THE TRANSFORMATION MATRIX FOR THE PERMUTATION GROUP AND THE CONSTRUCTION OF COORDINATE WAVE FUNCTIONS FOR A MULTISHELL CONFIGURATION

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We consider the orthogonal representation of the permutation group with an arbitrary type of reduction to subgroups. We introduce the matrix for transformation between representations with different types of reduction, which to a definite extent is the analog of the transformation matrix between different angular momentum coupling schemes, and we give a method for calculating this matrix in terms of the matrix elements of the standard Young-Yamanouchi representation. An expression is given for the coordinate wave function of a multishell configuration in terms of the vector-coupled coordinate wave functions of the individual shells.

1. INTRODUCTION

LET us consider a system of n identical particles placed in a central field. As examples of such a system, we have the nucleons in a nucleus (shell model) or the electrons in an atom. In those cases where the Hamiltonian of the system does not include spin interactions, all its properties are completely determined by assigning the coordinate wave function corresponding to a given value of the total orbital angular momentum and constructed including the spin and taking into account the Pauli principle (while for nucleons we must still also include the isotopic spin).* The splitting of the wave function into coordinate and spin parts is also often needed for a Hamiltonian of the most general type. Here the coordinate and spin functions must have permutation symmetry corresponding to dual Young patterns (associated representations).[1,2] However, until recently the problem of constructing a coordinate wave function for a configuration of several shells had not been solved in general form, except for those limiting cases which were treated by Jahn: 1) the particles have the same orbital angular momentum (a single shell);[3,4] 2) the particles have different orbital angular momenta, i.e., there is just one particle in each shell.[5] In [6] it is pointed out that Elliot in his dissertation treated the case where there is a single, unfilled, and several filled shells. However, unfortunately, these results were not published.

In the present paper we give a method for constructing the coordinate wave function of a multishell configuration in terms of the coordinate wave functions of the individual shells. In a succeeding paper we shall give the formulas for the fractional parentage coefficients of those configurations which make it possible to reduce the calculation of the matrix element of the energy operator and other physical quantities for a system of n particles to the already known matrix elements for two particles and one particle.

The problem of constructing functions with a definite permutation symmetry from the functions for subsystems, each of which has its own permutation symmetry, requires the study of the representations of the permutation group with arbitrary method of reduction to subgroups. In our work we introduce the transformation matrix which makes possible the transition between representations with different types of reduction to subgroups, and we give a method for calculating it. This matrix can be regarded as the analog of the matrix for transformation between different coupling schemes for angular momenta.[7]

Because the apparatus of the permutation group which is used in this paper is relatively little known to physicists, and also in order to systematize the basic definitions and notation, we felt it desirable to precede the presentation of our work

*We are talking about zeroth-order wave functions. By a coordinate function we mean a function which depends only on the spatial coordinates of the particles.

by giving the necessary information from the theory of the permutation group.

2. THE STANDARD REPRESENTATION OF THE PERMUTATION GROUP AND THE YOUNG OPERATORS

The irreducible representations of the permutation group on n symbols (S_n) are characterized by different symmetry schemes for the basis functions, the so-called Young patterns.[2,8] To described them we use the notation $[\lambda] \equiv [\lambda^{(1)}\lambda^{(2)} \ldots \lambda^{(m)}]$, where $\lambda^{(i)}$ is the number of boxes in the i-th row, $\lambda^{(1)} \geq \lambda^{(2)} \geq \ldots \geq \lambda^{(m)}$, and $\sum_{i=1}^{m} \lambda^{(i)} = n$. The number of linearly independent functions corresponding to a given Young pattern determines the dimensionality of the irreducible representation. The latter is equal to the number of ways of placing the integers from 1 to n into the boxes of the Young pattern in such a way that, reading from left to right in the rows and from top to bottom in the columns, the numbers will be arranged in increasing order. For example,

$$\begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline 4 & 5 \\ \cline{1-2}\end{array} \quad \begin{array}{|c|c|c|}\hline 1 & 2 & 4 \\ \hline 3 & 5 \\ \cline{1-2}\end{array} \quad \begin{array}{|c|c|c|}\hline 1 & 2 & 5 \\ \hline 3 & 4 \\ \cline{1-2}\end{array}$$

$$\begin{array}{|c|c|c|}\hline 1 & 3 & 4 \\ \hline 2 & 5 \\ \cline{1-2}\end{array} \quad \begin{array}{|c|c|c|}\hline 1 & 3 & 5 \\ \hline 2 & 4 \\ \cline{1-2}\end{array} \qquad (1)$$

