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On the symmetry properties of outer product reduction

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Abstract. The symmetry properties of outer product coupling coefficients for the symmetric group and of Clebsch-Gordan coefficients for the unitary group and of the corresponding isoscalar factors are discussed. A simple rule is given for determination of a phase factor of outer reduction symmetry of S_n and $U(N)$. The rule is provided with a relationship between the phase factor of a Young diagram with its subdiagrams.

1. Introduction

The symmetric and unitary group are two important groups which have been extensively used in describing the structure and properties of many-particle systems, in areas of theoretical physics and chemistry. The significance of the group SU(3) for the nuclear model is well known. In quantum chemistry, various approaches based on the unitary group and/or symmetric group to the many-electron correlation problem (Paldus 1974, Shavitt 1977, 1978, Hinze 1981, Matsen and Paunze 1986 and references therein) provide not only mathematically beautiful formalisms but also versatile, practical and powerful tools for handling many-electron systems. The approaches have been used in much of the methodology of quantum chemistry. These approaches are now developed to combine with other many-body theories, such as many-body perturbation theory, coupled cluster theory and propagator theory, in the hope of yielding more efficient and compact formalisms with a view towards implementation.

It is believed that further applications of these two groups to many-particle systems require better understanding of their mathematical structure. The construction of Clebsch-Gordan (CG) coefficients (or Wigner coefficients) for the relevant groups in an efficient way becomes a valuable topic. At present, much literature is concerned with the construction of CG coefficients for S_n and/or $U(N)$ from different points of view. Among these approaches are: Racah's infinitesimal operator (de Swart 1963, Haacke *et al* 1976), pattern calculus (Biedenharn and Louck 1968, 1981), diagonalisation of the representation matrix of certain operators such as CSCO (Bayman and Lande 1966, Chen *et al* 1985, 1987), build-up procedure for isoscalar factors (Wybourne 1974, Butler and Wybourne 1976), vector coherent state theory (Le Blanc and Hecht 1987), and some new developments (Karassiov 1987).

In recent papers, the inner and outer product coupling coefficients for S_n have been extensively discussed (Zhang and Li 1986, 1987, Li and Zhang 1987, 1989). Based

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on a double coset technique, we obtained two recursion formulae which lead to a simple and efficient construction of the corresponding isoscalar factors. Furthermore, the computation of isoscalar factors (reduced Wigner coefficients) for $U(N) \supset U(N-1)$ is carried out from a viewpoint of outer product isoscalar factors for S_n, by virtue of the duality between the outer product reduction of S_n and the Kronecker product reduction of $U(N)$ (Weyl 1946) and the duality of bases for the relevant groups.

Unlike the inner product coupling coefficients (IPCC) for S_n, the outer product coupling coefficients (OPCC) are rather new and suffer a lack of attention. However, the OPCC are useful in physics and quantum chemistry. For example, they appear naturally in a partitioning technique related to interaction theory of subsystems (Kaplan 1974, Paldus *et al* 1987). Using OPCC, one can generate any k-column Gelfand-Tsetlin state from k single-column states (Paldus and Sarma 1985, Sarma and Paldus 1985), which is the basis of a recently developed Clifford algebra unitary group approach to the many-electron correlation problem. It is therefore highly desirable that the relevant OPCC can be expressed by compact and closed formulae. Recently, a closed formula has been derived for coupling of two single-column states to generate two-column Gelfand-Tsetlin states (Li and Paldus 1989). The nature of this derivation tells us that any attempted search for a suitable algebraic formula shall require a better understanding of the structure and symmetry properties of OPCC. In a recent paper (Zhang and Li 1987), the computation of outer product isoscalar factors leads to an interesting rule for a phase factor of symmetry, in which the phase factor of a Young diagram is related to that of its subdiagrams. It is the purpose of the present paper to give a detailed description of symmetry and a proof of the rule of phase factors, based on some recent developments. The notation used in this paper is the same as that used earlier (Zhang and Li 1987).

