121)_2\}$	$[21](211)=(121)(321)$	$[21](211)=(211)(111)$
$[21](121)=\frac{1}{\sqrt{2}}\{(211)_1(121)_2+(121)_1(211)_2\}$	$[21](121)=-(211)(321)$	$[21](121)=(121)(111)$
$[111](321)=\frac{1}{\sqrt{2}}\{(211)_1(121)_2-(121)_1(211)_2\}$		

and using the symmetry-adapted functions of table 8, we have directly

$$\Psi(p^3\,{}^2P(211)[21])$$

$$= -\frac{1}{\sqrt{2}}\{\Phi^{[21]}_{(211)}\Gamma^{[21]}_{(211)} - \Phi^{[21]}_{(121)}\Gamma^{[21]}_{(121)}\}$$

$$= -(\sqrt{2}/3)\Phi(p^2\,{}^3S, p, {}^2P) + \sqrt{\tfrac{5}{18}}\,\Phi(p^2\,{}^3D, p, {}^2P) + (1/\sqrt{2})\Phi(p^2\,{}^1P, p, {}^2P) \qquad (29)$$

from which the U_{ij} matrix elements of (12) can be derived:

$$U_{34} = 1/\sqrt{2} \qquad U_{35} = \sqrt{\tfrac{5}{18}} \qquad U_{36} = -\sqrt{2}/3.$$

Similarly,

$$\Psi(p^3\,{}^2P(121)[21]) = \Phi^{[3]}_{(111)}\Gamma^{[21]}_{(121)}$$

$$= \sqrt{5}/3\Phi(p^2\,{}^1S, p, {}^2P) + \tfrac{2}{3}\,\Phi(p^2\,{}^1D, p, {}^2P) \qquad (30)$$

$$U_{62} = \tfrac{2}{3} \qquad U_{63} = \sqrt{5}/3.$$

We must point out here that the spatial fractional parentage coefficients calculated by Jahn and Van Wieringen are nothing other than the isoscalars needed for the approach of § 3 for the reduction $SU(2) \times U(3) \rightarrow SU(2) \times SO(3)$.

5. Conclusion

We have shown how to calculate the complete fractional parentage matrix by three different approaches. We now have a better understanding of the inverse transformation (3) which is needed for a complete formulation of Brillouin's theorem in complex atomic and molecular configurations (Godefroid *et al* 1987).

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References

Chisholm C D H 1976 *Group Theoretical Techniques in Quantum Chemistry* (New York: Academic)
Condon E U and Odabasi H 1980 *Atomic Structure* (Cambridge: Cambridge University Press)
Cotton F A 1971 *Chemical Applications of Group Theory* (New York: Wiley-Interscience)
Fano U 1965 *Phys. Rev.* **140** A67–75
Flowers 1952 *Proc. R. Soc.* A **210** 497–508
Godefroid M, Liévin J and Metz J-Y 1987 *J. Phys. B: At. Mol. Phys.* to be published
Jahn H A 1951 *Proc. R. Soc.* A **205** 192–235
Jahn H A and Van Wieringen 1951 *Proc. R. Soc.* A **209** 502–25
Judd B R 1963 *Operator Techniques in Atomic Spectroscopy* (New York: McGraw-Hill)
Racah G 1943 *Phys. Rev.* **63** 367–82
—— 1949 *Phys. Rev.* **76** 1352–65