PHYSICAL REVIEW VOLUME 96, NUMBER 4 NOVEMBER 15, 1954

Direct Evaluation of Fractional Parentage Coefficients Using Young Operators. General Theory and $<4|2,2>$ Coefficients

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(Received June 1, 1954)

General expressions for $\langle n|m,n-m\rangle$ fractional parentage coefficients are derived, for the special case where the state vectors are all different, by using normalized Young symmetry operators constructed out of permutation operators acting on the state vectors. The coefficients are given directly in terms of matrix elements of the permutations characterizing the cosets of the subgroup $S_m\times S_{n-m}$ of S_n multiplied by the corresponding permutation operator. The permutation operators themselves are expressible in terms of Racah W functions. Explicit expressions for the $\langle 4|2,2\rangle$ coefficients are given also for cases where some of the state vectors are identical.

1. INTRODUCTION

PROGRESS in the theory of nuclear structure requires, with the shell model, the setting up of energy matrices between many different single-particle configurations. The most direct way of setting up the energy matrices is by use of n-particle wave functions expressed as linear combinations of totally antisymmetric states of the first $n-2$ particles, vector coupled to totally antisymmetric states of the last two particles. Reduction in the size of energy matrices determining ground state properties requires the construction of states belonging to definite irreducible representations of the group of permutations of the space coordinates alone, so that the energy matrices can, in the first instance, be set up between states of maximum or near maximum orbital symmetry characteristic of the ground state. The coefficients of those linear combinations of vector coupled orbital states of $n-2$ and 2 particles of definite orbital symmetry, which give rise to states of definite orbital symmetry for n particles, are the $\langle n|n-2, 2\rangle$ orbital coefficients of fractional parentage. It is with the calculation of these, in mixed single-particle configurations, that we are mainly concerned.

2. PERMUTATIONS OF STATES AND PARTICLES. NORMALIZED YOUNG OPERATORS

If

$$\Phi_0=\Phi(j_1(1)j_2(2)J_2,\ j_3(3)J_3,\ \cdots,\ j_{n-1}(n-1)J_{n-1},\ j_n(n)JM) \quad (1)$$

is an n-particle vector coupled orbital state, with $j_1, j_2, \cdots, j_n$ all different, the numbers in parentheses being the particle numbers, we may form $n!$ distinct states from it by either permuting the particle numbers keeping the order of the states fixed, or by permuting the order of the states keeping the particle order unaltered. The relation between these two operations is the following. If P is a permutation of the particle nunbers, P^{-1} its inverse, then we define the corresponding permutation $\bar{P}$ of the states by

$$\begin{aligned}\bar{P}\Phi_0&=P^{-1}\Phi_0\\&=\Phi(j_1(P^{-1}1)j_2(P^{-1}2)J_2,\ j_3(P^{-1}3)J_3,\ \cdots\ J_{n-1},\ j_n(P^{-1}n)JM)\\&=\sum_{J_2'J_3'\cdots J_{n-1}'}\langle j_1j_2J_2j_3J_3\cdots J_{n-1}j_nJ|\,j_{P1}j_{P2}J_2'j_{P3}J_3'\cdots J_{n-1}'j_{Pn}J\rangle\\&\quad\times\Phi(j_{P1}(1)j_{P2}(2)J_2',\ j_{P3}(3)J_3',\ \cdots,\ J_{n-1}',\ j_{Pn}(n)JM).\end{aligned} \quad (2)$$

This is the basic operation of fractional parentage coefficient theory, where the particle order is always maintained.

There are now two distinct ways of operating on the state $\bar{P}\Phi_0$ by a further permutation, depending upon whether we take this to be (*a*) a permutation of the state vectors, or (*b*) a permutation of the particle numbers. These two operations commute and we have

(a) $$\bar{Q}(\bar{P}\Phi_0)=\overline{QP}\Phi_0=\bar{Q}\bar{P}\Phi_0, \quad (3)$$

(b) $$Q(\bar{P}\Phi_0)=\bar{P}Q\Phi_0=\bar{P}\bar{Q}^{-1}\Phi_0. \quad (4)$$

We see that the permutation of the state vectors $\bar{Q}$ operates by multiplication on the left of the operator $\bar{P}$, while the permutation Q of the particle numbers operates as $\bar{Q}^{-1}$ on the right of $\bar{P}$. We may say therefore that the $n!$ functions $\bar{P}\Phi_0$ can be subject to two commuting groups of permutations and it is possible to choose linear combinations of them so that they belong simultaneously to a definite row of a definite irreducible representation of each group.[1]

The linear combinations required are given directly by operating on Φ_0 by the $n!$ linear combinations of the permutations $\bar{P}$ characterizing the $n!$ distinct normalized Young tableau operators,[2]

$$\bar{\omega}_{rs}^{[\lambda]}=(f_\lambda/n!)^{\frac{1}{2}}\sum_P\theta_{rs}^{[\lambda]}(P)\bar{P}, \quad (5)$$

[1] Compare the analogous problem in molecular theory, where the rotational wave functions may be transformed by the two commuting groups of rotations (*a*) about axes fixed in space, (*b*) about axes fixed in the molecule; see, for instance, H. A. Jahn, Ann. Physik **23**, 529 (1935).