A Young pattern with a definite arrangement of numbers in it is called a Young tableau; in the following we shall use the abbreviation Y.T. The basis functions corresponding to each Y.T. can be chosen so that in making the transition from the group S_n to S_{n-1}, S_{n-2} etc., the irreducible representation $[\lambda]$ automatically splits into irreducible representations of the groups S_{n-1}, S_{n-2}, etc. The irreducible representation constructed in this fashion is said to be standard. Then each of the basis functions can be characterized by those irreducible representations to which it will belong in the reduction $S_n \to S_{n-1} \to S_{n-2} \to \ldots \to S_2$. This corresponds to the successive removal from the Y.T. of the boxes with the integers n, n − 1, ...

In place of the Y.T. it is convenient to characterize each of the basis functions by the Yamanouchi symbol (r) which is uniquely associated with the Y.T.[9] The symbol $(r) = (\sigma_1, \sigma_2, \ldots, \sigma_n)$, where σ_i is the number of the row in which the integer i appears. We shall say that $(r) = (\sigma_1 \ldots \sigma_n)$ lies higher than $(\bar{r}) = (\bar{\sigma}_1 \ldots \bar{\sigma}_n)$, if, for the first unequal pair of σ's we have the inequality $\sigma_i > \bar{\sigma}_i$.

The Young tableaux (1) correspond to the Yamanouchi symbols

$$(11122),\ (11212),\ (11221),\ (12112),\ (12121), \qquad (2)$$

which have been arranged in increasing order. The lowest Yamanouchi symbol corresponds to the Y.T. with the natural ordering of the integers. The Yamanouchi symbols corresponding to a given $[\lambda]$ can also be written without introducing the Y.T. if, in forming them, we remember that the arrangement of integers in the pattern must be subjected to the rule of lattice permutation which states: for any integer k appearing in the Yamanouchi symbol, we must satisfy the inequality $n(k) \geq n(k+1)$, where n(k) gives the number of times that one meets the integer k among the first l numbers in the Yamanouchi symbol.

It is easily verified that the five symbols (2) satisfy the rule for lattice permutations and that no other symbol for [32] will satisfy this rule.

If we apply the permutations of the group S_n to the function of n numbers $\Phi_0 = \varphi_1(1)\varphi_2(2)\ldots\varphi_n(n)$, where the $\varphi_i(i)$ form an orthonormal system,* we obtain n! linearly independent functions $\Phi_p = P\Phi_0$. These functions transform among themselves under the action of permutations according to the so-called regular representation.[2] Linear combinations of the functions Φ_p, forming a basis for the irreducible representation, can be obtained by using the normalized Young operators:[5]

$$\omega_{rs}^{[\lambda]} = \left(\frac{f_\lambda}{n!}\right)^{1/2} \sum_P \langle [\lambda]\,(r) \mid P \mid [\lambda]\,(s) \rangle P, \qquad (3)$$

where f_λ is the dimensionality of the representation $[\lambda]$; (r) and (s) are Yamanouchi symbols, and P runs through the n! permutations. The matrices appearing in (3) form the orthogonal representation of the permutation group S_n. Young and Yamanouchi[8,9] have given formulas for the matrix elements of the matrix of a transposition of the type $P_{i,i-1}$ (cf. also [4]). All the other permutations can always be obtained as the product of appropriate transpositions.

We can form $(f_\lambda)^2$ different operators (3) for each $[\lambda]$. Correspondingly we can form the $(f_\lambda)^2$ functions:

$$|[\lambda]\,(r \mid s)\rangle = \omega_{rs}^{[\lambda]}\Phi_0. \qquad (4)$$

However, only those functions will transform into one another under the action of a permutation which have the same second index:[5]

*The number i can, for example, denote the set of coordinates of the i-th particle.

