COORDINATE FRACTIONAL PARENTAGE COEFFICIENTS FOR MULTISHELL CONFIGURATIONS

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Expressions are found for the coordinate fractional parentage coefficients of an arbitrary multishell configuration in the form of a product of single-shell parentage coefficients and matrix elements of the transformation matrices of the permutation group and the rotation group. Formulas are presented for the matrix elements of the operators F and G in the case when they do not contain the spin variables.

THE problem of computing the energy and other characteristics of a system of n identical particles meets with difficulties in constructing the wave function and in the complexity of the computations. The introduction of fractional parentage coefficients in the papers of Racah[1] definitely simplified and systematized such computations. Later a whole series of papers appeared on the calculation of fractional parentage coefficients for identical particles (for a single shell).[2-7] Parentage coefficients for a configuration of several shells were obtained by Levinson,[8] and an expression for the fractional parentage coefficients of a two-shell configuration was used earlier by Elliott and Flowers.[9] Balashov, Tumanov, and Shirokov[10] obtained formulas for the matrix elements of configurations consisting of several shells by applying the methods of second quantization.

If the operators do not contain the spin variables, then to compute their matrix elements we need only know the parentage coefficients of the coordinate wave function. In the present paper we derive formulas for the coordinate fractional parentage coefficients of an arbitrary multishell configuration. We show that these coefficients are expressible as products of coordinate fractional parentage coefficients for a single shell and matrix elements of the transformation matrices of the permutation group and the rotation group. In addition we give formulas for the matrix elements of single-particle and two-particle operators which depend only on the spatial coordinates.

1. TWO-SHELL CONFIGURATION

The primary interest in quantum mechanical calculations is the computation of matrix elements of operators of the type[11]

$$F = \sum_{i=1}^{n} f_i, \quad G = \sum_{i<j}^{n} g_{ij}.$$

It is therefore convenient to represent the wave function of a system of n particles as an expansion in which one or two particles are separated out; the coefficients in such an expansion are called fractional parentage coefficients. We write the formal expansion of the coordinate wave function for a configuration consisting of two shells.*

a) Removal of a single particle, parentage coefficients of the type $\langle n-1, 1|\} n\rangle$:

$$\begin{aligned}
&\Phi((l_1^{n_1}[\lambda_1]\alpha_1L_1,\ l_2^{n_2}[\lambda_2]\alpha_2L_2)[\lambda](r)LM)\\
&\quad=\sum_{\lambda_2'}\sum_{\alpha_1'L_1'L'}\varphi((l_1^{n_1-1}[\lambda_1']\alpha_1'L_1',\ l_2^{n_2}[\lambda_2]\alpha_2L_2)[\lambda'](r')L',l_1;LM)\\
&\quad\times\langle(l_1^{n_1-1}[\lambda_1']\alpha_1'L_1',\ l_2^{n_2}[\lambda_2]\alpha_2L_2)[\lambda']L',l_1;L|\}\,l_1^{n_1}[\lambda_1]\\
&\quad\times\ \alpha_1L_1,l_2^{n_2}[\lambda_2]\alpha_2L_2;[\lambda]L\rangle\\
&\quad+\sum_{\lambda_2'}\sum_{\alpha_2'L_2'L'}\varphi((l_1^{n_1}[\lambda_1]\alpha_1L_1,\ l_2^{n_2-1}[\lambda_2']\alpha_2'L_2')[\lambda'](r')L',l_2;LM)\\
&\quad\times\langle(l_1^{n_1}[\lambda_1]\alpha_1L_1,\ l_2^{n_2-1}[\lambda_2']\alpha_2'L_2')[\lambda']L',l_2;L|\}\,l_1^{n_1}[\lambda_1]\\
&\quad\times\ \alpha_1L_1,l_2^{n_2}[\lambda_2]\alpha_2L_2;[\lambda]L\rangle. \qquad (1)
\end{aligned}$$

The function φ is formed as follows: we vector couple the wave function of n'th particle to the wave function with permutation symmetry $[\lambda'](r')$ for the configuration of $n-1$ particles. There is no summation over $[\lambda'](r')$ since the assignment of the Yamanouchi symbol (r)

*Throughout the paper we use the notation of our previous work,[12] references to which are indicated by a Roman numeral I. The quantum numbers of the configuration left after removal of a particle are indicated by a prime, those of the removed particle by a double prime.

uniquely determines the symmetry of the $(n-1)$ particles (cf.[2-3]).

b) Removal of two particles, parentage coefficients of the type $\langle n-2,\ 2\,|\}n\rangle$:

$$
\begin{aligned}
&\Phi\left((l_1^{n_1}[\lambda_1]\alpha_1L_1,\ l_2^{n_2}[\lambda_2]\alpha_2L_2)[\lambda](r'r'')LM\right)\\
&=\sum_{\lambda_1'}\ \sum_{\alpha_1'L_1'L_1''L'}\varphi\left((l_1^{n_1-2}[\lambda_1']\alpha_1'L_1',\ l_2^{n_2}[\lambda_2]\alpha_2L_2)[\lambda']\right.\\
&\times(r')L',\ l_1^2[\lambda'']L_1'';\ LM)\\
&\times\langle(l_1^{n_1-2}[\lambda_1']\alpha_1'L_1',\ l_2^{n_2}[\lambda_2]\alpha_2L_2)[\lambda']L',\\
&\to l_1^2[\lambda'']L_1'';L\,|\}\,l_1^{n_1}[\lambda_1]\alpha_1L_1,\ l_2^{n_2}[\lambda_2]\alpha_2L_2;\ [\lambda]L\rangle\\
&+\sum_{\lambda_2'}\ \sum_{\alpha_2'L_2'L_2''L'}\varphi\left((l_1^{n_1}[\lambda_1]\alpha_1L_1,\ l_2^{n_2-2}[\lambda_2']\alpha_2'L_2')[\lambda'](r')L',\right.\\
&\times l_2^2[\lambda'']L_2'';\ LM)\ \langle(l_1^{n_1}[\lambda_1]\alpha_1L_1,\ l_2^{n_2-2}[\lambda_2']\alpha_2'L_2')[\lambda']L',\\
&\to l_2^2[\lambda'']L_2'';L\,|\}\,l_1^{n_1}[\lambda_1]\alpha_1L_1,\ l_2^{n_2}[\lambda_2]\alpha_2L_2;\ [\lambda]L\rangle\\
&+\sum_{\lambda_1'\lambda_2'}\ \sum_{\alpha_1'L_1'\alpha_2'L_2'L'L''}\varphi\left((l_1^{n_1-1}[\lambda_1']\alpha_1'L_1',\ l_2^{n_2-1}[\lambda_2']\alpha_2'L_2')[\lambda']\right.\\
&\times(r')L',l_1l_2[\lambda'']L'';\ LM)\langle(l_1^{n_1-1}[\lambda_1']\alpha_1'L_1',\ l_2^{n_2-1}[\lambda_2']\alpha_2'L_2')\\
&\times[\lambda']L',\to l_1l_2[\lambda'']L'';L|\}\,l_1^{n_1}[\lambda_1]\alpha_1L_1,\ l_2^{n_2}\\
&\times[\lambda_2]\alpha_2L_2;\ [\lambda]L\rangle. \qquad (2)
\end{aligned}
$$

The choice of the representation $[\lambda']$, when reduced to the subgroup $S_{n-2}\times S_2$, corresponds to assigning the symmetry of $[\lambda'](r')$ and $[\lambda'']$, so there is no summation over these symbols.

To find the fractional parentage coefficients defined in (1) and (2) we shall start from formula I (20). Our problem is to transform it to the form (1) and (2).

Let us go through the derivation for the case of removal of two particles. For $(r)^A$ in I (20) we choose $(r'\,r'')$. Just as in[8], we divide the sum over Q into four sums, according to the effect of the permutations on the coordinates of the $(n-1)$-st and n-th particles: we denote by Q_1 those permutations which bring $n-1$ and n to the positions n_1-1 and n_1, by Q_2 those which bring $n-1$ to the position n_1, by Q_3 those which bring n to n_1, and by Q_4 those permutations which leave $n-1$ and n in their places. It is obvious that

$$
n(Q_1)=\frac{(n-2)!}{(n_1-2)!\,n_2!},\qquad n(Q_2)=n(Q_3)=\frac{(n-2)!}{(n_1-1)!\,(n_2-1)!},
$$

$$
n(Q_4)=\frac{(n-2)!}{n_1!\,(n_2-2)!},\qquad n(Q)=\sum_{i=1}^{4}n(Q_i)=\frac{n!}{n_1!n_2!}. \quad (3)
$$

Every permutation Q_i can be represented in the form of a product $Q_i'P_i$, where P_i brings $n-1$ and n to the appropriate places, while Q_i' does not act on them, i.e. $Q_i'\in S_{n-2}$. It is not difficult to show that we can choose the following permutations for P_i*

$$
P_1=\begin{cases}P_{n,\ n-2\ldots n_1-1,\ n-1,\ n-3\ldots n_1} & n_2\ \text{odd},\\ P_{n,\ n-2\ldots n_1}P_{n-1,\ n-3\ldots n_1-1} & n_2\ \text{even};\end{cases} \quad (4)
$$

$$
P_2=P_{n-1,\ n-2\ldots n_1},\qquad P_3=P_{n,\ n-1}P_2,\qquad P_4=1.
$$

Let us consider the sum over Q_1. When transformed appropriately, this sum should give explicit expressions for the fractional parentage coefficients of the type $\langle l_1^{n_1-2}\,l_2^{n_2},\ l_1^2\,|\}\,l_1^{n_1}l_2^{n_2}\rangle$. After applying P_1 to φ, we have

$$
\begin{aligned}
\sum\nolimits_1&=c\sum_{r_1r_2}\ \sum_{Q_1'}\langle[\lambda](r'r'')\,|\,Q_1\,|\,[\lambda](r_1r_2)\rangle\\
&\times Q_1'\varphi'(l_1^{n_1}[\lambda_1](r_1)\alpha_1L_1,\ l_2^{n_2}[\lambda_2](r_2)\alpha_2L_2;\\
&\to LM\,|\,1,2,\ldots,n_1-2,\ n-1,\ n;\ n_1-1,\ n_1,\ldots,n-2);
\end{aligned}
$$

$$
c=\left[\frac{f_\lambda}{f_{\lambda_1}f_{\lambda_2}}\ \frac{n_1!n_2!}{n!}\right]^{1/2}. \quad (5)
$$

The arrangement of the particle numbers in the argument of the function φ' corresponds to the distribution of the particles over the shells. Since we sum over the Yamanouchi symbols, the expression (5) can be replaced by the equivalent expression

$$
\begin{aligned}
\sum\nolimits_1&=c\sum_{\lambda_1'r_2'\lambda_1''r_1}\ \sum_{Q_1'}\langle[\lambda](r'r'')\,|\,Q_1\,|\,[\lambda]((r_1'r_1'')\lambda_1r_2)\rangle\\
&\times Q_1'\varphi'(l_1^{n_1}[\lambda_1](r_1'r_1'')\alpha_1L_1,\ l_2^{n_2}[\lambda_2](r_2)\alpha_2L_2;\\
&\to LM\,|\,1,\ 2,\ldots,\ n_1-2,\ n-1,\ n;\ n_1-1,\ n_1,\ldots,n-2).
\end{aligned} \quad (6)
$$