[2] The relation with the unnormalized orthogonal Young units $o_{rs}^{[\lambda]}$ as commonly defined [e.g., by D. E. Rutherford, *Substitutional Analysis* (University Press, Edinburgh, 1948)] is $\omega_{rs}^{[\lambda]}=(n!/f_\lambda)^{\frac{1}{2}}o_{rs}^{[\lambda]}$.

associated with the irreducible orthogonal matrix representations $\theta_{rs}^{[\lambda]}(P)$ of the symmetric group S_n, f_λ being the dimension of the representation. With the Young operators normalized in this way, the inverse relation,

$$\bar{P}=\sum_{\lambda rs}(f_\lambda/n!)^{\frac{1}{2}}\theta_{rs}^{[\lambda]}(P)\bar{\omega}_{rs}^{[\lambda]}, \tag{6}$$

expressing the $n!$ permutations in terms of the

$$\sum_\lambda(f_\lambda)^2=n! \tag{7}$$

symmetry operators, has the same coefficients as (5), showing that these transformation coefficients,

$$T_{\lambda rs,P}=(f_\lambda/n!)^{\frac{1}{2}}\theta_{rs}^{[\lambda]}(P), \tag{8}$$

describe an orthogonal transformation satisfying the relations:

$$\begin{aligned}\sum_{\lambda rs} T_{\lambda rs,P}T_{\lambda rs,Q}&=\sum_{\lambda rs}(f_\lambda/n!)\theta_{rs}^{[\lambda]}(P)\theta_{rs}^{[\lambda]}(Q)\\&=\delta(P,Q),\end{aligned} \tag{9}$$

$$\begin{aligned}\sum_P T_{\lambda rs,P}T_{\lambda' r's',P}&=\{(f_\lambda f_{\lambda'})^{\frac{1}{2}}/n!\}\sum_P\theta_{rs}^{[\lambda]}(P)\theta_{r's'}^{[\lambda']}(P)\\&=\delta(\lambda,\lambda')\delta(r,r')\delta(s,s').\end{aligned} \tag{10}$$

We may then form, for given $j_1j_2\cdots j_nJ_2J_3\cdots J_{n-1}JM$, the following $n!$ states,

$$\begin{aligned}\Phi_{rs}&\equiv\Phi(r|j_1j_2J_2j_3J_3\cdots j_{n-1}J_{n-1}j_nJM|s)\\&=\bar{\omega}_{rs}^{[\lambda]}\Phi_0,\end{aligned} \tag{11}$$

with the following properties:

(I) If Φ_0 is normalized and the state vectors $j_1, j_2, \cdots, j_n$ are all different, then the states Φ_{rs} are normalized and orthogonal.

(II) A permutation $\bar{P}$ of the state vectors acting as operator on Φ_{rs} transforms the first index r, leaving the second index s invariant:

$$\bar{P}\Phi_{rs}=\sum_t\Phi_{ts}\theta_{tr}^{[\lambda]}(P). \tag{12}$$

(III) A permutation P of the particle numbers acting as operator on Φ_{rs} transforms the second index s and leaves the first index unaltered:

$$P\Phi_{rs}=\sum_t\Phi_{rt}\theta_{ts}^{[\lambda]}(P). \tag{13}$$

The first property follows from the fact that under the conditions stated the $n!$ states $\bar{P}\Phi_0$ are all normalized and orthogonal. The second and third properties may be deduced easily from the following properties of the Young orthogonal units:

$$P=\sum_{\lambda rs}\theta_{rs}^{[\lambda]}(P)o_{rs}^{[\lambda]}, \tag{14}$$

$$o_{rs}^{[\lambda]}o_{r's'}^{[\lambda']}=\delta(\lambda,\lambda')\delta(s,r')o_{rs'}^{[\lambda]}. \tag{15}$$

In cases where some or all of the state vectors are identical it may be simpler to regard the Young operators as built up in the first place out of permutations of the particle numbers, rather than out of permutations of the state vectors. In this connection we may note that if we define for an orthogonal representation

$$\omega_{sr}^{[\lambda]}\Phi_0=(f_\lambda/n!)^{\frac{1}{2}}\sum_P\theta_{sr}^{[\lambda]}(P)P\Phi_0, \tag{16}$$

we will have simply

$$\bar{\omega}_{rs}^{[\lambda]}\Phi_0=\omega_{sr}^{[\lambda]}\Phi_0. \tag{17}$$

It is then in accordance with our notation to define

$$\Phi_{rs}^{[\lambda]}=N_r\omega_{sr}^{[\lambda]}\Phi_0, \tag{18}$$

the second label s describing as before the transformation properties with respect to permutation of the particle numbers. The factor N_r is introduced to allow of the renormalization that will be required when some of the state vectors are identical. Some of the state labels r may also become redundant, as the corresponding states may vanish identically or become identical with other states.

3. THE $\langle n|n-1, 1\rangle$ FRACTIONAL PARENTAGE COEFFICIENTS

We choose the orthogonal matrix representation $\theta_{rs}^{[\lambda]}(P)$ to have the standard Young-Yamanouchi form[3] appropriate to the regular partition,

$$[\lambda]=[\lambda_1\lambda_2\cdots\lambda_k], \tag{19}$$

of n:

$$n=\lambda_1+\lambda_2+\cdots+\lambda_k,\quad \lambda_1\geqslant\lambda_2\geqslant\cdots\geqslant\lambda_k. \tag{20}$$

We may then take the row and column indices r, s to be Yamanouchi symbols,[3]

$$(r)=(r_1r_2\cdots r_n),\quad (s)=(s_1s_2\cdots s_n), \tag{21}$$

where (r) is an arrangement of λ_1 integers 1, λ_2 integers 2, $\cdots$, λ_k integers k, such that, read from left to right,[4] the number of times the integer p has occurred at any stage is never less than the number of times the integer $p+1$ has occurred. Similarly for (s). The matrices of the transpositions P_{12}, P_{23}, $\cdots P_{n-1,n}$ can then be written down immediately by the Young-Yamanouchi rules and the matrix of any other permutation calculated.

We may then write

$$(s)=(s'\sigma), \tag{22}$$

where

$$\sigma=s_n \tag{23}$$

and

$$(s')=(s_1s_2\cdots s_{n-1}) \tag{24}$$

is a Yamanouchi symbol of a definite representation,

$$R[\lambda']=R[\lambda_1'\lambda_2'\cdots\lambda_{k'}'], \tag{25}$$

of S_{n-1}.