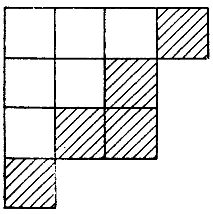
$$P\,|\,[\lambda]\,(r\,|\,s)\rangle = \sum_{(t)} |\,[\lambda]\,(t\,|\,s)\rangle\,\langle[\lambda]\,(t)\,|\,P\,|\,[\lambda]\,(r)\rangle. \tag{5}$$

For fixed (s) in Eq. (4), (r) runs through f_λ values which enumerate the basis functions of the $[\lambda]$ representation. Altogether, corresponding to the different values of (s), there are f_λ independent bases.* In those cases where there is no need to distinguish identical presentations, we shall agree to choose for the second index the lowest possible value and omit it in writing the symbol, for example, $|\,[\lambda]\,(r)\rangle$.

The Yamanouchi symbols considered above number the basis functions which transform according to the standard orthogonal Young-Yamanouchi representation. However, in constructing the wave function of a system with definite permutation symmetry from the wave functions of subsystems, each having their own permutation symmetry, one needs to know the representations with arbitrary type of reduction into subgroups. The next section of the paper will be devoted to the study of such representations and also of the matrix for transforming between them.

3. NON-STANDARD REPRESENTATION OF THE PERMUTATION GROUP AND THE TRANSFORMATION MATRIX

If in treating some standard representation of the group S_n we go over to a subgroup S_{n_1}, it will split into irreducible representations of this subgroup. However, in considering the permutation of only the last $n - n_1 = n_2$ integers, a splitting into irreducible representations of the group S_{n_2} can in general not be achieved. This is related to the fact that the last integers as a rule do not form standard Young patterns. In the figure, the shaded boxes refer to the last n_2 integers. They do not correspond to any standard Young pattern. In this case we say that the Yamanouchi symbols of the last n_2 numbers are non-standard, and in the following we shall denote them by the letter ρ. Then the Yamanouchi symbol of the representation $[\lambda]$ can be written as $(r) = (r_1\rho_2)$, where r_1 is a



standard Yamanouchi symbol for the first n_1 numbers and ρ_2 is a non-standard Yamanouchi symbol for the last n_2 numbers. (In special cases, it may also be standard.)

Let us suppose that we are required to find that representation of the group S_n which, in the transition to the subgroup $S_{n_1} \times S_{n_2}$, would split into the irreducible representations $[\lambda_1] \times [\lambda_2]$. The possible patterns $[\lambda_1]$ and $[\lambda_2]$ are determined from the expansion

$$[\lambda] = \sum_{\lambda_1\lambda_2} c\,(\lambda\lambda_1\lambda_2)\,[\lambda_1]\times[\lambda_2], \tag{6}$$

which can easily be established from the character tables or by using Littlewood's theorem (cf. the Appendix). Thus

$$[32] = [2]\ [3] + [2]\ [21] + [11]\ [21].$$

In place of the symbols (2), we shall now use the symbols (r_1r_2) to number the basis functions which are standard with respect to the first n_1 and the last n_2 numbers, namely,

$$((11)\ (111)),\ ((11)\ (112)),\ ((11)\ (121)),\ ((12)\ (112)),\ ((12)\ (121)). \tag{2a}$$

To find representations which are standard with respect to the last n_2 numbers, we apply the Young operator $\omega^{[\lambda_2]}_{r_2s_2}$ to the last n_2 numbers of the basis function of the standard representation $|\,[\lambda](r_1\bar{\rho}_2)\rangle$. For $\bar{\rho}_2$ we use the convention of choosing the symbol corresponding to the natural order of arrangement of the integers $n_1 + 1,\ n_1 + 2, \ldots, n_1 + n_2 = n$ in the Y.T., and for (s_2) the lowest symbol of the representation $[\lambda_2]$. Using formulas (3) and (5) we get

$$|[\lambda]\ (r_1r_2)\rangle = \text{const}\cdot\omega^{[\lambda_2]}_{r_2s_2}\,|[\lambda]\ (r_1\bar{\rho}_2)\ \rangle$$
$$= \sum_{\rho_2} |[\lambda]\ (r_1\rho_2)\rangle\,\langle[\lambda]\ (r_1\rho_2)\,|[\lambda]\ (r_1r_2)\rangle. \tag{7}$$