2. Symmetry properties

We shall denote an irrep of the symmetric and the unitary group by $[\lambda]$ and $\langle\lambda\rangle$, respectively. Consider groups S_{n_1} and S_{n_2}, the elements of which operate, respectively, on n_1 objects $\{1, 2, \ldots, n_1\} \equiv \omega_0^1$ and n_2 objects $\{n_1+1, n_2+2, \ldots, n_1+n_2=n\} \equiv \omega_0^2$. A standard Young-Yamanouchi basis for S_{n_1} and S_{n_2} is, respectively, $|[\lambda]r^1\rangle$ and $|[\lambda]r^2\rangle$. Replacing the index sets ω_0^1 and ω_0^2 by $\omega^1 \equiv \{i_1, i_2, \ldots, i_{n_1}\}$ and $\omega^2 \equiv \{j_1, j_2, \ldots, j_{n_2}\}$, respectively, from the standard bases for S_{n_1} and S_{n_2},

$$|[\lambda_k]r^k\omega^k\rangle = \begin{pmatrix} \omega_0^k \\ \omega^k \end{pmatrix} |[\lambda_k]r^k\rangle \qquad k = 1, 2 \tag{1}$$

we obtain the bases for groups $S_{n_1}(\omega^1)$ and $S_{n_2}(\omega^2)$, the groups consisting of all permutations operating on n_1 and n_2 objects labelled by ω^1 and ω^2, respectively. All those outer product states, i.e. $|[\lambda_1]r^1\omega^1\rangle|[\lambda_2]r^2\omega^2\rangle$, form a reducible space for S_n ($n = n_1 + n_2$) and we can use OPCC to decompose the space to obtain a basis for S_n:

$$|[\lambda]r\rangle = \sum_{r^1\omega^1} \sum_{r^2\omega^2} \begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ r^1\omega^1 & r^2\omega^2 & | & r \end{pmatrix} |[\lambda_1]r^1\omega^1\rangle|[\lambda_2]r^2\omega^2\rangle \tag{2}$$

where $[\lambda]$ is in the reduction of the outer product $[\lambda_1] \times [\lambda_2]$ described by the Littlewood rule.

The standard basis $|[\lambda]r\rangle$ is adapted to the subgroup chain

$$S_n \supset S_{n-1} \supset \cdots \supset S_1. \tag{3}$$

Moreover, the subduction of an outer product state $|[\lambda_1]r^1\omega^1\rangle|[\lambda_2]r^2\omega^2\rangle$ from S_n to S_{n-1} results in an outer product state for the group S_{n-1}. Hence, by using the Racah (1965) factorisation lemma, any OPCC is a successive product of I_o factors (outer product isoscalar factors or reduced OPCC):

$$\begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ r^1\omega^1 & r^2\omega^2 & | & r \end{pmatrix} = \prod_{m=1}^{n} I_o(S_{n-m+1} \supset S_{n-m} \otimes S_1). \tag{4}$$

The calculation of I_o factors has recently been described by Zhang and Li (1987) through a recursion formula which expresses $I_o(S_n \supset S_{n-1} \otimes S_1)$ in terms of $I_o(S_{n-1} \supset S_{n-2} \otimes S_1)$.

It is well known that an outer product reduction is independent of its order

$$[\lambda_1] \times [\lambda_2] = [\lambda_2] \times [\lambda_1]. \tag{5}$$

This implies

$$\begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ r^1\omega^1 & r^2\omega^2 & | & r \end{pmatrix} = \eta \begin{pmatrix} [\lambda_2] & [\lambda_1] & | & [\lambda] \\ r^2\omega^2 & r^1\omega^1 & | & r \end{pmatrix} \tag{6}$$

where $\eta = \pm 1$ is a phase factor of symmetry with respect to a permutation of the first two columns and depends on the irrep labels $[\lambda_1]$, $[\lambda_2]$ and $[\lambda]$. Generally speaking, the symmetric group S_n is not a simple reducible group (except for some smaller n). It is therefore not always possible to separate the phase factor η into three parts, such that each one depends only on one irrep label. However, for a given reduction which is multiplicity free, it is possible to define a phase factor for each irrep. Stated differently, we shall require a phase factor which is dependent on three irreps only when the relevant reduction is not multiplicity free. Hence we can define

$$\eta \equiv \eta([\lambda_1], [\lambda_2], [\lambda]) = (-1)^{[\lambda_1]+[\lambda_2]+[\lambda]} \tag{7}$$

for multiplicity-free cases, or more generally

$$\eta = (-1)^{[\lambda_1]+[\lambda_2]+[\lambda]} \theta([\lambda_1], [\lambda_2], [\lambda])_i \tag{8}$$