[3] H. A. Jahn, Proc. Roy. Soc. (London) **A205**, 192 (1951); H. A. Jahn and H. van Wieringen, Proc. Roy. Soc. (London) **A209**, 502 (1951).

[4] We have found it convenient to retain the natural order here, rather than the reverse of natural order previously used in reference 3.

We wish to express $\bar{\omega}_{r,s'\sigma}{}^{[\lambda]}$ in terms of the normalized Young operators $\bar{\omega}_{t's'}{}^{[\lambda']}$ of S_{n-1}, (t') being another Yamanouchi symbol for $R[\lambda']$. To do this we express the general permutation P of S_n as the product of a permutation R of S_{n-1} and a permutation Q taken from one of the $n-1$ cosets in S_n of the subgroup S_{n-1}. There is considerable arbitrariness in the choice of the permutations Q; we could for instance take simply

$$Q_1=I,\quad Q_2=P_{1n},\quad Q_3=P_{2n},\quad \cdots,\quad Q_n=P_{n-1,n}. \tag{26}$$

With such a choice of the Q's made, we have the unique expression,

$$P=QR, \tag{27}$$

for any permutation P of S_n. It follows that

$$\begin{aligned}
\bar{\omega}_{r,s'\sigma}{}^{[\lambda]} &= (f_\lambda/n!)^{\frac{1}{2}} \textstyle\sum_P \theta_{r,s'\sigma}{}^{[\lambda]}(P)\bar{P}\\
&= (f_\lambda/n!)^{\frac{1}{2}} \textstyle\sum_t [\sum_Q \theta_{rt}{}^{[\lambda]}(Q)\bar{Q}]\\
&\qquad\times[\textstyle\sum_R \theta_{t,s'\sigma}{}^{[\lambda]}(R)\bar{R}]\\
&= (f_\lambda/n!)^{\frac{1}{2}} \textstyle\sum_t [\sum_Q \theta_{rt}{}^{[\lambda]}(Q)\bar{Q}]\\
&\qquad\times[\textstyle\sum_R \delta(t,t'\sigma)\theta_{t's'}{}^{[\lambda']}(R)\bar{R}]\\
&= (f_\lambda/nf_{\lambda'})^{\frac{1}{2}} \textstyle\sum_{t'} [\sum_Q \theta_{r,t'\sigma}{}^{[\lambda]}(Q)\bar{Q}]\\
&\qquad\times\{[f_{\lambda'}/(n-1)!]^{\frac{1}{2}} \textstyle\sum_R \theta_{t's'}{}^{[\lambda']}(R)\bar{R}\}\\
&= (f_\lambda/nf_{\lambda'})^{\frac{1}{2}} \textstyle\sum_{t'} \sum_Q \theta_{r,t'\sigma}{}^{[\lambda]}(Q)\bar{Q}\bar{\omega}_{t's'}{}^{[\lambda']}.
\end{aligned} \tag{28}$$

The coefficients,

$$\langle rs'\sigma|Qt's'\rangle\bar{Q}\equiv\langle r|Qt'\rangle\bar{Q}=(f_\lambda/nf_{\lambda'})^{\frac{1}{2}}\theta_{r,t'\sigma}{}^{[\lambda]}(Q)\bar{Q}, \tag{29}$$

define the $\langle n|n-1,1\rangle$ fractional parentage coefficients of type $\langle[\lambda]|[\lambda']\times[1]\rangle$. It is seen that they are independent of the particular value of the Yamanouchi symbol (s'). Normalization and orthogonality require, for given s,

$$\begin{aligned}
&\textstyle\sum_Q\sum_{t'}\langle r|Qt'\rangle\langle p|Qt'\rangle\\
&=(f_\lambda/nf_{\lambda'})\textstyle\sum_Q\sum_{t'}\theta_{r,t'\sigma}{}^{[\lambda]}(Q)\theta_{p,t'\sigma}{}^{[\lambda]}(Q)=\delta(r,p).
\end{aligned} \tag{30}$$

This follows of course from the derivation, it may be deduced also directly from (10).

We have then

$$\begin{aligned}
&\Phi(r|j_1j_2J_2j_3J_3\cdots J_{n-1}j_nJM|s'\sigma)\\
&=\bar{\omega}_{r,s'\sigma}{}^{[\lambda]}\Phi(j_1(1)j_2(2)J_2,\, j_3(3)J_3,\,\cdots J_{n-1},\, j_n(n)JM)\\
&=(f_\lambda/nf_{\lambda'})^{\frac{1}{2}}\textstyle\sum_{t'}\sum_Q\theta_{r,t'\sigma}{}^{[\lambda]}(Q)\bar{Q}\bar{\omega}_{t's'}{}^{[\lambda']}\\
&\qquad\times\Phi(j_1(1)\cdots J_{n-1},\, j_n(n)JM)\\
&=(f_\lambda/nf_{\lambda'})^{\frac{1}{2}}\textstyle\sum_{t'}\sum_Q\theta_{r,t'\sigma}{}^{[\lambda]}(Q)\bar{Q}\\
&\qquad\times\Phi((t'|j_1j_2J_2j_3\cdots j_{n-1}J_{n-1}|s'),\, j_n(n)JM),
\end{aligned} \tag{31}$$

expressing an n-particle state of definite permutation symmetry as a linear combination of states of definite permutation symmetry of $n-1$ particles, vector coupled to the states of the nth particle.