The transformation matrix which accomplishes the transition from the basis functions of the standard representation to the basis functions of the representation with reduction type $S_{n_1} \times S_{n_2}$ is expressed in terms of the known matrix elements of the standard representation:

$$\langle[\lambda]\ (r_1\rho_2)\,|[\lambda]\ (r_1r_2)\rangle = N \sum_{P_2} \langle[\lambda_2]\ (r_2)\ |\ P_2\ |\ [\lambda_2]\ (s_2)\rangle$$
$$\times \langle[\lambda]\ (r_1\rho_2)\ |\ P_2\ |[\lambda]\ (r_1\bar{\rho}_2)\rangle. \tag{8}$$

The symbol $(r_1\rho_2)$ runs through all the Yamanouchi symbols of the pattern $[\lambda]$ which have for their first n_1 integers the symbol (r_1); P_2 are the permutations of the integers $n_1 + 1,\ n_1 + 2, \ldots, n$; N

*This is related to the fact that each irreducible representation appears in the resolution of the regular representation a number of times which is equal to its dimensionality. Consequently, in particular there follows the relation $\sum_\lambda (f_\lambda)^2 = n!$

is found from the condition of normalization of the function (7):

$$\sum_{\rho_2} (\langle [\lambda]\,(r_1\rho_2) \mid [\lambda]\,(r_1 r_2)\rangle)^2 = 1. \tag{9}$$

We note that the matrices of the representation according to which the functions (7) transform do not depend on the choice of $\bar{\rho}_2$ and (s_2). The matrix elements (8) are different from zero only for those (r_1), (r_2), which belong to the representations $[\lambda_1]$, $[\lambda_2]$ which appear in the expansion (6). We express this condition symbolically in the form of a curly bracket:

$$\{\lambda\,(\lambda_1\lambda_2)\}. \tag{10}$$

Obviously $\{\lambda_1(\lambda_1\lambda_2)\}$ is equivalent to $\{\lambda\,(\lambda_2\lambda_1)\}$. This symbol is in a certain sense analogous to the triangular condition for the addition of angular momenta. However, there is an essential difference from the addition of angular momenta. Whereas in the addition of angular momenta we are dealing with the direct product of representations of one and the same group (the rotation group), and in its expansion there appear the Clebsch-Gordan coefficients, in the expansion (6) a representation of the group S_n is expanded in representations of the subgroup $S_{n_1} \times S_{n_2}$. We cannot introduce Clebsch-Gordan coefficients in the usual sense.

In those cases where in the expansion of (6), $c(\lambda\lambda_1\lambda_2) > 1$, a further identification of the basis functions (7) is necessary. This is accomplished by the second index (s_2), which we choose starting from the lowest and so on. Then, the functions $|[\lambda](r_1(r_2|s_2))\rangle$ distinguished only by (s_2) will no longer be orthogonal to one another. However, the process of orthogonalization is easily carried out by considering the functions (7) as vectors in the orthogonal space of the standard basis (cf., for example, [10]). The scalar product of basis functions with different (s_2) is equal to

$$\sum_{\rho_2} \langle[\lambda]\,(r_1\rho_2) \mid [\lambda]\,(r_1(r_2 \mid s_2))\rangle\langle[\lambda[\,(r_1\rho_2) \mid [\lambda]\,(r_1(r_2 \mid \bar{s}_2))\rangle. \tag{9a}$$

For $n_2 = 2$, the matrix (8) has the simple form:

$$\langle[\lambda]\,(r_1\rho_2) \mid [\lambda]\,(r_1 r_2)\rangle = \begin{array}{c|cc|} & [2] & [11] \\ \rho_2' & \sqrt{\frac{d-1}{2d}} & -\sqrt{\frac{d+1}{2d}} \\ \rho_2'' & \sqrt{\frac{d+1}{2d}} & \sqrt{\frac{d-1}{2d}} \end{array}, \tag{11}$$

where $\rho_2 = (\sigma_{n-1}\sigma_n)$, and ρ_2' corresponds to $\sigma_{n-1} < \sigma_n$ and ρ_2'' to $\sigma_{n-1} \geq \sigma_n$; d is the axial distance between $n-1$ and n in the Y.T. corresponding to $(r_1\rho_2')$, and is defined as the number of single-box steps which are needed to move in the Y.T. from the integer $n-1$ to the integer n by moving from left to right and from top to bottom.[8]

