Memoirs of the College of Science, University of Kyoto, Series A,
Vol. XXVI, No. 3, Article 21, 1950.

On the Transformation of Spin Functions.

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(Received December 13, 1950)

SUMMARY

In order to determine the states of a system having several identical particles, each with any spin, we have essentially to consider the transformation of the spin functions of the system, and to treat the problem three principal methods may be expected. In the present paper we have treated the problem by the method of simultaneous reduction of both representations of rotation and symmetric groups, regarding the spin functions as the bases. The results of our calculation are given in Table I. By adopting these results it has been able to obtain, for example, the transformation of nuclear spin functions of a system having identical nuclei with any spatial symmetry.

1. Introduction

In quantum mechanics, for the purpose of determining the states of a system including several identical particles, we have essentially to find the transformation of the spin functions of the set in relation to the problem of permutation degeneracy and of statistical property subjected to the particle itself. The problem concerning a set of particles with spin $\frac{1}{2}\hbar$, e.g. many-electron problem, has been dealt with by the following methods: firstly, the wave method based upon the employment of explicit wave functions (**1**); secondly, the method of Dirac's character operator (**2**), which has been extended by Van Vleck (**3**), Serber (**4**), and Corson (**5**); and finally, a method which makes use of the representation matrices of the symmetric permutation group given by Serber (**6**) and by Yamanouchi (**7**).

In the present paper we have attempted to find the transformation of spin functions of a system composed of several identical particles, each having a higher spin. And we have treated especially along the line of the last method, performing the simultaneous reduction of both representations of rotation and symmetric groups regarding the spin functions as the bases, without having recourse to the construction of the representation matrices of the symmetric group. The results of our calculation are given in Table I.

By adopting these results we can obtain the transformation of nuclear spin functions of a system including identical nuclei with any spatial symmetry*. Then, some applications will be possible to the problem not only of nuclear spin degeneracy, nuclear quadrupole coupling, and nuclear spin-spin interaction in molecular and crystal systems, but also of nuclear shell structures.

2. General remarks on the simultaneous reduction of the two group representations

The spin space of a particle with spin s (taking $\hbar$ as unit) is expressed by the representation $\mathfrak{D}_s$ of a rotation group, diagonalizing the rotation about the z-axis in a $(2s+1)$-dimensional unitary space. The spin function of a system including f similar particles are made up of $(2s+1)^f$ independent bases:

$$U_\lambda^{(1)} U_\mu^{(2)} \cdots U_\nu^{(f)}, \text{ where } \lambda, \mu, \cdots, \nu = s, s-1, \cdots, -s. \qquad (1)$$

Therefore they make a $(2s+1)^f$-dimensional vector space $\mathfrak{R}$, in which they are linearly transformed not only by rotations of the space, but also by permutations of these identical particles. So we have two representations of the rotation and the symmetric groups in the space $\mathfrak{R}$ at the same time: the former, $[\mathfrak{D}_s]_f$, the Kronecker f-th power of $\mathfrak{D}_s$, and the latter, π_f of degree f. In the reduction of $\mathfrak{R}$ the following theorem is employed: the reduction of either representation can be carried out simultaneously, since the operations of these two groups are commutative with each other. This means, as regards the basis vectors, that it is possible to divide into a set of rectangles with the following form:

$$\begin{matrix} V_{11}, \cdots, V_{1n} \\ \cdot \quad\quad \cdot \\ \cdot \quad\quad \cdot \\ V_{k1}, \cdots, V_{kn} \end{matrix} ; \quad \begin{matrix} V'_{11}, \cdots, V'_{1n'} \\ \cdot \quad\quad \cdot \\ \cdot \quad\quad \cdot \\ V'_{k'1}, \cdots, V'_{k'n'} \end{matrix} ; \quad \cdots\cdots\cdots \qquad (2)$$

Every set of basis vectors belonging to every row in one of the rectangles appertains together to a certain irreducible representation of a group. And in the same way it holds between every column in one of the

* The spatial symmetry of the fixed nuclei is expressed by the *symmetry group* $\mathfrak{G}$ (8), which is a finite or continuous sub-group of the three-dimensional full rotation-reflection group.

rectangles and another group representation. Consequently either irreducible representation of the two groups corresponds to one of the rectangles (**10**).

