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Coupling coefficient for the symmetric and unitary groups

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Abstract. Two recursion formulae are deduced for the construction of inner- and outer-product isoscalar factors, respectively, for the symmetric group, by which the corresponding coupling coefficients can be easily obtained. A formula for the evaluation of the isoscalar factor for the subgroup chain $U(N) \supset U(N-1)$ is proposed based on the relation between the outer-product coupling coefficient for the standard basis of the symmetric group and Clebsch-Gordan coefficient for the canonical basis of the unitary group. The calculation procedures are presented and the properties of those coefficients are investigated.

1. Introduction

The group theoretical techniques of the symmetric and unitary groups play a very important role in physics and quantum chemistry for describing the properties of many-particle systems. Wigner and Racah have emphasised that one of the major problems standing in the way of the application of group theory to physical and chemical topics is the construction of Clebsch-Gordan (CG) coefficients which reduce the direct product of irreducible representation matrices. CG coefficients for finite groups and compact Lie groups can be obtained by the projection operator method (Koster *et al* 1963, Schindler and Mirman 1977, 1978), diagonalisation of the representation matrix of certain operators such as the Dirac character (Bayman and Lande 1966, Chen *et al* 1985), Racah's infinitesimal operator (de Swart 1963, Haacke *et al* 1976) and the build-up principle for the isoscalar factor based on the recoupling relations (Wybourne 1974). The double coset analysis for the coefficients for the groups S_n and $U(N)$ was given by Sullivan (1973, 1975, 1978a, b, 1980).

At present, an extensive literature exists on the computation of CG coefficients based on these approaches. Recent progress has been made by Chen *et al* (1985), who introduced the EF method for the calculation of CG coefficients for the symmetric and unitary groups by solving linear eigenfunction equations of the so-called CSCO which are formally similar to the eigenfunction equations in quantum mechanics, or equivalently, by diagonalising the CSCO. Nevertheless, those methods have some serious drawbacks. The major one is that they can only provide tables of calculated CG coefficients rather than a direct computational formula from which CG coefficients for the related group can be conveniently evaluated, as one always desires such a formula for simplifying the numerical calculation programmes of quantum mechanics and chemistry.

The main point of the projection operator method, which is also frequently used for construction of CG coefficients, can be briefly described as follows. For some types

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of symmetry adapted bases $|\Gamma(\gamma)^A\rangle$ of group G, such as the standard Young-Yamanouchi basis of group S_n, we define a projection operator

$$\hat{\omega}^{\Gamma}_{(\gamma)^A,(\gamma')^A} = \frac{f_\Gamma}{g} \sum_R D^{\Gamma}_{(\gamma)^A,(\gamma')^A}(\hat{R})^* \hat{R}. \tag{1}$$

The basis $|\Gamma(\gamma)^A\rangle$ can be expanded by an orthonormal complete set $|c\rangle$

$$|\Gamma(\gamma)^A\rangle = \sum_c |c\rangle\langle c|\Gamma(\gamma)^A\rangle. \tag{2}$$

It is easy to prove that the symmetry coefficient in the above expansion is

$$\langle c|\Gamma(\gamma)^A\rangle = N\frac{f_\Gamma}{g}\sum_R \langle c|\hat{R}|c'\rangle\langle\Gamma(\gamma)^A|\hat{R}|\Gamma(\gamma')^A\rangle \tag{3}$$

and the normalisation factor is

$$N = [\langle\Gamma(\gamma')^A|c'\rangle]^{-1}. \tag{4}$$

This shows that when projection operators are exploited to calculate some symmetry coefficients, the normalisation factor is just another coefficient. If $|c\rangle$ is chosen as the direct product function of two states, we have

$$\langle\Gamma_1\Gamma_2\gamma_1\gamma_2|\Gamma\gamma\rangle = [\langle\Gamma\gamma'|\Gamma_1\Gamma_2\gamma_1'\gamma_2'\rangle]^{-1}\frac{f_\Gamma}{g}\sum_R \langle\Gamma_1\gamma_1|\hat{R}|\Gamma_1\gamma_1'\rangle\langle\Gamma_2\gamma_2|\hat{R}|\Gamma_2\gamma_2'\rangle\langle\Gamma\gamma|\hat{R}|\Gamma\gamma'\rangle$$

i.e. the symmetry coefficient is just a CG coefficient. Equation (3) can also be used to evaluate the transformation coefficients which relate different symmetry adapted bases. It seems that the application of the projection operator method requires a knowledge of the representation matrix of every group element and takes the summation over all the group elements, so that it is complex and tedious for a high-order group, especially for the symmetric group of large n.

It is evident that if the group summation can be greatly simplified and made easier to carry out, equation (3) provides a direct computation formula for CG and other symmetry coefficients. It has been shown (Li and Zhang 1986, Zhang and Li 1986) that the powerful double coset technique can be used to simplify greatly the required computation. The following sections describe the method for the construction of the various coupling coefficients for the symmetric and unitary groups using the double coset technique.