For various questions associated with the treatment of configurations consisting of several shells, one needs to know the representations with arbitrary type of reduction to subgroups. We shall denote the type of reduction by Latin capitals; for example, $(r)^A$, $(r)^B$ denote Yamanouchi symbols with reduction types A and B. The absence of such a notation on the Yamanouchi symbol means that it refers to the standard type of reduction. Then, if the representation $[\lambda]$ is reduced to the subgroup $S_{n_1} \times S_{n_2} \times \ldots \times S_{n_k}$ where $(n_1 + n_2 + \ldots + n_k = n)$, then for its complete characterization we must give, in addition to the Young patterns $[\lambda_1], \ldots [\lambda_k]$, $k-2$ intermediate Young patterns and also the method for combining the $[\lambda_i]$ in the intermediate patterns (a situation which is analogous to the addition of k angular momenta, cf. [7,11]).

For example, for the case of the reduction type $(S_{n_1} \times S_{n_2}) \times S_{n_3}$, the basis functions of the transformed representation are obtained by applying two Young operators to the basis function of the standard representation, with an intermediate Young pattern of the first $n_1 + n_2$ numbers equal to $[\lambda_{12}]$. We write the Yamanouchi symbol of the standard representation in the form $(r_1\rho_2\rho_3)$, where $(r_1\rho_2) = (r_{12})$.* Then

$$\begin{aligned} |\,[\lambda]\,((r_1r_2)\,\lambda_{12}r_3)\rangle &= \text{const}\cdot\omega^{[\lambda_3]}_{r_3s_3}\omega^{[\lambda_2]}_{r_2s_2}\,|\,[\lambda]\,(r_1\bar{\rho}_2\bar{\rho}_3)\rangle \\ &= \sum_{\rho_2\rho_3} |\,[\lambda]\,(r_1\rho_2\rho_3)\rangle\langle[\lambda]\,(r_1\rho_2\rho_3) \mid [\lambda]\,((r_1r_2)\,\lambda_{12}r_3)\rangle. \end{aligned} \tag{12}$$

The transformation matrix is reduced to a product of two simpler matrices, which are obtained from formula (8):

$$\begin{aligned} &\langle[\lambda]\,(r_1\rho_2\rho_3) \mid [\lambda]\,((r_1r_2)\,\lambda_{12}r_3)\rangle \\ &= \langle[\lambda_{12}]\,(r_1\rho_2) \mid [\lambda_{12}]\,(r_1r_2)\rangle\langle[\lambda](r_{12}\rho_3) \mid [\lambda](r_{12}r_3)\rangle. \end{aligned} \tag{13}$$

The transformation matrices for the transition to the basis of a representation with a more complicated reduction type is found in similar fashion by applying appropriate sets of Young operators. The matrices of the transformed representation are calculated as usual from the formula

$$\begin{aligned} \langle[\lambda]\,(r)^A \mid P \mid [\lambda]\,(\bar{r})^A\rangle &= \sum_{r,\bar{r}} \langle[\lambda]\,(r)^A \mid [\lambda]\,(r)\rangle \\ &\times \langle[\lambda]\,(r) \mid P \mid [\lambda]\,(\bar{r})\rangle\langle[\lambda]\,(\bar{r}) \mid [\lambda]\,(\bar{r})^A\rangle. \end{aligned} \tag{14}$$

*Since the assignment of the Yamanouchi symbol automatically determines the Young pattern, to abbreviate the writing we shall omit the symbol for the Young pattern $[\lambda_i]$ in all those cases where no confusion can arise.