According to the above theorem, to each rectangle corresponds an irreducible representation specified by a certain resultant spin value S of the rotation group and one of the symmetric group, taking suitable linear combinations of (1) as the bases. In our case, however, to all the columns of each rectangle belongs not always an irreducible representation of a group, that is to say, the representation of the symmetric group belonging to a rectangle is not irreducible in general. If the representation of the rotation group has been completely reduced, each rectangle has one-to-one correspondence with each S which is given by the reduction of the product representation:

$$[\mathfrak{D}_s]_f = \sum_S c(S, f)\, \mathfrak{D}_S; \quad S = fs - g\,, \tag{3}$$

where $g = 0, 1, 2, \cdots, fs$, or $fs - \frac{1}{2}$ for all the possible resultant spin values S's, and $c(S, f)$ is the number of times of the appearance of an irreducible representation $\mathfrak{D}_S$.

Now we take

$$U_\lambda^{(i)} = \frac{(u_1^{(i)})^{s+\lambda}(u_2^{(i)})^{s-\lambda}}{\sqrt{(s+\lambda)!\,(s-\lambda)!}}\,, \tag{4}$$

as the unitary base vector of the spin space of each particle, where $i = 1, 2, \cdots, f$ and $\lambda = s, s-1, \cdots, -s$. And if we introduce the contragradient variables x_1 and x_2 to $u_1^{(i)}$ and $u_2^{(i)}$, respectively, the following invariant formula can be established:

$$I = \prod_{i<j}(u_1^{(i)}u_2^{(j)} - u_2^{(i)}u_1^{(j)})^{\sigma_{ij}} \prod_k (u_1^{(k)}x_1 + u_2^{(k)}x_2)^{2s-g_k}\,, \tag{5}$$

where $\prod_{i<j}$ means the product with respect to i less than j, subject to the condition that $\sum_{i<j}\sigma_{ij} = g$, and

$$g_k = \begin{cases} \sum' \sigma_{ij} & (\text{for } k = i, \text{ or } j) \\ 0 & (\text{for } k \neq i, \text{ and } j)\,, \end{cases}$$

$\sum'$ being the summation with respect to all k's. Then it is easily proved that the basis vector of the representation $\mathfrak{D}_S$ is given for $M = S, S-1, \cdots, -S$ by the coefficient of

$$X_M^S = \frac{x_1^{S+M}\, x_2^{S-M}}{\sqrt{(S+M)!\,(S-M)!}} \tag{6}$$

in the expansion of the invariant formula (5). Thereby we can explicitly obtain each column in every rectangle (2) except for common numerical factor.

From the fact that the characters of the representations in $\mathfrak{R}$ are invariant for any set of linear combinations, those characters of a transformation AP in the spin space can be calculated by the following two methods: first, by the bases (2) reduced only for the rotation group, and secondly, by the basis vectors of the type (1); where A means a set of unitary transformations:

$$U_s = \zeta^s U_s, \; U_{s-1} = \zeta^{s-1} U_{s-1}, \; \cdots, \; U_{-s} = \zeta^{-s} U_{-s}, \tag{7}$$

on remembering that the representation $R_z(\varphi)$ of the rotation (angle φ) about the z-axis with the bases $U_s, U_{s-1}, \cdots, U_{-s}$ can be given by

$$R_z(\varphi) = \begin{pmatrix} e^{is\varphi} & & & 0 \\ & e^{i(s-1)\varphi} & & \\ & & \ddots & \\ 0 & & & e^{-is\varphi} \end{pmatrix}.$$