We strip off the particles $n-1$ and n from the first shell using the fractional parentage coefficients for that shell, and then change the order of coupling of the orbital angular momenta so that the group $l_1^{n_1-2}$ is coupled to $l_2^{n_2}$. When we do this, we get a transformation matrix for the rotation group, in other words, a matrix which transforms between different schemes for coupling the orbital angular momenta:[13]

$$
\begin{aligned}
\varphi'&=\sum_{\alpha_1'L_1'L_1''L'}\varphi''\left((l_1^{n_1-2}[\lambda_1'](r_1')\alpha_1'L_1',\ l_2^{n_2}[\lambda_2](r_2)\alpha_2L_2)L',\right.\\
&\times l_1^2[\lambda_1'']L_1'';\ LM)\langle l_1^{n_1-2}[\lambda_1']\alpha_1'L_1',\ l_1^2[\lambda_1'']L_1'';L_1|\}l_1^{n_1}\\
&\times[\lambda_1]\alpha_1L_1\rangle\langle((L_1'L_2)L'L_1'')L\,|\,((L_1'L_1'')L_1L_2)L\rangle.
\end{aligned} \quad (7)
$$

We write the matrix element as $Q_1=Q_1'P_1$ according to the formula for multiplication of the matrices chosen for the intermediate state with permutation symmetry of the function φ'' and a

*We choose for Q the permutations which preserve the increasing order of numbering of particles within each shell.

definite permutation symmetry $[\bar{\lambda}']$ for the first n − 2 numbers:

$$\langle[\lambda](r'r'')\,|\,Q_1'P_1\,|\,[\lambda]((r_1'r_1'')\,\lambda_1 r_2)\rangle$$
$$=\sum\langle[\lambda](r'r'')|\,Q_1'|\,[\lambda]((\bar{r}_1'\bar{r}_2)\,\bar{\lambda}'\bar{r}_1''))\rangle$$
$$\times\ \langle[\lambda]((\bar{r}_1'\bar{r}_2)\,\bar{\lambda}'\bar{r}_1'')\,|\,P_1\,|\,[\lambda]((r_1'r_1'')\,\lambda_1 r_2)\rangle. \qquad (8)$$

Since $Q_1'\in S_{n-2}$, the sum over $\bar{\lambda}'$ is replaced by $\delta_{\bar{\lambda}'\lambda'}$ and in addition we also get $\delta_{r_1'' r''}$. It is not difficult to show that P_1 is a matrix of type I (18), i.e. it is diagonal in $[\lambda_i](r_i)$ and is independent of the Yamanouchi symbols. Consequently the summation in (8) drops out.

We substitute (7) and (8) in (6). Since

$$\sum_{r_1'r_2}\sum_{Q_1'}\langle[\lambda'](r')\,|\,Q_1'\,|[\lambda'](r_1'r_2)\rangle\, Q_1'\varphi''([\lambda_1'](r_1'),\ [\lambda_2](r_2),\ [\lambda''])$$
$$=c'\Phi\,(([\lambda_1'][\lambda_2])\,[\lambda'](r'),\ [\lambda'']),$$
$$c'=\left\{\frac{f_{\lambda_1'}f_{\lambda_2}}{f_{\lambda'}}\frac{(n-2)!}{(n_1-2)!\,n_2!}\right\}^{1/2}, \qquad (9)$$

the summation $\sum_1$ finally takes the following form*

$$\sum\nolimits_1=cc'\sum_{\lambda_1'}\ \sum_{\alpha_1'L_1'L_1''L'}\Phi\,((l_1^{n_1-2}[\lambda_1']\,\alpha_1'L_1',\ l_2^{n_2}[\lambda_2]\,\alpha_2L_2)\,[\lambda'](r')\,L',$$
$$\times\ l_1^2[\lambda'']\,L_1'';\ LM)\langle l_1^{n_1-2}[\lambda_1']\alpha_1'L_1',\ l_1^2[\lambda'']\,L_1'';\,L_1|\}\,l_1^{n_1}[\lambda_1]$$
$$\times\ \alpha_1L_1\rangle\,\langle[\lambda]((\lambda_1'\lambda_2)\lambda'\lambda'')\,\|\,P_1\,\|\,[\lambda]((\lambda_1'\lambda'')\lambda_1\lambda_2)\rangle$$
$$\times\ \langle((L_1'L_2)\,L'L_1'')\,L\,|\,((L_1'L_1'')L_1L_2)L\rangle. \qquad (10)$$

Comparing this expression with the first term in (2), we get the following formula for the fractional parentage coefficients:

$$\langle(l_1^{n_1-2}[\lambda_1']\,\alpha_1'L_1',\ l_2^{n_2}[\lambda_2]\,\alpha_2L_2)\,[\lambda']\,L',\ \ l_1^2[\lambda'']L_1'';L_1|\}\,l_1^{n_1}[\lambda_1]$$
$$\times\alpha_1L_1,\rightarrow l_2^{n_2}[\lambda_2]\,\alpha_2L_2;\ [\lambda]\,L\rangle=\left\{\frac{f_\lambda f_{\lambda_1'}}{f_{\lambda'}f_{\lambda_1}}\frac{n_1\,(n_1-1)}{n\,(n-1)}\right\}^{1/2}$$
$$\times\ \langle l_1^{n_1-2}[\lambda_1']\,\alpha_1'L_1',\ l_1^2[\lambda'']\,L_1'';\ L_1|\}\,l_1^{n_1}[\lambda_1]\,\alpha_1L_1\rangle$$
$$\times\ \langle[\lambda]\,((\lambda_1'\lambda_2)\,\lambda'\lambda'')\,\|\,P_1\,\|\,[\lambda]\,((\lambda_1'\lambda'')\,\lambda_1\lambda_2)\rangle$$
$$\times\ \langle((L_1'L_2)\,L'L_1'')\,L\,|\,((L_1'L_1'')\,L_1L_2)\,L\rangle. \qquad (11)$$