if multiplicity arises. Here, in (8), i is a multiplicity index. It shows that a phase factor which is dependent on three irreps can be defined by introducing a new phase factor to modify the original phase without multiplicity. Taking (7) and (8) into account, I_o factors have symmetry

$$I_o \begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ [\mu_1] & [\mu_2] & | & [\mu] \end{pmatrix} = (-1)^{[\lambda_1]+[\lambda_2]+[\lambda]+[\mu_1]+[\mu_2]+[\mu]} I_o \begin{pmatrix} [\lambda_2] & [\lambda_1] & | & [\lambda] \\ [\mu_2] & [\mu_1] & | & [\mu] \end{pmatrix} \tag{9}$$

under the permutation of the first two columns. Generally, we shall require

$$I_o \begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda]_i \\ [\mu_1] & [\mu_2] & | & [\mu]_j \end{pmatrix} = (-1)^{[\lambda_1]+[\lambda_2]+[\lambda]+[\mu_1]+[\mu_2]+[\mu]} \times \theta([\lambda_1], [\lambda_2], [\lambda])_i \theta([\mu_1], [\mu_2], [\mu])_j I_o \begin{pmatrix} [\lambda_2] & [\lambda_1] & | & [\lambda]_i \\ [\mu_2] & [\mu_1] & | & [\mu]_j \end{pmatrix} \tag{10}$$

where i and j are multiplicity indices.

The phases of (7) and (9) can be completely determined by the group itself. On the other hand, when multiplicity appears, there is no unique solution to this problem. We cannot determine the phases within the group. Solutions are usually obtained based on an *ad hoc* procedure. Therefore we shall pay special attention to the phases in (7) and (9).

The significance of I_o factors is evident. Due to the duality between the bases for S_n and $U(N)$ and the fact that both the reductions of the outer product of S_n and of the Kronecker product of $U(N)$ are determined by the Littlewood rule, it was shown (Chen 1984, Chen *et al* 1987) that CG coefficients for $U(N)$ are related with OPCC for S_n. It follows that the isoscalar factors for $U(N) \supset U(N-1)$ (I_u factor for short) can be expressed in terms of I_o factors (Zhang and Li 1987). From (37) of Zhang and Li (1987), it can easily be verified that the symmetry of I_u factors for multiplicity-free cases is given by

$$I_u\begin{pmatrix} \langle\lambda\rangle & \langle\mu\rangle \\ \langle\lambda_1\rangle & \langle\mu_1\rangle \end{pmatrix} \begin{vmatrix} \langle\nu\rangle \\ \langle\nu_1\rangle \end{pmatrix} = (-1)^{[\lambda]+[\mu]+[\nu]+[\lambda_1]+[\mu_1]+[\nu_1]} I_u\begin{pmatrix} \langle\mu\rangle & \langle\lambda\rangle \\ \langle\mu_1\rangle & \langle\lambda_1\rangle \end{pmatrix} \begin{vmatrix} \langle\nu\rangle \\ \langle\nu_1\rangle \end{pmatrix} \tag{11}$$

with the same phase factors $(-1)^{[\lambda]}$ as used for I_o factors when considered in terms of Young diagrams for irreps of $U(N)$. Generally, we require another phase θ given by (10). It is indicated that we can examine the phases either from the viewpoint of I_o factors or of I_u factors.

3. Phase factor

The symmetry properties of inner product coupling coefficients or IPCC for S_n have been examined by Hamermesh (1962) and recently by Zhang and Li (1987). The conclusions are: (i) when three irreps involved are different, one can arbitrarily choose the phase; (ii) when two of them are identical, we must distinguish two different spaces, namely the spaces of symmetric and antisymmetric squares; (iii) when all three irreps are identical, there are three different possibilities for symmetry properties, namely symmetry [3], antisymmetry $[1^3]$ and mixed symmetry [21].