P is a set of permutations which have various cycle structures $(\alpha_1, \alpha_2, \cdots, \alpha_\rho)$, provided that $\alpha_1 + 2\alpha_2 + \cdots + \rho\alpha_\rho = f$ (9). Let $\chi_S(P)$ be a set of characters of the representation of the permutations P belonging to a rectangle specified by a given S. Then as both results must be equal, we can find the following identities, namely, for an integral value of S:

$$\sum_S \chi_S(P) (\zeta^S + \zeta^{S-1} + \cdots + \zeta^{-S}) = \prod_{i=1}^{\rho} (\zeta^{s\alpha_i} + \zeta^{(s-1)\alpha_i} + \cdots + \zeta^{-s\alpha_i}), \tag{8 a}$$

and for a half-integral value of S:

$$\sum_S \chi_S(P) (\zeta^{2S} + \zeta^{(2S-2)} + \cdots + \zeta^{-2S})$$
$$= \prod_{i=1}^{\rho} (\zeta^{2s\alpha_i} + \zeta^{(2s-2)\alpha_i} + \cdots + \zeta^{-2s\alpha_i}), \tag{8 b}$$

respectively, where $\sum_S$ is a summation about all possible $S = fs - g \geqq 0$. Thereupon $\chi_S(P)$ can be obtained as the coefficient of ζ^g in a polynomial:

$$\prod_{i=1}^{\rho} (1-\zeta)(\zeta^{2s\alpha_i} + \zeta^{(2s-1)\alpha_i} + \cdots + 1), \tag{9}$$

if both sides of (8 a) and (8 b) are multiplied by $\zeta^{sf}(1-\zeta)$, and $\zeta^{2sf} \times (1-\zeta^2)$ for $s =$ an integer and a half-integer, respectively, and ζ^2 is replaced by ζ for the latter.

Thus we can calculate $\chi_S(P)$ about every class of the symmetric group over all possible S. The calculations have been carried out within the limits of the problem of some part of the nuclear spins and of $f \leqq 6$. It is shown that the results are equal to those found from branching diagrams. In addition, a character of the unit element is the degree of dimension of the representation matrix of the symmetric group belonging to a given S, being just equal to $c(S, f)$ in (3).

Finally, the complete reductions of π_f are given by resolving every $\chi_S(P)$ calculated above into simple characters of the symmetric group (**9**). The final results of the simultaneous reductions are inserted in Table I, where in case of $s = 1$, $f = 6$, and $S = 2$, the result is given by the direct sum:

$$\{6\} + \{5, 1\} + 2\{4, 2\} + \{3, 2, 1\}$$

and every $\{\alpha_1, \cdots, \alpha_\rho\}$ means an irreducible representation of the symmetric group, above all $\{f\}$ is always an identical one. In these illustrations we can find the fact that, if $2s + 1 \geqq f$, every irreducible representation is at least once included in the direct sum.

TABLE I. The results of the simultaneous reduction.

The first row of each sub-table gives the irreducible representations of each symmetric group $\mathfrak{S}_f$, and the first column of them means the resultant spins characterizing the irreducible representations of the rotation group. In case when $f = 6$, χ_i's give $\{6\}$, $\{5, 1\}$, $\{4, 2\}$, $\{4, 1^2\}$, $\{3^2\}$, $\{3, 2, 1\}$, $\{3, 1^3\}$, $\{2^3\}$, $\{2^2, 1^2\}$, $\{2, 1^4\}$, and $\{1^6\}$ with the order of i. In case when $f = 5$, they give $\{5\}$, $\{4, 1\}$, $\{3, 2\}$, $\{3, 1^2\}$, $\{2^2, 1\}$, $\{2, 1^3\}$, and $\{1^5\}$, respectively. And in case when $f = 4$, $\chi_2 = \{3, 1\}$, $\chi_3 = \{2^2\}$, $\chi_4 = \{2, 1^2\}$, and $\chi_5 = \{1^4\}$. In the following table any column of χ_i is omitted, whenever its elements are all zero. Besides we put the table of $s = 1/2$ only as a reference.

a) $s = 1/2$.