Proceeding similarly with the fourth sum, which contains a summation over Q_4, and comparing it with the second term in (2), we get

$$\langle(l_1^{n_1}[\lambda_1]\,\alpha_1L_1,\ l_2^{n_2-2}[\lambda_2']\,\alpha_2'L_2')\,[\lambda']L',\,l_2^2[\lambda'']\,L_2'';L\,|\}$$
$$\times\,l_1^{n_1}[\lambda_1]\,\alpha_1L_1,\rightarrow l_2^{n_2}[\lambda_2]\,\alpha_2L_2;\ [\lambda]\,L\rangle$$
$$=\left\{\frac{f_\lambda f_{\lambda_2'}}{f_{\lambda'}f_{\lambda_2}}\frac{n_2\,(n_2-1)}{n\,(n-1)}\right\}^{1/2}\langle l_2^{n_2-2}[\lambda_2']\,\alpha_2'L_2',\,l_2^2[\lambda'']\,L_2'';L_1|\}$$
$$\times\ l_2^{n_2}[\lambda_2]\alpha_2L_2\rangle\langle[\lambda]((\lambda_1\lambda_2')\lambda'\lambda'')\,|\,[\lambda](\lambda_1(\lambda_2'\lambda'')\,\lambda_2)\rangle$$
$$\times\ \langle((L_1L_2')\,L'L_2'')L\,|\,(L_1\,(L_2'L_2'')\,L_2)\,L\rangle. \qquad (12)$$

*To simplify the writing, in indicating the method of reduction we write all the intermediate $[\lambda_i]$ without the square brackets.

To find the parentage coefficients $\langle l_1^{n_1-1}l_2^{n_2-1},\ l_1l_2\,|\}\,l_1^{n_1}l_2^{n_2}\rangle$ we must combine the second and third sums. First we transform the third sum:

$$\sum\nolimits_3=c\sum_{r_1r_2}\sum_{Q_2'}\langle[\lambda]\,(r'r'')\,|\,P_{n,\,n-1}\,Q_2\,|\,[\lambda]\,(r_1r_2)\rangle\,Q_3\varphi$$
$$=c\sum_{r_1r_2}\sum_{Q_2'}\langle[\lambda'']\,|\,P_{n,\,n-1}\,|[\lambda'']\rangle\langle[\lambda]\,(r'r'')|\,Q_2\,|[\lambda]\,(r_1r_2)\rangle Q_3\varphi. \qquad (13)$$

Combining it with the second, we obtain

$$\sum\nolimits_2+\sum\nolimits_3=c\sum_{r_1r_2}\sum_{Q_2'}(1+\langle[\lambda'']\,|\,P_{n,\,n-1}\,|\,[\lambda'']\rangle\,P_{n,\,n-1})$$
$$\times\ \langle[\lambda]\,(r'r'')\,|\,Q_2\,|\,[\lambda]\,(r_1r_2)\rangle\,Q_2'\varphi\,(l_1^{n_1}[\lambda_1]\,(r_1)\,\alpha_1L_1,$$
$$\rightarrow l_2^{n_2}[\lambda_2]\,(r_2)\ \alpha_2L_2;\ LM\,|\,1,\ 2\ldots n_1-1,\ n-1;\ n_1,$$
$$n_1+1\ldots\ \ n-2,\ \ n). \qquad (14)$$

Next, separating off the particles n-1 and n from the first and second shells by using the single-shell parentage coefficients and carrying out some transformations, we get the required expression:

$$\langle(l_1^{n_1-1}[\lambda_1']\,\alpha_1'L_1',\ l_2^{n_2-1}[\lambda_2']\,\alpha_2'L_2')\,[\lambda']\,L',\ l_1l_2\,[\lambda'']\,L'';\,L|\}$$
$$\times\,l_1^{n_1}[\lambda_1]\,\alpha_1L_1\rightarrow l_2^{n_2}[\lambda_2]\,\alpha_2L_2;\ [\lambda]\,L\rangle$$
$$=\left\{\frac{f_\lambda f_{\lambda_1'}f_{\lambda_2'}}{f_{\lambda'}f_{\lambda_1}f_{\lambda_2}}\frac{2n_1n_2}{n\,(n-1)}\right\}^{1/2}$$
$$\times\ \langle l_1^{n_1-1}[\lambda_1']\,\alpha_1'L_1',\,l_1;\,L_1|\}\,l_1^{n_1}[\lambda_1]\,\alpha_1L_1\rangle$$
$$\times\,\langle l_2^{n_2-1}[\lambda_2']\,\alpha_2'L_2',\,l_2;\,L_2|\}\,l_2^{n_2}[\lambda_2]\,\alpha_2L_2\rangle$$
$$\times\ \langle[\lambda]\,((\lambda_1'\lambda_2')\,\lambda'\lambda'')\,\|\,P_2\,\|\,[\lambda]\,((\lambda_1'1)\,\lambda_1\,(\lambda_2'1)\,\lambda_2)\rangle$$
$$\times\ \langle((L_1'L_2')\,L'L'')\,L\,|\,((L_1'l_1)\,L_1\,(L_2'l_2)\,L_2)\,L\rangle. \qquad (15)$$