I_o and I_u factors of the outer reduction have similar symmetries. Equations (9)-(11) show that the permutation of the first two columns only causes a change in the phase, the value of which can be chosen arbitrarily to be positive or negative in most cases. However, unlike the IPCC, there are not the spaces of symmetric and antisymmetric squares for the outer product reduction. But a similar restriction of the phases appears when $[\lambda_1]=[\lambda_2]$ in (9) (or $\langle\lambda\rangle=\langle\mu\rangle$ in (11)). In fact, if we let $\langle\lambda\rangle=\langle\mu\rangle$ and $\langle\lambda_1\rangle=\langle\mu_1\rangle$ in (11), we have

$$I_u\begin{pmatrix} \langle\lambda\rangle & \langle\lambda\rangle \\ \langle\lambda_1\rangle & \langle\lambda_1\rangle \end{pmatrix} \begin{vmatrix} \langle\nu\rangle \\ \langle\nu_1\rangle \end{pmatrix} = (-1)^{[\nu]+[\nu_1]} I_u\begin{pmatrix} \langle\lambda\rangle & \langle\lambda\rangle \\ \langle\lambda_1\rangle & \langle\lambda_1\rangle \end{pmatrix} \begin{vmatrix} \langle\nu\rangle \\ \langle\nu_1\rangle \end{pmatrix}. \tag{12}$$

It shall require

$$(-1)^{[\nu]} = (-1)^{[\nu_1]}. \tag{13}$$

In order to better understand the symmetry properties, we first consider some simple examples for I_o factors. For the reduction of $[1]\times[1]=[2]+[1^2]$, we have following symmetry of OPCC

$$(\boxed{1}\ \boxed{2}\mid \boxed{1}\boxed{2}) = (\boxed{2}\ \boxed{1}\mid \boxed{1}\boxed{2}) \qquad \left(\boxed{1}\ \boxed{2}\ \middle|\ \begin{matrix}\boxed{1}\\ \boxed{2}\end{matrix}\right) = -\left(\boxed{2}\ \boxed{1}\ \middle|\ \begin{matrix}\boxed{1}\\ \boxed{2}\end{matrix}\right).$$

In terms of I_o factors, we get

$$I_o\begin{pmatrix}[1] & [1] & | & [2]\\ [1] & 0 & | & [1]\end{pmatrix} = I_o\begin{pmatrix}[1] & [1] & | & [2]\\ 0 & [1] & | & [1]\end{pmatrix} \tag{14a}$$

$$I_o\begin{pmatrix}[1] & [1] & | & [1^2]\\ [1] & 0 & | & [1]\end{pmatrix} = -I_o\begin{pmatrix}[1] & [1] & | & [1^2]\\ 0 & [1] & | & [1]\end{pmatrix}. \tag{14b}$$

Therefore

$$(-1)^{[2]} = 1 \qquad (-1)^{[1^2]} = -1. \tag{15}$$

Similar analysis leads to the following phase factors:

$$(-1)^{[2k]} = 1 \qquad (k = 1, 2, 3, \ldots) \tag{16}$$

$$(-1)^{[1^{2k}]} = -1 \qquad (k = 1, 3, 5, \ldots) \tag{17}$$

$$(-1)^{[1^{4k}]} = 1 \qquad (k = 1, 3, 5, \ldots). \tag{18}$$

The above phase factors are provided with some built-up features. The phase factor of a Young diagram indicates a relation with its Young subdiagrams. This fact motivates us to search for such a relationship by which the phase of an arbitrary irrep of group S_n can be determined from the phase factors of its subgroup S_{n-1}. For this purpose, it is found that a realisation of the $U(N)$ basis in terms of the embedding $U(2^N) \supset SO(M)$ basis is beneficial.

Exploiting the subgroup chain

$$U(2^N) \supset SO(M) \supset U(N) \supset U(N-1) \supset \cdots \supset U(1) \tag{19}$$

where $M = 2N$ or $2N+1$, it was found (Sarma and Paldus 1985, Paldus and Sarma 1985) that every basis state of any k-column irrep of $U(N)$ can be realised as a multispinor basis state of $SO(M)$ and the Lie algebra of $SO(M)$ can be realised by using the embedding $U(2^N) \supset SO(M)$ and only totally symmetric representations of $U(2^N)$ are required to generate any $U(N)$ irreducible basis.