$f = 2$

	χ_1	χ_2
$S = 0$	0	1
1	1	0

$f = 3$

	χ_1	χ_2
$S = 1/2$	0	1
3/2	1	0

$f = 4$

	χ_1	χ_2	χ_3
$S = 0$	0	0	1
1	0	1	0
2	1	0	0

$f = 5$

	χ_1	χ_2	χ_3
$S = 1/2$	0	0	1
3/2	0	1	0
5/2	1	0	0

$f = 6$

	χ_1	χ_2	χ_3	χ_5
$S = 0$	0	0	0	1
1	0	0	1	0
2	0	1	0	0
3	1	0	0	0

b) $s = 1$

$f = 2$

	χ_1	χ_2
$S = 0$	1	0
1	0	1
2	1	0

$f = 3$

	χ_1	χ_2	χ_3
$S = 0$	0	0	1
1	1	1	0
2	0	1	0
3	1	0	0

$f = 4$

	χ_1	χ_2	χ_3	χ_4
$S = 0$	1	0	1	0
1	0	1	0	1
2	1	1	1	0
3	0	1	0	0
4	1	0	0	0

$f = 5$

	χ_1	χ_2	χ_3	χ_4	χ_5
$S = 0$	0	0	0	1	0
1	1	1	1	0	1
2	0	1	1	1	0
3	1	1	1	0	0
4	0	1	0	0	0
5	1	0	0	0	0

$f = 6$

	χ_1	χ_2	χ_3	χ_4	χ_5	χ_6	χ_8
$S = 0$	1	0	1	0	0	0	1
1	0	1	0	1	1	1	0
2	1	1	2	0	0	1	0
3	0	1	1	1	1	0	0
4	1	1	1	0	0	0	0
5	0	1	0	0	0	0	0
6	1	0	0	0	0	0	0

c) $s = 3/2$

$f = 2$

	χ_1	χ_2
$S = 0$	0	1
1	1	0
2	0	1
3	1	0

$f = 3$

	χ_1	χ_2	χ_3
$S = 1/2$	0	1	0
3/2	1	1	1
5/2	1	1	0
7/2	0	1	0
9/2	1	0	0

$f = 4$

	χ_1	χ_2	χ_3	χ_4	χ_5
$S = 0$	1	0	0	0	1
1	0	2	0	1	0
2	1	1	2	1	0
3	1	2	0	1	0
4	1	1	1	0	0
5	0	1	0	0	0
6	1	0	0	0	0

$f = 5$

	χ_1	χ_2	χ_3	χ_4	χ_5	χ_6
$S = 1/2$	0	1	1	1	1	0
3/2	1	2	2	1	1	1
5/2	1	2	2	2	1	0
7/2	1	2	2	1	1	0
9/2	1	2	1	1	0	0
11/2	1	1	1	0	0	0
13/2	0	1	0	0	0	0
15/2	1	0	0	0	0	0

$f = 6$

	χ_1	χ_2	χ_3	χ_4	χ_5	χ_6	χ_7	χ_8	χ_9
$S = 0$	0	1	0	1	2	0	0	0	1
1	1	1	3	1	0	0	1	1	0
2	0	3	2	2	2	3	0	0	1
3	2	2	4	2	1	2	1	1	0
4	1	3	2	2	2	2	0	0	0
5	1	2	3	1	0	1	0	0	0
6	1	2	1	1	1	0	0	0	0
7	1	1	1	0	0	0	0	0	0
8	0	1	0	0	0	0	0	0	0
9	1	0	0	0	0	0	0	0	0

d) $s = 5/2$.