To obtain the fractional parentage coefficients $\langle n-1,\ 1\,|\}\,n\rangle$, we divide the sum over Q in I (20) into two sums. In the first sum we include the permutations which bring particle n to position n_1. From it we obtain the form of the coefficients $\langle l_1^{n_1-1}l_2^{n_2},\ l_1\,|\}\,l_1^{n_1}l_2^{n_2}\rangle$. The second sum includes those permutations which leave the n-th particle fixed, and gives us $\langle l_1^{n_1}l_2^{n_2-1},\ l_2\,|\}\,l_1^{n_1}l_2^{n_2}\rangle$. As a result we have

$$\langle(l_1^{n_1-1}[\lambda_1']\,\alpha_1'L_1',\ l_2^{n_2}[\lambda_2]\,\alpha_2L_2)\,[\lambda']\,L',\ l_1;\,L|\}\,l_1^{n_1}[\lambda_1]\,\alpha_1L_1,$$
$$\rightarrow l_2^{n_2}[\lambda_2]\,\alpha_2L_2;\ [\lambda]\,L\rangle=\left\{\frac{f_\lambda f_{\lambda_1'}}{f_{\lambda'}f_{\lambda_1}}\frac{n_1}{n}\right\}^{1/2}\langle l_1^{n_1-1}[\lambda_1']\,\alpha_1'L_1',\ l_1;$$
$$L_1\,|\}\,l_1^{n_1}[\lambda_1]\,\alpha_1L_1\rangle\ \langle[\lambda]\,((\lambda_1'\lambda_2)\,\lambda'1)\,\|\,P_{n,\,n-1\ldots n_1}\|\,[\lambda]$$
$$\times((\lambda_1'\ 1)\lambda_1\lambda_2)\rangle\,\langle((L_1'L_2)L'l_1)\,L((L_1'l_1)L_1L_2)L\rangle; \qquad (16)$$

$$\langle(l_1^{n_1}[\lambda_1]\,\alpha_1L_1,\ l_2^{n_2-1}[\lambda_2']\,\alpha_2'L_2')\,[\lambda']\,L',\ l_2;\ \ L\,|\}\,l_1^{n_1}[\lambda_1]\,\alpha_1L_1,$$
$$\rightarrow l_2^{n_2}[\lambda_2]\,\alpha_2L_2;\ [\lambda]\,L\rangle=\left\{\frac{f_\lambda f_{\lambda_2'}}{f_{\lambda'}f_{\lambda_2}}\frac{n_2}{n}\right\}^{1/2}\langle l_2^{n_2-1}[\lambda_2']\,\alpha_2'L_2'l_2;$$
$$L_2\,|\}\ l_2^{n_2}[\lambda_2]\,\alpha_2L_2\rangle\,\langle[\lambda]\,((\lambda_1\lambda_2')\,\lambda'1)\,|\,[\lambda]\,(\lambda_1\,(\lambda_2'1)\,\lambda_2)\rangle$$
$$\times\,\langle((L_1L_2')\,L'l_2)\,L\,|\,(L_1\,(L_2'l_2)\,L_2)\,L\rangle. \qquad (17)$$

All our formulas for the parentage coefficients are diagonal in the shells from which no particles were split off, and the transformation matrices repeat the coupling scheme in the two parts of the parentage coefficient. It is not hard to see that for the special case of the antisymmetric representation [λ] = [11 . . . 1] the formulas for the parentage coefficients go over into the corresponding formulas in the paper of Levinson,[8] since, for the one-dimensional representations the transformation matrices of the permutation group, which appear in the formulas, are equal to unity except for a phase factor.

2. ARBITRARY MULTISHELL CONFIGURATION

When there are k shells present, to characterize a state with a given permutation symmetry and total orbital angular momentum we must also give k-2 intermediate symmetry patterns and k-2 intermediate orbital angular momenta. We shall define the fractional parentage coefficients for such a configuration by generalizing the expansion of the coordinate wave function for two shells given in (1) and (2):

$$\Phi((l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_k^{n_k}[\lambda_k]\,\alpha_kL_k)^B\,b_\lambda\,[\lambda]\,(r)\,b_LLM)$$
$$=\sum_{i=1}^{k}\sum_{\lambda_i' b_{\lambda'}}\sum_{\alpha_i'L_i'b_{L'}L'}\Phi((l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_i^{n_i-1}[\lambda_i']\,\alpha_i'L_i'\ldots$$
$$\to l_k^{n_k}[\lambda_k]\,\alpha_kL_k)^{B'}\,b_{\lambda'}\,[\lambda']\,(r')\,b_{L'}L',\ l_i;\ LM)$$
$$\times\langle(l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_i^{n_i-1}[\lambda_i']\,\alpha_i'L_i'\ldots l_k^{n_k}[\lambda_k]$$
$$\times\ \alpha_kL_k)^{B'}b_{\lambda'}\,[\lambda']\,b_{L'}L',$$
$$\to l_i;\ L|\}\,(l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots)^B\,b_\lambda\,[\lambda]\,b_LL\rangle. \qquad (18)$$

B and B′ are the coupling schemes for the shell symmetry patterns and orbital angular momenta (cf. I); b_λ and b_L are respectively the sets of intermediate symmetry patterns and intermediate orbital angular momenta. The summation extends only over those symmetry patterns and orbital angular momenta in $b_{\lambda'}$ and $b_{L'}$ which appear when we strip off a particle. Furthermore,

$$\Phi((l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_k^{n_k}[\lambda_k]\,\alpha_kL_k)^B\,b_\lambda\,[\lambda]\,(r'r'')\,b_LLM)$$
$$=\sum_{i=1}^{k}\sum_{\lambda_i' b_{\lambda'}}\sum_{\alpha_i'L_i'L_i''b_{L'}L'}\Phi((l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_i^{n_i-2}[\lambda_i']$$
$$\times\ \alpha_i'L_i'\ldots l_k^{n_k}[\lambda_k]\,\alpha_kL_k)^{B'}\to b_{\lambda'}\,[\lambda']\,(r')\,b_{L'},L',\ l_i^2\,[\lambda'']$$
$$\times\ L_i'';\ LM)\,\langle(l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_i^{n_i-2}[\lambda_i']\,\alpha_i'L_i'\ldots l_k^{n_k}[\lambda_k]$$
$$\times\ \alpha_kL_k)^{B'}\,b_{\lambda'}\,[\lambda']\,b_{L'}L',\ \to l_i^2\,[\lambda'']\,L_i'';\,L|\}$$
$$\times\ (l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots)^B\,b_\lambda\,[\lambda]\,b_LL\rangle$$
$$+\sum_{i<j}\ \sum_{\lambda_i'\lambda_j'b_{\lambda'}}\ \sum_{\alpha_i'L_i'\alpha_j'L_j'b_{L'}L'L''}\Phi((l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_i^{n_i-1}[\lambda_i']$$
$$\times\ \alpha_i'L_i'\ldots\to l_j^{n_j-1}[\lambda_j']\,\alpha_j'L_j'\ldots l_k^{n_k}[\lambda_k]\,\alpha_kL_k)^{B'}\,b_{\lambda'}\,[\lambda']$$
$$\times\ (r')\,b_{L'}L',\ l_il_j\,[\lambda'']\,L'';\ LM)\,\langle(l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_i^{n_i-1}[\lambda_i']$$
$$\times\ \alpha_i'L_i'\ldots l_j^{n_j-1}[\lambda_j']\,\alpha_j'L_j'\ldots l_k^{n_k}[\lambda_k]\,\alpha_kL_k)^{B'}$$
$$\to b_{\lambda'}\,[\lambda']\,b_{L'}L',\ \ l_il_j\,[\lambda'']\,L'';\,L|\}\,(l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots)^B\,b_\lambda$$
$$\times\ [\lambda]\,b_LL\rangle. \qquad (19)$$