In applications it is frequently convenient to use the matrices for permutation operators constructed from "non-diagonal" matrix elements, in which the wave functions on the left and right sides have different types of reduction into subgroups:

$$\langle [\lambda]\,(r)^A \,|\, P \,|\, [\lambda]\,(r)^B\rangle. \quad (15)$$

These matrix elements appear as the coefficients in the expansion of the result of the operation of a permutation P on a function with reduction type B in terms of functions with reduction type A:

$$P\,|\,[\lambda]\,(r)^B\rangle = \sum_{(r)^A} |\,[\lambda]\,(r)^A\rangle\langle[\lambda]\,(r)^A\,|\,P\,|[\lambda]\,(r)^B\rangle. \quad (16)$$

The transformation matrices (8) and (13) may be regarded as special cases of the matrices (15) with P ≡ 1. The obvious generalization of formula (14) is

$$\langle [\lambda]\,(r)^A \,|\, P \,|\, [\lambda]\,(r)^B\rangle = \sum_{r,\,\bar r} \langle [\lambda]\,(r)^A \,|\, [\lambda]\,(r)\rangle$$

$$\times \langle [\lambda]\,(r)\,|\,P\,|\,[\lambda]\,(\bar r)\rangle\langle[\lambda]\,(\bar r)\,|\,[\lambda]\,(r)^B\rangle. \quad (14a)$$

Let us consider a special class of matrices (15), which we shall need in the following to find the coordinate fractional parentage coefficients of mixed configurations. Let us suppose that, under the action of the permutation P on $|\,[\lambda](r)^B\rangle$, we obtain a function in which the numbers are split up into the same groups as in $|\,[\lambda](r)^A\rangle$. Then we can apply the Wigner-Eckart[5] theorem* to each of these groups (its extension to finite groups has been given by Koster[12]). The matrix element (15) can be written as an integral of the product of two functions. If we choose P to be the identity operator, then from the point of view of the permutation group this is an irreducible tensor operator transforming according to the completely symmetric representation $[\lambda_g] \equiv [n]$; we denote such an operator by T^g. Since the direct product $[\lambda_g] \times [\lambda_i] = [\lambda_i]$ (there are no multiple representations in the expansion of the direct product), the Wigner-Eckart theorem takes the form

$$\langle [\lambda_i]\,(r_i)\,|\,T^g\,|\,[\bar\lambda_i]\,(\bar r_i)\rangle = \langle[\lambda_i]\,\|\,T^g\,\|\,[\lambda_i]\rangle\,\delta_{\lambda_i\bar\lambda_i}\delta_{r_i\bar r_i}, \quad (17)$$

i.e., the matrix element is diagonal with respect to $[\lambda_i](r_i)$ and does not depend on the Yamanouchi symbols. Therefore in this case equation (15) can be written in the form †

$$\langle [\lambda]^A \,\|\, P \,\|\, [\lambda]^B\rangle, \quad (18)$$

where the double bar means that the expression is independent of the Yamanouchi symbols, while A and B as before denote the types of reductions into subgroups, and the expressions are diagonal with respect to the $[\lambda_i]$ of the individual groups of numbers.

The simplest example of the matrix (18) is

$$\langle [\lambda]\,(r_1r_2)\,|\,P\,|\,[\lambda]\,(\bar r_2\bar r_1)\rangle$$

$$= \int \Phi^*([\lambda]\,(r_1r_2)\,|\,12\,345)\,P_{13524}\Phi([\lambda]\,(\bar r_2\bar r_1)\,|\,123\,45)\,d\tau$$

$$= \int \Phi^*([\lambda]\,(r_1r_2)\,|\,12\,345)\,\Phi([\lambda]\,(\bar r_2\bar r_1)\,|\,345\,12)\,d\tau, \quad (19)$$

Applying the Wigner-Eckart theorem individually to the groups of permutations of the numbers 12 and 345, we find that the expression is diagonal with respect to $[\lambda_1]$, $[\lambda_2]$ and independent of the Yamanouchi symbols.

4. CONSTRUCTION OF COORDINATE WAVE FUNCTIONS

Suppose we have a configuration consisting of two shells $l_1^{n_1}l_2^{n_2}$. In the absence of spin interactions, the energy levels are classified by assigning the permutation symmetry $[\lambda]$ of the whole configuration and the total orbital angular momentum L, and, in addition, a set of quantum numbers characterizing the energy levels of the individual shells $[\lambda_i]\,\alpha_i L_i$ (where the α_i distinguish terms with the same $[\lambda_i]\,L_i$). In the case of k shells it is necessary in addition to give k − 2 intermediate symmetry patterns and intermediate orbital angular momenta.