4. THE $\langle n|m,\ n-m\rangle$ COEFFICIENTS

The determination of the $\langle n|m,\ n-m\rangle$ coefficients of type $\langle[\lambda]|[\lambda']\times[\lambda'']\rangle$ proceeds in a similar manner. Instead of the standard Young-Yamanouchi representation of S_n, in which the subgroups $S_{n-1}, S_{n-2}, \cdots, S_2$ appear in standard form, we use a transformed representation in which the matrices of the group S_m of permutations R of the first m integers appear in standard Yamanouchi form and the group S_{n-m} of permutations S of the last $n-m$ integers appears also in standard form. In place of the labels r, s of the original representation, we may use modified labels,

$$(r)=(\alpha,\beta),\quad (s)=(\rho,\sigma), \tag{32}$$

built up out of the same set of integers as the original labels, with

$$(\alpha)=(r_1r_2\cdots r_m)\quad\text{and}\quad(\rho)=(s_1s_2\cdots s_m) \tag{33}$$

being standard Yamanouchi symbols associated with a definite row and a definite column of the representation $R[\lambda']$ of S_m (this is a property of the original Young-Yamanouchi representation), and with

$$(\beta)=(r_{m+1}r_{m+2}\cdots r_n)\quad\text{and}\quad(\sigma)=(s_{m+1}s_{m+2}\cdots s_n) \tag{34}$$

involving the remaining integers. Although these latter symbols are not necessarily of the form of standard Yamanouchi symbols, they may nevertheless be used, by prescription, to specify a definite row and a definite column of a definite representation $R[\lambda'']$ of S_{n-m}. The reason that such a prescription is always possible is that the total number of states before and after the transformation is the same, and after the transformation each state belongs to a definite row of a definite representation of each group.

The permutations RS form the subgroup $S_m\times S_{n-m}$ of S_n of dimension $m!(n-m)!$, and, as before, we may introduce

$$\binom{n}{m}=n!/[m!(n-m)!] \tag{35}$$

permutations Q characterizing the cosets of this subgroup (taking again $Q_1=I$, counting the subgroup itself as coset). We may then express any permutation P of S_n in the form

$$P=QRS, \tag{36}$$

and we have

$$\begin{aligned}
\bar{\omega}_{\alpha\beta,\rho\sigma}{}^{[\lambda]}&=(f_\lambda/n!)^{\frac{1}{2}}\sum_{QRS}\theta_{\alpha\beta,\rho\sigma}{}^{[\lambda]}(QRS)\bar{Q}\bar{R}\bar{S}\\
&=(f_\lambda/n!)^{\frac{1}{2}}\sum_{uvxy}[\textstyle\sum_Q\theta_{\alpha\beta,uv}{}^{[\lambda]}(Q)\bar{Q}]\\
&\quad\times[\textstyle\sum_R\theta_{uv,xy}{}^{[\lambda]}(R)\bar{R}][\sum_S\theta_{xy,\rho\sigma}{}^{[\lambda]}(S)\bar{S}]\\
&=(f_\lambda/n!)^{\frac{1}{2}}\sum_{uvxy}[\textstyle\sum_Q\theta_{\alpha\beta,uv}{}^{[\lambda]}(Q)\bar{Q}]\\
&\quad\times[\delta(v,y)\textstyle\sum_R\theta_{ux}{}^{[\lambda']}(R)\bar{R}]\\
&\qquad\times[\delta(x,\rho)\textstyle\sum_S\theta_{y\sigma}{}^{[\lambda'']}(S)\bar{S}]\\
&=\left\{f_\lambda\Big/\left[\binom{n}{m}f_{\lambda'}f_{\lambda''}\right]\right\}^{\frac{1}{2}}\sum_{uvQ}\theta_{\alpha\beta,uv}{}^{[\lambda]}(Q)\bar{Q}\\
&\qquad\times\bar{\omega}_{u\rho}{}^{[\lambda']}\bar{\omega}_{v\sigma}{}^{[\lambda'']}.
\end{aligned} \tag{37}$$

The coefficients $\langle n|m, n-m\rangle$ of fractional parentage of type $\langle[\lambda]|[\lambda']\times[\lambda'']\rangle$ are hence given by

$$\langle\alpha\beta\rho\sigma|Quv\rho\sigma\rangle\bar{Q}\equiv\langle\alpha\beta|Quv\rangle\bar{Q}$$
$$=\left\{f_\lambda\Big/\left[\binom{n}{m}f_{\lambda'}f_{\lambda''}\right]\right\}^{\frac{1}{2}}\theta_{\alpha\beta,\,uv}{}^{[\lambda]}(Q)\bar{Q}, \quad (38)$$

and are independent of the value of the Yamanouchi symbols ρ and σ. We have then

$$\Phi(\alpha,\beta|(j_1j_2J_2j_3J_3\cdots J_{m-1}j_mJ_m),$$
$$(j_{m+1}j_{m+2}J_{m+2}j_{m+3}J_{m+3}\cdots j_nJ_n), JM|\rho,\sigma)$$
$$=\bar{\omega}_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}\Phi\{(j_1(1)j_2(2)J_2,\cdots j_m(m)J_m),$$
$$(j_{m+1}(m+1)j_{m+2}(m+2)$$
$$J_{m+2},\cdots,j_n(n)J_n), JM\}$$
$$=\left\{f_\lambda\Big/\left[\binom{n}{m}f_{\lambda'}f_{\lambda''}\right]\right\}^{\frac{1}{2}}\sum_{uv}\sum_{Q}\theta_{\alpha\beta,\,uv}{}^{[\lambda]}(Q)\bar{Q}$$
$$\times\Phi((u|j_1j_2J_2\cdots j_mJ_m|\rho),$$
$$(v|j_{m+1}j_{m+2}J_{m+2}\cdots J_n|\sigma), JM), \quad (39)$$

which expresses the n-particle state of definite permutation symmetry as a linear combination of states of definite permutation symmetry of the first m particles, vector coupled to states of definite permutation symmetry of the last $n-m$ particles. Orthogonality and normalization require

$$\left\{f_\lambda\Big/\left[\binom{n}{m}f_{\lambda'}f_{\lambda''}\right]\right\}\sum_{Q}\sum_{uv}\theta_{\alpha\beta,\,uv}{}^{[\lambda]}(Q)\theta_{\alpha'\beta',\,uv}{}^{[\lambda]}(Q)$$
$$=\delta(\alpha,\alpha')\delta(\beta,\beta'), \quad (40)$$

which also, as before, may be deduced directly from (10).