To obtain the fractional parentage coefficients defined in (18) and (19) we shall start from the expression I (21) for the wave function. The computations are similar to those for the case of two shells, but are more complicated. We shall give only the results.

In the case of $\langle n-1,\ 1\,|\}\,n\rangle$,

$$\langle(l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_i^{n_i-1}[\lambda_i']\,\alpha_i'L_i'\ldots l_k^{n_k}[\lambda_k]\,\alpha_kL_k)^B\,b_{\lambda'}\,[\lambda']\,b_{L'}L',$$
$$\to l_i;\ L_i|\}(l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots)^B\,b_\lambda\,[\lambda]\,b_LL\rangle$$
$$=\left\{\frac{f_\lambda f_{\lambda_i'}}{f_{\lambda'}f_{\lambda_i}}\frac{n_i}{n}\right\}^{1/2}\langle l_i^{n_i-1}[\lambda_i']\,\alpha_i'L_i',\ l_i;\ L_i|\}\,l_i^{n_i}[\lambda_i]\alpha_iL_i\rangle$$
$$\times\langle[\lambda]\,((\lambda_1\ldots\lambda_i'\ldots\lambda_k)^{B'}\,b_{\lambda'}\lambda'1)\,\|\,P_i^{(1)}\,\|\,[\lambda]\,((\lambda_1\ldots(\lambda_i'\,1)$$
$$\times\ \lambda_i\ldots\lambda_k)^B\,b_\lambda)\rangle\langle((L_1\ldots L_i'\ldots L_k)^{B'}\,b_{L'}\,L'l_i)$$
$$\times\ L\,|\,(L_1\ldots(L_i'l_i)\ L_i\ldots L_k)^B\,b_LL\rangle. \qquad (20)$$

In the case of $\langle n-2,\ 2\,|\}\,n\rangle$, for the stripping off of two particles from the same shell,

$$\langle(l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_i^{n_i-2}\,[\lambda_i']\,\alpha_i'L_i'\ldots l_k^{n_k}[\lambda_k]\,\alpha_kL_k)^{B'}\,b_{\lambda'}\,[\lambda']$$
$$\times\,b_{L'}L',\to l_i^2\,[\lambda'']\,L_i'';\,L|\}\,(l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots)^B\,b_\lambda\,[\lambda]\,b_LL\rangle$$
$$=\left\{\frac{f_\lambda f_{\lambda_i'}}{f_{\lambda'}f_{\lambda_i}}\frac{n_i\,(n_i-1)}{n\,(n-1)}\right\}^{1/2}\langle l_i^{n_i-2}\,[\lambda_i']\,\alpha_iL_i,\ \ l_i^2\,[\lambda'']\,L_i'';\ L_i|\}\,l_i^{n_i}$$
$$\times\,[\lambda_i]\,\alpha_iL_i\rangle\langle[\lambda]\,((\lambda_1\ldots\lambda_i'\ldots\lambda_k)^{B'}\,b_{\lambda'}\lambda'\lambda'')\,\|\,P_i^{(2)}\,\|\,[\lambda]$$
$$\times((\lambda_1\ldots(\lambda_i'\lambda'')\ \lambda_i\ldots\lambda_k)^B\,b_\lambda)\rangle\langle((L_1\ldots L_i'\ldots L_k)^{B'}$$
$$\times\,b_{L'}L'L_i'')\,L\,|\,(L_1\ldots(L_i'L_i'')\,L_i\ldots L_k)^B\,b_LL\rangle. \qquad (21)$$

For stripping off from different shells,

$$\langle(l_1^{n_1}[\lambda_1]\,\alpha_1L_1\ldots l_i^{n_i-1}[\lambda_i']\,\alpha_i'L_i'\ldots l_j^{n_j-1}[\lambda_j']\,\alpha_j'L_j'\ldots$$
$$\ldots l_k^{n_k}[\lambda_k]\,\alpha_kL_k)^{B'}\,b_{\lambda'}\,[\lambda']\,b_{L'}L',\to l_il_j\,[\lambda'']\,L'';\,L|\}\,(l_1^{n_1}[\lambda_1]$$
$$\times\ \alpha_1L_1\ldots)^B\,b_\lambda\,[\lambda]\,b_LL\rangle=\left\{\frac{f_\lambda f_{\lambda_i'}f_{\lambda_j'}}{f_{\lambda'}f_{\lambda_i}f_{\lambda_j}}\frac{2n_in_j}{n\,(n-1)}\right\}^{1/2}$$
$$\times\langle l_i^{n_i-1}\,[\lambda_i']\,\alpha_i'L_i,\,l_i;\,L_i|\}\,l_i^{n_i}\,[\lambda_i]\ \alpha_iL_i\rangle\ \langle l_j^{n_j-1}\,[\lambda_j']\,\alpha_j'L_j',\ l_j;$$
$$\times\ L_j|\}\,l_j^{n_j}\,[\lambda_j]\,\alpha_jL_j\rangle\langle[\lambda]((\lambda_1\ldots\lambda_i'\ldots\lambda_j'\ldots\lambda_k)^{B'}\,b_{\lambda'}\lambda'\lambda'')\,\|\,P_{ij}^{(2)}\|$$
$$\times\,[\lambda]\,((\lambda_1\ldots(\lambda_i'1)\,\lambda_i\ldots(\lambda_j'1)\,\lambda_j\ldots\lambda_k)^B\,b_\lambda)\rangle$$
$$\times\langle((L_1\ldots L_i'\ldots L_j'\ldots L_k)^{B'}\,b_{L'}L'L'')\,L\,|\,(L_1\ldots(L_i'l_i)\,L_i\ldots(L_j'l_j)$$
$$\times\,L_j\ldots L_k)^B\,b_LL\rangle. \qquad (22)$$