In the work of Jahn,[5] for the case when all the orbital angular momenta of the particles are different, a formula was given which makes it possible to construct functions with symmetry $[\lambda]$ from functions with symmetries $[\lambda_1]$ and $[\lambda_2]$. In the final expression there enters the matrix whose calculation was not shown (except for the case of $n_2 = 2$). If in place of permutations of the orbital angular momenta we permute the coordinates of the particles and introduce a matrix of type (15), then by means of computations which are analogous to those carried out by Jahn we obtain the following expression for the orbital wave function of a two-shell configuration:

$$\Phi\,((l_1^{n_1}\,[\lambda_1]\,\alpha_1L_1,\ l_2^{n_2}\,[\lambda_2]\,\alpha_2L_2)\ [\lambda]\ (r)^A LM)$$

$$= \left\{\frac{f_\lambda}{f_{\lambda_1}f_{\lambda_2}}\,\frac{n_1!\,n_2!}{n!}\right\}^{1/2} \sum_{r_1r_2}\sum_{Q} \langle[\lambda]\ (r)^A\,|Q|\ [\lambda]\ (r_1r_2)\rangle\ Q$$

$$\times\ \varphi\,(l_1^{n_1}\ [\lambda_1]\ (r_1)\ \alpha_1L_1,\ l_2^{n_2}[\lambda_2]\ (r_2)\ \alpha_2L_2;\ LM). \quad (20)$$

The function φ describes the vector-coupled state

*This fact was brought to the author's attention by I. B. Levinson.

†The result (17) of the Wigner-Eckart theorem is trivial, since it follows from the orthonormality of the basis of the standard representation ($\langle[\lambda_i]\|\,T^g\|\,[\lambda_i]\rangle = 1$). However, the application of the theorem to the class of matrices (15) which we are considering gives the non-trivial result that (18) is independent of the Yamanouchi symbols and is diagonal with respect to $[\lambda_i]$.

with total angular momentum L and projection M. The symbols (r_1), (r_2) run through all the Yamanouchi symbols of the patterns $[\lambda_1]$ and $[\lambda_2]$, and Q are permutations of the coordinates of the particles between the shells. The choice of Q is not unique. We may choose for them any $n!/n_1!n_2!$ permutations from the set which are conjugate with respect to the subgroup $S_{n_1} \times S_{n_2}$.

As an example let us consider the case of $S_2 \times S_2$. We denote this subgroup of S_4 by H. It forms an invariant subgroup. The other elements can be obtained by multiplying the elements of H by the elements of the group S_4 which do not appear in it, until we exhaust the whole group:[10]

H:	1	P_{12}	P_{34}	$P_{12}P_{34}$
$P_{13}H$:	P_{13}	P_{123}	P_{134}	P_{1234}
$P_{23}H$:	P_{23}	P_{132}	P_{234}	P_{1342}
$P_{14}H$:	P_{14}	P_{124}	P_{143}	P_{1243}
$P_{24}H$:	P_{24}	P_{142}	P_{243}	P_{1432}
$P_{13}P_{24}H$:	$P_{13}P_{24}$	P_{1432}	P_{1324}	$P_{14}P_{23}$

Jahn uses the first column; we shall choose the permutations preserving the increasing order of enumeration of the particles within each shell:

Q	1	P_{123}	P_{23}	P_{1243}	P_{243}	$P_{13}P_{24}$
first shell	12	23	13	24	14	34
second shell	34	14	24	13	23	12

This choice of Q is made so that it is convenient for the later expansion of the wave function in terms of the fractional parentage coefficients, for which one has to split off the last particle from each of the shells.