5. THE $\langle n|n-2, 2\rangle$ COEFFICIENTS

In the important case of the $\langle n|n-2, 2\rangle$ coefficients, some simplification is possible since the group S_2 has only two irreducible representations each of which is one dimensional. Hence, in (39) applied to this case the summation over v is not required, since we must have here $v=\sigma$. Taking then the $n(n-1)/2$ operators Q to be

$$I,\ P_{k,\,n-1},\ P_{kn},\ P_{k,\,n-1}P_{ln},\ (l>k=1,2,\cdots n-2), \quad (41)$$

we have the general $\langle n|n-2, 2\rangle$ fractional parentage coefficients given us by

$$\Phi(\alpha,\beta|j_1j_2J_2j_3J_3\cdots j_{n-2}J_{n-2},\ j_{n-1}j_nJ_n,\ JM|\rho,\sigma)$$
$$=\left\{f_\lambda\Big/\left[\binom{n}{2}f_{\lambda'}\right]\right\}^{\frac{1}{2}}\sum_{u}\sum_{Q}\theta_{\alpha\beta,\,u\sigma}{}^{[\lambda]}(Q)\bar{Q}$$
$$\times\Phi((u|j_1j_2J_2\cdots j_{n-2}J_{n-2}|\rho),(\sigma|j_{n-1}j_nJ_n|\sigma),JM)$$
$$=\left\{f_\lambda\Big/\left[\binom{n}{2}f_{\lambda'}\right]\right\}^{\frac{1}{2}}\sum_{u}\Bigg\{\delta(\alpha,u)\delta(\beta,\sigma)$$
$$+\sum_{l>k=1}^{n-2}\theta_{\alpha\beta,\,u\sigma}{}^{[\lambda]}(P_{k,\,n-1}P_{ln})\bar{P}_{k,\,n-1}\bar{P}_{ln}$$
$$+\sum_{k=1}^{n-2}[\theta_{\alpha\beta,\,u\sigma}{}^{[\lambda]}(P_{k,\,n-1})\bar{P}_{k,\,n-1}+\theta_{\alpha\beta,\,u\sigma}{}^{[\lambda]}(P_{kn})\bar{P}_{kn}]\Bigg\}$$
$$\times\Phi\{(u|j_1j_2J_2j_3J_3\cdots j_{n-2}J_{n-2}|\rho),$$
$$(\sigma|j_{n-1}j_nJ_n|\sigma), JM\}, \quad (42)$$

where the effect of the permutations $\bar{P}$ of the state vectors can be expressed in terms of Racah W functions.

For normalized two-particle states of definite symmetry, such as occur here, it is convenient to introduce the following special notation

$$\Phi(j_a(i)j_b(k)\sigma JM)\equiv\Phi(\sigma|j_a(i)j_b(k)JM|\sigma)$$
$$=(1/\sqrt{2})[I+(-1)^\sigma P_{ik}]\Phi(j_a(i)j_b(k)JM), \quad (43)$$

with the convention

$$\left.\begin{aligned}&(-1)^\sigma=+1,\ \text{when } \sigma \text{ denotes a symmetrical two-particle state,}\\&(-1)^\sigma=-1,\ \text{when } \sigma \text{ denotes an antisymmetrical state.}\end{aligned}\right\} \quad (44)$$

It is easy to verify that

$$\Phi(j_a(i)j_b(k)\sigma JM)$$
$$=(-1)^\sigma(-1)^{j_a+j_b-J}\Phi(j_b(i)j_a(k)\sigma JM). \quad (45)$$

Further, in the standard $(P_{n-1,\,n})$-diagonalized Young-Yamanouchi representation,[5] we may make the prescription mentioned in connection with (34) so that $(\beta)=(r_{n-1}r_n)$ is interpreted in the following simple form:

(i) if $r_{n-1}<r_n$ then β describes an antisymmetrical state,
(ii) if $r_{n-1}\geqslant r_n$ then β describes a symmetric state. (46)

That this is so may be seen as follows.

(*A*) If $|r_1r_2\cdots r_{n-2}rs\rangle$ and $|r_1r_2\cdots r_{n-2}sr\rangle$, with $r<s$, are both allowed Yamanouchi symbols, we may define[5] the orthogonal transformation diagonalizing $P_{n-1,\,n}$ by means of

$$\left.\begin{aligned}|r_1r_2\cdots r_{n-2},rs\rangle&=[(\mu-1)/(2\mu)]^{\frac{1}{2}}|r_1r_2\cdots r_{n-2}sr\rangle\\&\quad-[(\mu+1)/(2\mu)]^{\frac{1}{2}}|r_1r_2\cdots r_{n-2}rs\rangle,\\|r_1r_2\cdots r_{n-2},sr\rangle&=[(\mu+1)/(2\mu)]^{\frac{1}{2}}|r_1r_2\cdots r_{n-2}sr\rangle\\&\quad+[(\mu-1)/(2\mu)]^{\frac{1}{2}}|r_1r_2\cdots r_{n-2}rs\rangle,\end{aligned}\right\} \quad (47)$$

with

$$\mu=\lambda_r-\lambda_s+s-r, \quad (48)$$

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

so that, for $r<s$, we have

$$\begin{aligned}\langle r_1r_2\cdots r_{n-2}, rs|P_{n-1,\,n}|r_1r_2\cdots r_{n-2}, rs\rangle &= -1,\\ \langle r_1r_2\cdots r_{n-2}, sr|P_{n-1,\,n}|r_1r_2\cdots r_{n-2}, sr\rangle &= +1.\end{aligned} \tag{49}$$