Based on such a realisation, it was further shown (Paldus *et al* 1987) that any two-column Gelfand-Tsetlin (GT) basis can be represented by coupling two single-column states. Let us give this formalism by writing

$$|\langle 2^b 1^{a-b}\rangle W\rangle = \sum_{W_1 W_2} \begin{pmatrix}\langle 1^a\rangle & \langle 1^b\rangle & | & \langle 2^b 1^{a-b}\rangle\\ W_1 & W_2 & | & W\end{pmatrix} \{|\langle 1^a\rangle W_1\rangle |\langle 1^b\rangle W_2\rangle\}_s \tag{20}$$

where the GT bases are denoted by Weyl tableaux W_1, W_2, W. $\{|\langle 1^a\rangle W_1\rangle|\langle 1^b\rangle W_2\rangle\}_s$ is a normalised symmetrised product of $|\langle 1^a\rangle W_1\rangle$ and $|\langle 1^b\rangle W_2\rangle$, namely

$$\{|\langle 1^a\rangle W_1\rangle|\langle 1^b\rangle W_2\rangle\}_s = 2^{-1/2}\{|\langle 1^a\rangle W_1\rangle|\langle 1^b\rangle W_2\rangle + |\langle 1^b\rangle W_2\rangle|\langle 1^a\rangle W_1\rangle\}. \tag{21}$$

One can extend this formalism to more general k-column states by successively coupling k single-column states.

Changing the sequence of coupling in (20) and using the symmetry properties, we have

$$\begin{aligned}|\langle 2^b 1^{a-b}\rangle W\rangle &= \sum_{W_2 W_1} \begin{pmatrix}\langle 1^b\rangle & \langle 1^a\rangle & | & \langle 2^b 1^{a-b}\rangle\\ W_2 & W_1 & | & W\end{pmatrix} \{|\langle 1^b\rangle W_2\rangle|\langle 1^a\rangle W_1\rangle\}_s\\ &= \sum_{W_1 W_2} (-1)^{[1^a]+[1^b]+[2^b 1^{a-b}]} \begin{pmatrix}\langle 1^a\rangle & \langle 1^b\rangle & | & \langle 2^b 1^{a-b}\rangle\\ W_1 & W_2 & | & W\end{pmatrix} \{|\langle 1^b\rangle W_2\rangle|\langle 1^a\rangle W_1\rangle\}_s.\end{aligned} \tag{22}$$

It follows that

$$(-1)^{[1^a]+[1^b]+[2^b1^{a-b}]}=1 \tag{23}$$

or

$$(-1)^{[2^b1^{a-b}]}=(-1)^{[1^a]+[1^b]} \tag{24}$$

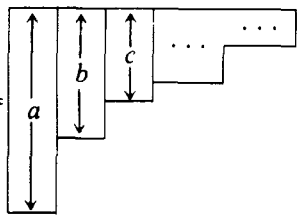
since

$$\langle\{\langle 1^a\rangle W_1,\langle 1^b\rangle W_2\}_s|\langle 2^b1^{a-b}\rangle W\rangle=\langle\{\langle 1^b\rangle W_2,\langle 1^a\rangle W_1\}_s|\langle 2^b1^{a-b}\rangle W\rangle. \tag{25}$$

Extending this result to general cases, the phase of any irrep of S_n and $U(N)$ is expressed as a product of the phases of its component k single-column irreps:

$$(-1)^{[\lambda]}=(-1)^{[1^a]+[1^b]+[1^c]+\cdots} \tag{26}$$

where $[\lambda]$ is schematically given by

$\langle\lambda\rangle =$ 

(27)

Let us examine the phase factor of a single-column irrep $[1^m]$ from the viewpoint of the I_o factors. We shall adopt the convention $(-1)^{[1]}=1$ and use one of the orthogonal relations (Zhang and Li 1987) of I_o factors which is

$$\sum_{\mu_1\mu_2} I_o\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]\\ [\mu_1] & [\mu_2] & | & [\mu]\end{pmatrix} I_o\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda']\\ [\mu_1] & [\mu_2] & | & [\mu]\end{pmatrix}=\delta_{[\lambda][\lambda']}. \tag{28}$$

Consider the reduction

$$[1^m]\times[1]=[2\,1^{m-1}]+[1^{m+1}]. \tag{29}$$

Using (28) we get

$$I_o\begin{pmatrix}[1^m] & [1] & | & [2\,1^{m-1}]\\ [1^m] & [0] & | & [1^m]\end{pmatrix} I_o\begin{pmatrix}[1^m] & [1] & | & [1^{m+1}]\\ [1^m] & [0] & | & [1^m]\end{pmatrix}$$
$$=-I_o\begin{pmatrix}[1^m] & [1] & | & [2\,1^{m-1}]\\ [1^{m-1}] & [1] & | & [1^m]\end{pmatrix} I_o\begin{pmatrix}[1^m] & [1] & | & [1^{m+1}]\\ [1^{m-1}] & [1] & | & [1^m]\end{pmatrix}. \tag{30}$$