For the case of k shells one can prove the following generalization of formula (20):

$$\Phi\left((l_1^{n_1}[\lambda_1]\,\alpha_1 L_1 \ldots l_k^{n_k}[\lambda_k]\,\alpha_k L_k)^B b_\lambda\,[\lambda]\,(r)^A b_L LM\right)$$
$$= c\sum_{r_1\ldots r_k}\sum_{Q^B}\langle [\lambda]\,(r)^A\,|\,Q^B\,|\,[\lambda]\,(r_1\ldots r_k)^B\rangle$$
$$\times\, Q^B\varphi\left(l_1^{n_1}[\lambda_1](r_1)\ldots l_k^{n_k}[\lambda_k](r_k)\right.$$
$$\times\left.(\alpha_1 L_1\ldots\alpha_k L_k)^B b_L LM\right),$$
$$c=\left\{\frac{f_\lambda}{f_{\lambda_1}\cdots f_{\lambda_k}}\,\frac{n_1!\ldots n_k!}{n!}\right\}^{1/2}. \tag{21}$$

Here A is the type of reduction of the representation $[\lambda]$ into subgroups, B is the method of coupling the $[\lambda_i]$ to form $[\lambda]$ and L_i to form L, which characterizes the structure of the function Φ; b_λ and b_L are sets of intermediate symmetry patterns and intermediate angular momenta necessary for complete characterization of a state, Q^B is the set of permutations which interchange the coordinates of particles between the shells and is determined by the method of coupling, B, of the shells. Thus, for successive symmetrization of the shells

$$Q^B = Q_{12\ldots k-1,\,k}\,Q_{12\ldots k-2,\,k-1}\ldots Q_{12},$$

where $Q_{12\ldots m-1,m}$ are the permutations of exchange between sets of particles of the first $m-1$ shells and the m-th shell.

APPENDIX

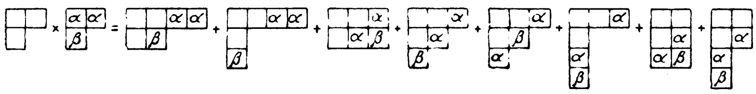
THE LITTLEWOOD THEOREM FOR THE PERMUTATION GROUP

To find all the possible $[\lambda]$ for the transition from the irreducible representation $[\lambda_1]\times[\lambda_2]$ of the subgroup $S_{n_1}\times S_{n_2}$ to the total group S_n, one can use Littlewood's theorem.[13] This theorem was proven by Littlewood for the group of linear transformations, and gives the expansion of the direct product of two irreducible representations of the linear group:

$$[\lambda_1]\times[\lambda_2]=\sum_\lambda c(\lambda_1\lambda_2\lambda)\,[\lambda]. \tag{22}$$

Weyl showed that the bases of all irreducible representations of the linear group can be obtained by symmetrization of an arbitrary tensor of rank n according to the Young patterns with n boxes.[14] However, the n-th rank tensor symmetrized according to some Young pattern can simultaneously also serve as the basis for an irreducible representation of the group of permutations of n symbols, if we fix the components of the tensor and carry out the symmetrization over all Young tableaux. The fact that the expansion of the direct product of representations of the linear group contains the representation symmetrized according to some pattern $[\lambda]$ shows that for the permutation group also the representation $[\lambda]$ will appear in the symmetrization of the product $[\lambda_1]\times[\lambda_2]$. It can be shown that $c(\lambda\lambda_1\lambda_2)$ from Eq. (6) is equal to $c(\lambda_1\lambda_2\lambda)$ from (22), and therefore, to obtain the expansion (6), one can also use Littlewood's theorem, which is formulated as follows: to find the irreducible representations contained in the expansion of the direct product of the representations $[\lambda_1]\equiv[\lambda_1^{(1)}\lambda_1^{(2)}\ldots]$ and $[\lambda_2]\equiv[\lambda_2^{(1)}\lambda_2^{(2)}\ldots]$, we must successively add to the pattern $[\lambda_1]$, in all possible ways, $\lambda_2^{(1)}$ boxes with indices α, $\lambda_2^{(2)}$ boxes with indices β, etc., in such order that in the standard Young patterns which are formed the added indices satisfy the following two conditions: 1) there shall be no two identical indices in one column; 2) if we enumerate all the added indices from right to left successively through the rows, we obtain a lattice permutation of the expression $\alpha^{\lambda_2^{(1)}}\beta^{\lambda_2^{(2)}}\ldots$, i.e., among any m first terms the number of times we encounter α

is no less than the number of times that we encounter β, etc. As an example: $[21] \times [21]$:



Collecting like terms, we finally get

$$[21] \times [21] = [42] + [411] + [33] + 2\,[321] + [3111] + [222] + [2211]. \qquad (23)$$

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