(B) If $|r_1r_2\cdots r_{n-2}rs\rangle$ is an allowed symbol, but not $|r_1r_2\cdots r_{n-2}sr\rangle$, then we must have $r<s$ and we may put here

$$|r_1r_2\cdots r_{n-2}, rs\rangle = |r_1r_2\cdots r_{n-2}rs\rangle \quad (\text{when } |r_1r_2\cdots r_{n-2}sr\rangle \text{ not allowed}). \tag{50}$$

(C) Finally we write

$$|r_1r_2\cdots r_{n-2}, rr\rangle = |r_1r_2\cdots r_{n-2}rr\rangle. \tag{51}$$

It follows then from the properties of the standard Young-Yamanouchi representation[3,4] that the prescription (46) is valid in all cases. This process and prescription can be extended to the case where $P_{n-1,\,n}$, $P_{n-3,\,n-2}$, $\cdots$, P_{12} (n even) or P_{23} (n odd) are taken to be diagonal matrices, thus defining the $(\cdots P_{n-3,\,n-2},\ P_{n-1,\,n})$-diagonal Young-Yamanouchi representation with standard phases.

6. EXPLICIT EXPRESSIONS FOR THE $\langle 4|2,2\rangle$ COEFFICIENTS

In the particular case of the $\langle 4|2,2\rangle$ coefficients the sum over both u and v in (39) become unnecessary and we have simply, $f_{\lambda'}$ and $f_{\lambda''}$ being here both unity,

$$\begin{aligned}\Phi(\alpha,\beta|j_1j_2J_1j_3j_4J_2JM|\rho,\sigma) &= (f_\lambda/6)^{\frac{1}{2}}[\delta(\alpha,\rho)\delta(\beta,\sigma)+\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{13}P_{24})\bar{P}_{13}\bar{P}_{24}\\ &\quad+\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{13})\bar{P}_{13}+\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{14})\bar{P}_{14}\\ &\quad+\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{23})\bar{P}_{23}+\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{24})\bar{P}_{24}]\\ &\quad\times\Phi(j_1(1)j_2(2)\rho J_1,\ j_3(3)j_4(4)\sigma J_2,\ JM).\end{aligned} \tag{52}$$

From (47), (48), (50), and (51) the basic vectors,

$$|\alpha,\beta\rangle \equiv |r_1r_2,\ r_3r_4\rangle, \tag{53}$$

of the standard (P_{12}, P_{34})-diagonal Young-Yamanouchi representation are given in terms of the vectors $|r_1r_2r_3r_4\rangle$ of the standard Young-Yamanouchi representation by

$$\begin{aligned}
&[\lambda]=[4]: && |11,11\rangle=|1111\rangle;\\
&[\lambda]=[1111]: && |12,34\rangle=|1234\rangle,\\
&[\lambda]=[31]: && |11,21\rangle=(2/3)^{\frac{1}{2}}|1121\rangle+(1/3)^{\frac{1}{2}}|1112\rangle,\\
& && |11,12\rangle=(1/3)^{\frac{1}{2}}|1121\rangle-(2/3)^{\frac{1}{2}}|1112\rangle,\\
& && |12,11\rangle=|1211\rangle,\\
&[\lambda]=[211]: && |12,13\rangle=(1/3)^{\frac{1}{2}}|1231\rangle-(2/3)^{\frac{1}{2}}|1213\rangle,\\
& && |12,31\rangle=(2/3)^{\frac{1}{2}}|1231\rangle+(1/3)^{\frac{1}{2}}|1213\rangle,\\
& && |11,23\rangle=|1123\rangle,\\
&[\lambda]=[22]: && |11,22\rangle=|1122\rangle;\quad |12,12\rangle=|1212\rangle.
\end{aligned} \tag{54}$$

Since then, with the convention of (44), we have

$$P_{12}|\alpha,\beta\rangle=(-1)^\alpha|\alpha,\beta\rangle;\quad P_{34}|\alpha,\beta\rangle=(-1)^\beta|\alpha,\beta\rangle, \tag{55}$$

it follows that the matrices of P_{13}, P_{14}, and P_{24} are simply expressible as follows in terms of the matrices of P_{23}.

$$\begin{aligned}\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{13}) &= \theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{12}P_{23}P_{12})\\ &= (-1)^{\alpha+\rho}\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{23}),\\ \theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{14}) &= \theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{12}P_{34}P_{23}P_{12}P_{34})\\ &= (-1)^{\alpha+\beta+\rho+\sigma}\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{23}),\\ \theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{24}) &= \theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{34}P_{23}P_{34})\\ &= (-1)^{\beta+\sigma}\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{23}).\end{aligned} \tag{56}$$

In order, however, to obtain a simple general expression for the matrix element of $P_{13}P_{24}$, it is desirable to make an additional phase change: we change the sign of the representation vector $|12,31\rangle$. We may do this by using in place of the vector $|12,31\rangle$ a nonstandard vector $|23,11\rangle$ defined by

$$|23,11\rangle \equiv -|12,31\rangle, \tag{57}$$

this still being in agreement with the prescription (46). It may be verified then that

$$\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{13}P_{24}) = S(\lambda)\delta_p(\alpha,\sigma)\delta_p(\beta,\rho), \tag{58}$$

where

$$\begin{aligned}S(\lambda) &= +1 \text{ for } [\lambda]=[4],\ [22],\ [1111],\\ &= -1 \text{ for } [\lambda]=[31],\ [211],\end{aligned} \tag{59}$$

and

$$\begin{aligned}\delta_p(x,y) &= \tfrac{1}{2}[1+(-1)^{x+y}]\\ &= +1, \text{ when } x \text{ and } y \text{ have the same parity, zero otherwise.}\end{aligned} \tag{60}$$