$f = 2$

	χ_1	χ_2
$S = 0$	0	1
1	1	0
2	0	1
3	1	0
4	0	1
5	1	0

$f = 3$

	χ_1	χ_2	χ_3
$S = 1/2$	0	1	0
3/2	1	1	1
5/2	1	2	1
7/2	1	2	0
9/2	1	1	1
11/2	1	1	0
13/2	0	1	0
15/2	1	0	0

$f = 4$

	χ_1	χ_2	χ_3	χ_4	χ_5
$S = 0$	1	0	2	0	1
1	0	3	0	2	0
2	2	2	3	2	1
3	1	4	1	3	0
4	2	3	3	2	1
5	1	4	1	2	0
6	2	2	2	1	0
7	1	2	0	1	0
8	1	1	1	0	0
9	0	1	0	0	0
10	1	0	0	0	0

$f = 5$

	χ_1	χ_2	χ_3	χ_4	χ_5	χ_6	χ_7
$S = 1/2$	1	2	2	2	2	1	0
3/2	1	4	4	4	3	2	0
5/2	2	5	6	5	4	2	1
7/2	2	6	6	6	4	2	0
9/2	3	6	6	5	4	2	0
11/2	2	6	5	5	3	1	0
13/2	2	5	5	3	2	1	0
15/2	2	4	3	3	1	0	0
17/2	2	3	2	1	1	0	0
19/2	1	2	1	1	0	0	0
21/2	1	1	1	0	0	0	0
23/2	0	1	0	0	0	0	0
25/2	1	0	0	0	0	0	0

$f = 6$

	χ_1	χ_2	χ_3	χ_4	χ_5	χ_6	χ_7	χ_8	χ_9	χ_{10}	χ_{11}
$S = 0$	0	2	0	3	4	2	0	0	2	0	1
1	2	3	8	4	1	7	4	3	1	1	0
2	1	8	7	8	6	11	3	1	5	1	0
3	4	7	13	9	4	12	6	5	3	1	0
4	2	10	11	11	8	13	4	2	5	1	0
5	4	9	14	9	4	13	5	3	2	1	0
6	3	10	10	10	7	10	3	2	3	0	0
7	4	8	11	7	3	8	3	2	1	0	0
8	2	8	7	6	4	6	1	0	0	0	0
9	3	5	7	4	2	3	1	1	0	0	0
10	2	5	3	3	2	2	0	0	0	0	0
11	2	3	3	1	0	1	0	0	0	0	0
12	1	2	1	1	1	0	0	0	0	0	0
13	1	1	1	0	0	0	0	0	0	0	0
14	0	1	0	0	0	0	0	0	0	0	0
15	1	0	0	0	0	0	0	0	0	0	0

3. Transformation of nuclear spin functions

As an example of applications of the above results, we can obtain the transformation of nuclear spin functions of a system including several identical (relatively) fixed nuclei with a certain spatial symmetry, each nucleous having a higher spin. The symmetry group $\mathfrak{G}$ expressing the spatial symmetry of nuclear architecture of a molecular system can be always represented with homomorphic correspondence by a permutation group $\mathfrak{P}$, which is generally a sub-group of a symmetric group $\mathfrak{S}_f$. It is easily proved, however, that the followings correspond isomorphically to each other:

$$\left.\begin{array}{c}\mathfrak{P} \cong \mathfrak{G} \equiv C_i, C_s, C_2, C_{3v}, D_3, C_4, C_{4v}, V_d, D_4, D_6, \\ T, T_d, O, O_h, \text{ etc.}\end{array}\right\} \qquad (10)$$

Therefore, the irreducible representations of the grovp $\mathfrak{S}_f$ are not always irreducible for the representations of $\mathfrak{P}$, or isomorphically represented group $\mathfrak{G}$, and so by considering the spatial symmetry of equivalent nuclear system the irreducible representations of $\mathfrak{S}_f$ can be reduced in general to those of $\mathfrak{G}$. If $\mathfrak{P}$ is homomorphic to $\mathfrak{G}$, the reduction must be carried out in regard to the class elements corresponding to the permutations of equivalent nuclei. And in the case of $\mathfrak{P} \equiv \mathfrak{S}_f$, the reduction is not necessary. The correspondence of the irreducible representations of $\mathfrak{S}_f$ to the typical $\mathfrak{G}$ is given by the following Table II.