All the permutations in formulas (20)—(22) preserve the increasing order of numbering of particles within the shells. $P_i^{(1)}$ moves n to the position of the last particle in the i-th shell, whose number we denote by $m_i = \sum_{t=1}^{i} n_t$; $P_i^{(2)}$ shifts n and n-1 into the i-th shell; $P_{ij}^{(2)}$ takes particle n-1 into the i-th shell and particle n into the j-th shell, $m_i < m_j$:

$$P_i^{(1)} = P_{n,\, n-1 \ldots m_i};$$

$$P_i^{(2)} = \begin{cases} P_{n,\, n-2 \ldots m_i-1,\, n-1,\, n-3 \ldots m_i} & (n-m_i) \text{ odd,} \\ P_{n,\, n-2 \ldots m_i} P_{n-1,\, n-3 \ldots m_i-1} & (n-m_i) \text{ even,} \end{cases}$$

$$P_{ij}^{(2)} = \begin{cases} P_{n,\, n-2 \ldots m_j-1,\, m_j-2 \ldots m_i,\, n-1,\, n-3 \ldots m_j} & (n-m_j) \text{ odd,} \\ P_{n,\, n-2 \ldots m_j} P_{n-1,\, n-3 \ldots m_j-1,\, m_j-2 \ldots m_i} & (n-m_j) \text{ even.} \end{cases} \tag{23}$$

3. COMPUTATION OF FRACTIONAL PARENTAGE COEFFICIENTS

The expressions found for the fractional parentage coefficients consist of four factors: 1) a normalization factor, 2) parentage coefficients for a single shell, 3) matrix elements of transformation matrices of the permutation group, and 4) matrix elements of transformation matrices of the rotation group. $[\lambda] \equiv [\lambda^{(1)}\lambda^{(2)} \ldots \lambda^{(m)}]$ of the permutation group S_n is given by the formula

$$f_\lambda = n! \prod_{i<j}^{m} (h_i - h_j) / h_1! \ldots h_m!, \qquad h_i = \lambda^{(i)} + m - i. \tag{24}$$

Single-shell parentage coefficients for stripping off of one particle for the d and p shells are given in[2] and[3]; those for stripping off two particles for the p shell are in[5]. Coefficients for stripping of two particles can be found from those for stripping off one particle by using the formulas of[5]. The transformation matrices for the rotation group are studied in detail in the monograph of Yutsis, Levinson, and Vanagas,[13] who also give a complete bibliography of available tables of these matrices.

The transformation matrices of the permutation group can be calculated in terms of the matrices of the standard Young-Yamanouchi[3,15] representation by using the method developed in I.* Let us consider some examples:

$$\langle [\lambda] ((\lambda_1'\lambda_2)\lambda'\lambda'') \| P_1 \| [\lambda] ((\lambda_1'\lambda'')\lambda_1\lambda_2)\rangle = \sum_{r,\bar{r}} \langle [\lambda] ((r_1'r_2)\lambda'r'') | [\lambda](r)\rangle \langle [\lambda](r) | P_1 | [\lambda](\bar{r})\rangle \langle [\lambda](\bar{r}) | [\lambda]((r_1'r'')\lambda_1 r_2)\rangle. \tag{25}$$

*Calculations are being made at present of tables of transformation matrices of the permutation group which appear in the formulas for fractional parentage coefficients of two-shell configurations with N = 3 – 6. Tables are also being prepared of coordinate parentage coefficients for vector-uncoupled states with numbers of particles from three to six.

The Yamanouchi symbols in the matrices for transition from the standard basis to the nonstandard one can be chosen in any convenient manner, since the final expression does not depend on them. The two transformation matrices are found from formulas I (13) and I (8). Conditions like I (10):

$$\{\lambda_1(\lambda_1'\lambda'')\}, \quad \{\lambda(\lambda_1\lambda_2)\}, \quad \{\lambda'(\lambda_1'\lambda_2)\}, \quad \{\lambda(\lambda'\lambda'')\} \tag{26}$$

are imposed on the symmetry patterns in (25). We find the matrix appearing in (12) by choosing as the intermediate state the one with the standard pattern in the reduction:

$$\langle [\lambda]((\lambda_1\lambda_2')\lambda'\lambda'') | [\lambda](\lambda_1(\lambda_2'\lambda'')\lambda_2)\rangle = \sum_{(r)} \langle [\lambda]((r_1r_2')\lambda'r'') | [\lambda](r)\rangle \langle [\lambda](r) | [\lambda](r_1(r_2'r'')\lambda_2)\rangle. \tag{27}$$

Similarly we find the matrices with more complicated reduction types.