Then

$$I_o\begin{pmatrix}[1^m] & [1] & | & [2\,1^{m-1}]\\ [1^m] & [0] & | & [1^m]\end{pmatrix} I_o\begin{pmatrix}[1^m] & [1] & | & [1^{m+1}]\\ [1^m] & [0] & | & [1^m]\end{pmatrix}$$
$$=-(-1)^{[2\,1^{m-1}]+[1^{m+1}]} I_o\begin{pmatrix}[1] & [1^m] & | & [2\,1^{m-1}]\\ [1] & [1^{m-1}] & | & [1^m]\end{pmatrix} I_o\begin{pmatrix}[1] & [1^m] & | & [1^{m+1}]\\ [1] & [1^{m-1}] & | & [1^m]\end{pmatrix}. \tag{31}$$

The absolute values on the right- and left-hand sides of (31) will cancel. In accordance with the extended Condon-Shortley convention (Zhang and Li 1987), the I_o factors on the LHS and the second I_o factor on the RHS of (31) are positive. Thus, (31) requires

$$-(-1)^{[2\,1^{m-1}]+[1^{m+1}]}\times \operatorname{sgn} I_o\begin{pmatrix}[1] & [1^{m-1}] \\ [1] & [1^{m-1}]\end{pmatrix}\begin{vmatrix}[2\,1^{m-1}] \\ [1^m]\end{vmatrix} = 1. \tag{32}$$

Using (23) in Zhang and Li (1987), we have

$$I_o\begin{pmatrix}[1] & [1^m] \\ [1] & [1^{m-1}]\end{pmatrix}\begin{vmatrix}[2\,1^{m-1}] \\ [1^m]\end{vmatrix} I_o\begin{pmatrix}[1] & [1^m] \\ [1] & [1^{m-1}]\end{pmatrix}\begin{vmatrix}[2\,1^{m-1}] \\ [2\,1^{m-2}]\end{vmatrix}$$
$$= -\frac{m}{(m^2-1)^{1/2}} I_o\begin{pmatrix}[1] & [1^{m-1}] \\ [1] & [1^{m-2}]\end{pmatrix}\begin{vmatrix}[1^m] \\ [1^{m-1}]\end{vmatrix} I_o\begin{pmatrix}[1] & [1^{m-1}] \\ [1] & [1^{m-2}]\end{pmatrix}\begin{vmatrix}[2\,1^{m-2}] \\ [1^{m-1}]\end{vmatrix}. \tag{33}$$

Therefore

$$\operatorname{sgn} I_o\begin{pmatrix}[1] & [1^m] \\ [1] & [1^{m-1}]\end{pmatrix}\begin{vmatrix}[2\,1^{m-1}] \\ [1^m]\end{vmatrix} = -\operatorname{sgn} I_o\begin{pmatrix}[1] & [1^{m-1}] \\ [1] & [1^{m-2}]\end{pmatrix}\begin{vmatrix}[2\,1^{m-2}] \\ [1^{m-1}]\end{vmatrix}. \tag{34}$$

Successively using (34), we have

$$\operatorname{sgn} I_o\begin{pmatrix}[1] & [1^m] \\ [1] & [1^{m-1}]\end{pmatrix}\begin{vmatrix}[2\,1^{m-1}] \\ [1^m]\end{vmatrix} = (-1)^{m-1} \operatorname{sgn} I_o\begin{pmatrix}[1] & [1] \\ [1] & 0\end{pmatrix}\begin{vmatrix}[2] \\ [1]\end{vmatrix} = (-1)^{m-1}. \tag{35}$$

Taking (35) into account, we get from (32)

$$(-1)^{[2\,1^{m-1}]+[1^{m+1}]} = (-1)^m. \tag{36}$$

Using (24), we obtain

$$(-1)^{[1^{m+1}]} = (-1)^{[1^m]+m} = (-1)^{[1^m]+(m+1)+1}. \tag{37}$$

We can also rewrite (37) as

$$(-1)^{[1^m]} = (-1)^{1+2+\ldots+m+m} = (-1)^{m(m-1)/2}. \tag{38}$$

Using (26) and (38), the phase factors of any irrep are now determined.