We may call the representation with this modification the modified (P_{12},P_{34})-diagonal representation and it may be verified that in this representation the matrix elements of P_{23} are as follows:

$$\begin{array}{llllll}
[\lambda]: & [4] & [22] & [1111] & [31] & [211]\\
\theta_{\alpha\beta,\,\rho\sigma}{}^{[\lambda]}(P_{23}): &
\begin{array}{r}11,11\end{array}\!\begin{bmatrix}1\end{bmatrix} &
\begin{array}{r}11,22\\12,12\end{array}\!\begin{bmatrix}-\frac{1}{2} & \sqrt{3}/2\\ \sqrt{3}/2 & \frac{1}{2}\end{bmatrix} &
\begin{array}{r}12,34\end{array}\!\begin{bmatrix}-1\end{bmatrix} &
\begin{array}{r}11,21\\11,12\\12,11\end{array}\!\begin{bmatrix}0 & -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}}\\ -\sqrt{\frac{1}{2}} & \frac{1}{2} & \frac{1}{2}\\ \sqrt{\frac{1}{2}} & \frac{1}{2} & \frac{1}{2}\end{bmatrix} &
\begin{array}{r}12,13\\23,11\\11,23\end{array}\!\begin{bmatrix}0 & \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}}\\ \sqrt{\frac{1}{2}} & -\frac{1}{2} & -\frac{1}{2}\\ -\sqrt{\frac{1}{2}} & -\frac{1}{2} & -\frac{1}{2}\end{bmatrix}.
\end{array} \tag{61}$$

Using this representation, we obtain from (52), on evaluating the transformations $\bar{P}$ of the state vectors, the general $\langle 4|2,2\rangle$ expansion as follows:

$$\Phi(\alpha,\beta|j_1j_2J_1j_3j_4J_2JM|\rho,\sigma)$$

$$=(f_\lambda/6)^{\frac{1}{2}}\Bigg\{\delta(\alpha,\rho)\delta(\beta,\sigma)\Phi(j_1j_2\rho J_1j_3j_4\sigma J_2JM)+S(\lambda)\delta_p(\alpha,\sigma)\delta_p(\beta,\rho)(-1)^{J_1+J_2-J}\Phi(j_3j_4\rho J_2j_1j_2\sigma J_1JM)$$

$$+2\theta_{\alpha\beta,\rho\sigma}{}^{[\lambda]}(P_{23})\times\tfrac{1}{2}\Bigg[\sum_{J_3J_4}\chi\begin{pmatrix}j_1j_2J_1\\ j_3j_4J_2\\ J_3J_4J\end{pmatrix}(\Phi(j_1j_3\rho J_3j_2j_4\sigma J_4JM)+(-1)^{\alpha+\beta+J_3+J_4-J}\Phi(j_2j_4\rho J_4j_1j_3\sigma J_3JM)$$

$$+\sum_{J_5J_6}\chi\begin{pmatrix}j_1j_2J_1\\ j_4j_3J_2\\ J_5J_6J\end{pmatrix}[(-1)^{\alpha+j_3+j_4-J_2+J_5+J_6-J}\Phi(j_2j_3\rho J_6j_1j_4\sigma J_5JM)$$

$$+(-1)^{\beta+j_3+j_4-J_2}\Phi(j_1j_4\rho J_5j_2j_3\sigma J_6JM)]\Bigg]\Bigg\},\quad (62\mathrm{A})$$

where

$$\chi\begin{pmatrix}abe\\ cdf\\ ghk\end{pmatrix}=[(2e+1)(2f+1)(2g+1)(2h+1)]^{\frac{1}{2}}\begin{Bmatrix}abe\\ cdf\\ ghk\end{Bmatrix}=\langle(ab)e,(cd)f,kq|(ac)g,(bd)h,kq\rangle \quad (63)$$

is the Hope χ function.[6] The normalization of the function (62A) is assured by the relation

$$(f_\lambda/6)[\delta(\alpha,\rho)\delta(\beta,\sigma)+\delta_p(\alpha,\sigma)\delta_p(\beta,\rho)+4\{\theta_{\alpha\beta,\rho\sigma}{}^{[\lambda]}(P_{23})\}^2]=1, \quad (64)$$

which follows from (10) and may be verified also directly from (61).

It is easy to deduce from (62A) the corresponding expansions when some or all of the state vectors become equal. This may be done by removing, for the time being, the labels ρ and σ in the functions on the right-hand side by inserting the corresponding factors

$$(1/\sqrt{2})[I+(-1)^\rho P_{12}],\quad (1/\sqrt{2})[I+(-1)^\sigma P_{34}] \quad (65)$$

and then making the vectors equal. Then on reapplying the operators (65) allowance has to be made for the renormalization that may be required. In the process of collecting together identical states use is made of the fundamental symmetry relation of the Hope χ function:[6]

$$\chi\begin{pmatrix}abe\\ cdf\\ ghk\end{pmatrix}=(-1)^{a+b-e+c+d-f+g+h-k}\chi\begin{pmatrix}cdf\\ abe\\ ghk\end{pmatrix}. \quad (66)$$

Equations (62B, C, D, and E) below give the resulting $\langle 4|2,2\rangle$ expansions for the configurations $j_1j_2j_3{}^2$, $j_1{}^2j_2{}^2$, $j_1{}^3j_2$, and j^4, respectively. For the last two cases the over-all normalizing factor is not here determined,[7] for the first two normalization is assured by (64).