4. COMPUTATION OF MATRIX ELEMENTS

In those cases where the operators do not depend on the spin coordinates, a knowledge of the coordinate wave functions is sufficient for computing the matrix elements. We start from the expression for the antisymmetric total wave function in the form of a sum of products of coordinate and spin functions,* symmetrized according to associated representations:[3]

$$\Psi = \frac{1}{\sqrt{f_\lambda}} \sum_{(r)} \Phi_{(r)}^{[\lambda]} \chi_{(\tilde{r})}^{[\tilde{\lambda}]}. \tag{28}$$

Using the orthonormality of the spin functions and the expansions (18) and (19), we can express the matrix elements of the operators F and G for an arbitrary multishell configuration in terms of the fractional parentage coefficients and matrix elements for one or two particles. Here, because of the identity of the particles or, what amounts to the same thing, because of the antisymmetry of the total wave function, the operator F can be replaced by nf_n, and G by $\frac{1}{2}n(n-1)g_{n-1,n}$. The operator f_n acts only on the coordinates of the last (n-th) particle, and $g_{n-1,n}$ on the coordinates of the last two particles; we shall assume it to be a scalar, and denote it simply by g.

For the matrix elements of the operator F we get

*For nucleons we have a spin-charge function in place of the spin function, so in the following formulas we must write the isotopic spin T in addition to the spin S in the matrix elements.

$$\langle\alpha\,[\lambda]\,LM_L\beta\,SM_S\,|\,F\,|\,\bar{\alpha}\,[\lambda]\,\bar{L}\bar{M}_L\,\bar{\beta}\bar{S}\bar{M}_{\bar{S}}\rangle = \delta\,(\beta SM_S,\ \bar{\beta}\bar{S}\bar{M}_{\bar{S}})\,n\sum_{i=1}^{k}\sum_{\alpha'\lambda'L'}\frac{f_{\lambda'}}{f_\lambda}\langle\alpha\,[\lambda]\,L\,\{|\,\alpha'\,[\lambda']\,L',\ l_i;\,L\rangle\,\langle\alpha'\,[\lambda']\,L',\ l_i;\ \ LM\,|\,f_n\,|\,\alpha'\,[\lambda']\,L',\ l_i;\ \bar{L}\bar{M}\rangle \times\langle\alpha'\,[\lambda']\,L',\ l_i;\,\bar{L}\,|\}\,\bar{\alpha}\,[\lambda]\,\bar{L}\rangle. \quad (29)$$

To shorten the writing we have omitted the designation of the configurations; the sets of orbital quantum numbers which distinguish terms of the same type are denoted by α, and the set of spin quantum numbers by β. The matrix elements of the operator f_n can be determined by using the algebra of tensor operators developed by Racah.[16] For the scalar operator G we have

$$\langle\alpha\,[\lambda]\,L\beta S\,|\,G\,|\,\bar{\alpha}\,[\lambda]\,L\beta S\rangle = \frac{n\,(n-1)}{2}\sum_{i\leqslant j}^{k}\sum_{\alpha'\lambda'L'\lambda''L''}\frac{f_{\lambda'}}{f_\lambda} \times\langle\alpha\,[\lambda]\,L\{|\,\alpha'\,[\lambda']\,L',\ l_il_j\,[\lambda'']\,L'';\,L\rangle \times\langle l_i\,l_j\,[\lambda'']\,L''\,|\,g\,|\,l_il_j\,[\lambda'']\,L''\rangle \times\langle\alpha'\,[\lambda']\,L',\ l_il_j\,[\lambda'']\,L'';\,L|\}\,\bar{\alpha}\,[\lambda]\,L\rangle. \quad (30)$$

A detailed description of the computation of orbital matrix elements of the operator g can be found, for example, in the paper of Elliott and Lane (cf.[17]). In the matrix element formulas (29) and (30) it is assumed that the same configuration appears on the right and left hand sides. In a similar way one can obtain formulas for the nonvanishing matrix elements with configurations which differ by having one or two particles permuted between the shells.

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[1] G. Racah, Phys. Rev. **63**, 367 (1943); **76**, 1352 (1949).

[2] H. A. Jahn, Proc. Roy. Soc. (London) **A205**, 192 (1951).

[3] H. A. Jahn and H. van Wieringen, Proc. Roy. Soc. (London) **A209**, 502 (1951).

[4] A. R. Edmonds and B. H. Flowers, Proc. Roy. Soc. (London) **A214**, 515 (1952).

[5] Elliott, Hope and Jahn, Phil. Trans. Roy. Soc. **A246**, 241 (1953).

[6] P. J. Redmond, Proc. Roy. Soc. (London) **A222**, 84 (1954).

[7] A. Hassitt, Proc. Roy. Soc. (London) **A229**, 110 (1955).

[8] I. B. Levinson, Reports of the Academy of Sciences, Lithuanian SSR, **B4**, 17 (1957).

[9] J. P. Elliott and B. H. Flowers, Proc. Roy. Soc. (London) **A229**, 536 (1955).

[10] Balashov, Tumanov and Shirokov, Nuclear Reactions at Low and Medium Energies, Reports of the All-Union Conference, 1957-58, p. 548.

[11] E. U. Condon and G. H. Shortley, The Theory of Atomic Spectra, Cambridge, University Press, 1935.

[12] I. G. Kaplan, JETP **41**, 560 (1961). Soviet Phys. JETP **14**, 401 (1962).

[13] Yutsis, Levinson and Vanagas, Matematicheskii Apparat Teori Momenta Kolichestva Dvizheniya (Mathematical Apparatus of the Theory of Angular Momentum) Vilna, 1960.

[14] F. Murnaghan, The Theory of Group Representations, The Johns Hopkins Press, Baltimore, 1938.

[15] D. E. Rutherford, Substitutional Analysis, Edinburgh University Press, 1948.

[16] G. Racah, Phys. Rev. **62**, 438 (1942). G. Racah, Group Theory and Spectroscopy, mimeographed lecture notes, Princeton, 1951.

[17] J. P. Elliott and A. M. Lane, Handbuch der Physik, Vol. 39, 1957.

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