In concluding the discussion, we can easily express the phase factor by writing

$$(-1)^{[\lambda+1,r_{n+1}]} = (-1)^{[\lambda]+r_{n+1}+1}. \tag{39}$$

The rule given by Zhang and Li (1987), which relates the phase factor of the Young diagram $[\lambda+1,\ r_{n+1}]$ with that of diagram $[\lambda]$, if $[\lambda+1,\ r_{n+1}]$ is obtained by adding one box to the (r_{n+1})th row of $[\lambda]$. In terms of the shift notation used for U(N), it is

$$(-1)^{\{[\lambda]+[\Delta(\tau)]\}} = (-1)^{[\lambda]+\tau+1}. \tag{40}$$

4. Discussion

In principle, only the overall phase factor η can be uniquely determined by the group itself, while the choice of $(-1)^{[\lambda]}$ is not unique. The above rule can be considered as one possible solution among all possibilities. However, this rule is clearly reasonable due to its build-up structure. Based on Cartan's works, it was known (Biedenharn and Louck 1968) that there are two types of building blocks from which any irrep can be constructed. They are the fundamental irrep [1] and the elementary irreps $[1^k]$. The present rule ((26) and (39) respectively) reveals a distinct composite structure of the phase factors from these two kinds of building blocks.

With regard to phase factors described by other authors, it is found that in a recent book (Chen *et al* 1987) the phase factors (their ε_2 factors) are not separated into three parts, and phases which depends on three irreps are always required, even though without multiplicity. Moreover, there is not a general rule for the determination of the phases. Each of them must be examined individually and hence only the phases for groups S_2-S_6 are known. Even so, if one expresses their factors by

$$\varepsilon_2([\lambda_1],[\lambda_2],[\lambda]) = (-1)^{[\lambda_1]+[\lambda_2]+[\lambda]} \tag{41}$$

and uses the present rule, one can easily observe that table 5 of Chen *et al* (1987) satisfies the rule. It is also found that Hecht *et al* (1987) introduced (without proof) a phase convention $\phi([\lambda])_N$, which is similar but not equal to $(-1)^{[\lambda]}$. However, the overall phase is clearly identical, i.e.

$$(-1)^{\phi([\lambda_1])_N+\phi([\lambda_2])_N-\phi([\lambda])_N} = (-1)^{[\lambda_1]+[\lambda_2]+[\lambda]} \tag{42}$$

when considered in terms of Young diagrams. Different from $\phi([\lambda])_N$, the present phases are N independent. This is obviously a beneficial feature, since N can be fairly large in molecular electronic structure calculations (where N is the size of the basis set). These comparisons and relationships reveal the validity of the present phase factors.

Applications of the representation theory rely heavily on our ability to construct various kinds of coupling coefficients. However, the determination of suitable phases of CG coefficients is sometimes more difficult than that of their absolute values. In a recent paper (Gould 1986), for example, only the absolute values of CG coefficients for $U(N)$ are discussed and the author seems unable to fix the phases. The present rule of phases provides new insight into the structure of coupling coefficients for both S_n and $U(N)$ and will be beneficial for an efficient construction of coupling coefficients and their applications.

Finally, we emphasise that the representation theory of S_n and $U(N)$ for large n and N seems to be more useful in many-electron systems than in other areas of theoretical physics (except, of course, some smaller-N cases as SU(3), etc). The applications of the unitary group approach (UGA) to the many-electron correlation problem in the past decade have proven its versatility and efficiency. Recently, it has been possible to obtain highly accurate calculations of electronic structure for molecules in such a way that the exact molecular wavefunctions are expressed as linear combinations of several millions of Gelfand states (Saxe *et al* 1982). It is indeed unbelievable to carry out such large-scale computations without UGA. It is presently realised that the UGA is, in fact, an irreducible tensor method for $U(N)$ and the so-called segment values in the UGA are isoscalar factors. Detailed discussion of this topic is beyond the scope of the present paper. We intend to publish systematically a series of papers in the near future in which we will discuss how one can efficiently construct CG coefficients for $U(N)$ purely based on a symmetric group technique and how the Racah-Wigner tensor operator calculus for $U(N)$ for large N can be carried out for many-electron problems. In those developments, the rule of phases will play a non-trivial role.

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