$$\Phi(\alpha,\beta|j_1j_2J_1j_3{}^2J_2JM|\rho,\sigma)$$

$$=\delta_p(\beta,2j_3-J_2)(f_\lambda/6)^{\frac{1}{2}}\Bigg\{\delta(\alpha,\rho)\delta(\beta,\sigma)\Phi(j_1j_2\rho J_1j_3{}^2J_2JM)+S(\lambda)\delta_p(\alpha,\sigma)\delta_p(\beta,\rho)(-1)^{J_1+J_2-J}\Phi(j_3{}^2J_2j_1j_2\sigma J_1JM)$$

$$+2\theta_{\alpha\beta,\rho\sigma}{}^{[\lambda]}(P_{23})\sum_{J_3J_4}\chi\begin{pmatrix}j_1j_2J_1\\ j_3j_3J_2\\ J_3J_4J\end{pmatrix}(1/\sqrt{2})[\Phi(j_1j_3\rho J_3j_2j_3\sigma J_4JM)+(-1)^{\alpha+\beta+J_3+J_4-J}\Phi(j_2j_3\rho J_4j_1j_3\sigma J_3JM)]\Bigg\},\quad (62\mathrm{B})$$

[6] H. A. Jahn and J. Hope, Phys. Rev. 93, 318 (1954).
[7] It has been evaluated by M. J. Englefield (to be published).

$$\Phi(\alpha,\beta|j_1^2J_1j_2^2J_2JM|\rho,\sigma)$$
$$=\delta_p(\alpha,2j_1-J_1)\delta_p(\beta,2j_2-J_2)(f_\lambda/6)^{\frac{1}{2}}\Bigg[\delta(\alpha,\rho)\delta(\beta,\sigma)\Phi(j_1^2J_1j_2^2J_2JM)+S(\lambda)\delta_p(\alpha,\sigma)\delta_p(\beta,\rho)(-1)^{J_1+J_2-J}$$
$$\times\Phi(j_2^2J_2j_1^2J_1JM)+2\theta_{\alpha\beta,\rho\sigma}{}^{[\lambda]}(P_{23})\sum_{J_3J_4}\chi\begin{pmatrix}j_1j_1J_1\\ j_2j_2J_2\\ J_3J_4J\end{pmatrix}\Phi(j_1j_2\rho J_3j_1j_2\sigma J_4JM)\Bigg], \quad (62\mathrm{C})$$

$$\Phi(\alpha,\beta|j_1^2J_1j_1j_2J_2JM|\rho,\sigma)$$
$$=N_{\alpha\beta}(f_\lambda/6)^{\frac{1}{2}}\delta_p(\alpha,2j_1-J_1)\Bigg\{\delta(\alpha,\rho)\delta(\beta,\sigma)\Phi(j_1^2J_1j_1j_2\sigma J_2JM)+S(\lambda)\delta_p(\alpha,\sigma)\delta_p(\beta,\rho)(-1)^{J_1+J_2-J}$$
$$\times\Phi(j_1j_2\rho J_2j_1^2J_1JM)+2\theta_{\alpha\beta,\rho\sigma}{}^{[\lambda]}(P_{23})\sum_{J_3J_4}\chi\begin{pmatrix}j_1j_1J_1\\ j_1j_2J_2\\ J_3J_4J\end{pmatrix}[\delta_p(\rho,2j_1-J_3)\Phi(j_1^2J_3j_1j_2\sigma J_4JM)$$
$$+\delta_p(\sigma,2j_1-J_3)(-1)^{\alpha+\beta+J_3+J_4-J}\Phi(j_1j_2\rho J_4j_1^2J_3JM)]\Bigg\}, \quad (62\mathrm{D})$$

$$\Phi(\alpha,\beta|j^2J_1j^2J_2JM|\rho,\sigma)$$
$$=N_{\alpha\beta}(f_\lambda/6)^{\frac{1}{2}}\delta_p(\alpha,2j-J_1)\delta_p(\beta,2j-J_2)\Bigg\{\delta(\alpha,\rho)\delta(\beta,\sigma)\Phi(j^2J_1j^2J_2JM)+S(\lambda)\delta_p(\alpha,\sigma)\delta_p(\beta,\rho)(-1)^{J_1+J_2-J}$$
$$\times\Phi(j^2J_2j^2J_1JM)+2\theta_{\alpha\beta,\rho\sigma}{}^{[\lambda]}(P_{23})\sum_{J_3J_4}\chi\begin{pmatrix}jjJ_1\\ jjJ_2\\ J_3J_4J\end{pmatrix}[\delta_p(\rho,2j-J_3)\delta_p(\sigma,2j-J_4)\Phi(j^2J_3j^2J_4JM)$$
$$+\delta_p(\sigma,2j-J_3)\delta_p(\rho,2j-J_4)(-1)^{\alpha+\beta+J_3+J_4-J}\Phi(j^2J_4j^2J_3JM)]\Bigg\}. \quad (62\mathrm{E})$$

CONCLUSION

We may note finally that it is not always simpler to construct all the states required by means of Young operators: when one state has been constructed, others may be obtained from it by operating on it by a suitably chosen permutation. Using this mixed method and the standard (P_{12},P_{34},P_{56})-diagonal representation the writer has constructed, using the $\langle 4|2,2\rangle$ expansion given here, a complete set of $\langle 6|4,2\rangle$ coefficients for states of maximum symmetry [42] arising from the mixed configurations s^4l^2, $s^4l_1l_2$ and $s^3l_1^2l_2$. These are being used,[8] in conjunction with numerical tables[5] of charge and spin coefficients and numerical tables of $\langle 6|4,2\rangle$ coefficients for s^2p^4 previously obtained, to set up the energy matrix, with central and tensor forces, for Li^6 with ten S states, six P states, and fifteen D states, all of symmetry type [42], even parity, $T=0$, $S=1$, $J=1$, obtained from the assumed lowest configuration s^4p^2 under the restriction of not more than two quanta of single-particle excitation. It is considered that it will be of some interest to see how much binding energy can be obtained for the ground state of Li^6 using this 31×31 matrix with the charge symmetric Pease-Feshbach or Hu-Massey mixture of central and tensor forces with oscillator well wave functions.

[8] This work is being undertaken mainly by P. G. Wakely, A. E. Lee, and R. Fielder.