TABLE II.

a) $\mathfrak{S}_2$.

	$\mathfrak{G} \equiv C_i$	C_s	C_2	C_{2v}	D_{2v}	$D_{\infty h}$
χ_1	A_g	A'	A	A_1	A_{1g}	Σ_g^+
χ_2	A_u	A''	B	B_2	B_{2u}	Σ_u^+

b) $\mathfrak{S}_3$.

	$\mathfrak{G} \equiv C_{3v}, D_3$	D_3
χ_1	A_1	A_{1g}
χ_2	E	E_g
χ_3	A_2	A_{2g}

c) $\mathfrak{S}_4$.

	$\mathfrak{G} \equiv C_{4v}, D_4, V_d$	D_{4h}	T_d
χ_1	A_1	A_{1g}	A_1
χ_2	$B_1 + E$	$B_{1g} + E_{1u}$	T_2
χ_3	$A_1 + B_1$	$A_{1g} + B_{2g}$	E
χ_4	$A_2 + E$	$A_{2g} + E_{1u}$	T_1
χ_5	B_1	B_{2g}	A_2

d) $\mathfrak{S}_6$.

$\mathfrak{G} \equiv D_{6v}$:

$\chi_1 = A_{1g}$, $\chi_2 = B_{1u} + E_{1g} + E_{2u}$, $\chi_3 = 2A_{1g} + B_{2u} + 2E_{1g} + E_{2u}$,
$\chi_4 = 2A_{2g} + B_{1u} + B_{2u} + E_{1g} + 2E_{2u}$, $\chi_5 = A_{2g} + 2B_{1u} + E_{2u}$,
$\chi_6 = A_{1g} + A_{2g} + B_{1u} + B_{2u} + 3E_{1g} + 3E_{2u}$,
$\chi_7 = A_{1g} + A_{2g} + 2B_{2u} + 2E_{1g} + E_{2u}$,
$\chi_8 = 2A_{1g} + E_{1g} + B_{2u}$, $\chi_9 = A_{2g} + 2B_{1u} + E_{1g} + 2E_{2u}$,
$\chi_{10} = A_{1g} + E_{1g} + E_{2u}$, $\chi_{11} = B_{1u}$.

$\mathfrak{G} \equiv O_h$:

$\chi_1 = A_{1g}$, $\chi_2 = E_g + T_{1u}$, $\chi_3 = A_{1g} + E_g + T_{2g} + T_{2u}$,
$\chi_4 = A_{2g} + T_{1g} + T_{1u} + T_{2u}$, $\chi_5 = A_{2g} + A_{2u} + T_{1u}$,
$\chi_6 = E_g + E_u + T_{1g} + T_{1u} + T_{2g} + T_{2u}$, $\chi_7 = A_{1u} + T_{1g} + T_{2g} + T_{2u}$,
$\chi_8 = A_{1g} + A_{1u} + T_{2g}$, $\chi_9 = A_{2u} + E_u + T_{1u} + T_{1g}$,
$\chi_{10} = E_u + T_{2g}$, $\chi_{11} = A_{2u}$.

By making use of the above relations, the transformation of nuclear spin functions is given in terms of a direct sum of irreducible representations Γ_j of $\mathfrak{G}$: the results are generally obtained by the formula:

$$\sum_S (2S+1) \sum_j \gamma(j, S)\, \Gamma_j, \tag{11}$$

where the factor $(2S+1)$ is the nuclear spin multiplicity corresponding to a given resultant spin S, and $\gamma(j, S)$ are always positive integer, or the number of times in which each irreducible representation of $\mathfrak{G}$ specified by j appears.

In conclusion, the authors should like to express his deep gratitude to Professor H. Yukawa for his kind interest and encouragement.

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