2. Inner-product coupling coefficient for the symmetric group

In handling some many-particle problems, one is interested in a coupled wavefunction of subspaces characterised by an irreducible representation of the symmetric group S_n, i.e. in the coupled function

$$|[\nu]t\rangle = \sum_{rs} ([\lambda][\mu]rs|[\nu]t)|[\lambda]r\rangle|[\mu]s\rangle \tag{5}$$

where the coefficients $([\lambda][\mu]rs|[\nu]t)$ are called the inner-product coupling coefficients (IPCC). Hamermesh (1962) developed a recursion equation for IPCC for S_n by introducing a so-called K coefficient, but the computation method is practically too complex and tedious to carry out. In the following we propose a new convenient recursion formula from which the IPCC can easily be calculated.

Define the V coefficient (3-j or 3-jm symbol) for S_n as follows:

$$V\begin{pmatrix}[\lambda] & [\mu] & [\nu]\\ r & s & t\end{pmatrix}=\frac{1}{\sqrt{f_{[\nu]}}}([\lambda][\mu]rs|[\nu]t) \tag{6}$$

where $f_{[\nu]}$ is the dimension of the representation $[\nu]$. Since $|[\lambda]r\rangle, [\mu]s\rangle, |[\nu]t\rangle$ are the standard basis vectors which are denoted by Young tableaux or Yamanouchi symbols and adapted to the subgroup chain $S_n \supset S_{n-1} \supset \ldots \supset S_1$, the V coefficient for S_n can be expressed by the product of the V coefficient for S_{n-1} and an isoscalar factor (also called the coupling factor, 3-jm factor or reduced coupling coefficient) for the subgroup chain $S_n \supset S_{n-1}$ (I_i coefficient for short):

$$V\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ r & s & t\end{pmatrix}=\sum_j I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ [\lambda-1, r_n] & [\mu-1, s_n] & [\nu-1, t_n]_j\end{pmatrix} \times V\begin{pmatrix}[\lambda-1, r_n] & [\mu-1, s_n] & [\nu-1, t_n]_j\\ r/r_n & s/s_n & t/t_n\end{pmatrix} \tag{7}$$

where i and j are the multiplicity indices. Then V coefficients can be obtained by successive products of the corresponding I_i coefficients. By using equation (3), we have

$$\sum_i V\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ r & s & t\end{pmatrix} V\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ u & v & w\end{pmatrix}=\frac{1}{n!}\sum_P D^{[\lambda]}_{ru}(\hat{P})D^{[\mu]}_{sv}(\hat{P})D^{[\nu]}_{tw}(\hat{P}). \tag{8}$$

In the double coset decomposition $S_{n-1}\backslash/S_{n-1}$ of S_n, there are two distinct double cosets which are represented by two double coset generators $\hat{e}$ (the identity element) and the transposition $(n-1, n)$ respectively. Considering the effects of the operation of group elements both to the left and the right of matrix elements in equation (8), we obtain a recursion formula of I_i coefficients:

$$\begin{aligned}\sum_i I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ [\lambda-1, r_n] & [\mu-1, s_n] & [\nu-1, t_n]_j\end{pmatrix} I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ [\lambda-1, u_n] & [\mu-1, v_n] & [\nu-1, w_n]_m\end{pmatrix}\\ =\frac{1}{n}\Bigg[\delta_{jm}\delta_{r_nu_n}\delta_{s_nv_n}\delta_{t_nw_n}+(n-1)\sum_{\substack{r_{n-1}s_{n-1}t_{n-1}p\\ u_{n-1}v_{n-1}w_{n-1}}}\sum\sum\\ \times I_i\begin{pmatrix}[\lambda-1, r_n] & [\mu-1, s_n] & [\nu-1, t_n]_j\\ [\lambda-2, r_nr_{n-1}] & [\mu-2, s_ns_{n-1}] & [\nu-2, t_nt_{n-1}]_p\end{pmatrix}\\ \times I_i\begin{pmatrix}[\lambda-1, u_n] & [\mu-1, v_n] & [\nu-1, w_n]_m\\ [\lambda-2, u_nu_{n-1}] & [\mu-2, v_nv_{n-1}] & [\nu-2, w_nw_{n-1}]_p\end{pmatrix}\\ \times D^{[\lambda]}_{r_nr_{n-1},u_nu_{n-1}}(n-1, n)D^{[\mu]}_{s_ns_{n-1},v_nv_{n-1}}(n-1, n)D^{[\nu]}_{t_nt_{n-1},w_nw_{n-1}}(n-1, n)\Bigg]\end{aligned} \tag{9}$$

where the labels i, j, m, p are the multiplicity indices which are required when the multiplicity in the reduction of the direct product of two representations is greater than one. $[\lambda-1, r_n]$ is the Young diagram of S_{n-1} which is deduced by detaching the square for the location of the index n from the Young diagram $[\lambda]$ of S_n. The Young diagrams of S_{n-2} in equation (9) must satisfy the following relations: $[\lambda-2, r_nr_{n-1}]=[\lambda-2, u_nu_{n-1}]$, $[\mu-2, s_ns_{n-1}]=[\mu-2, v_nv_{n-1}]$ and $[\nu-2, t_nt_{n-1}]=[\nu-2, w_nw_{n-1}]$. Due to the simple expression for the matrix elements of transposition $(n-1, n)$, the formally complicated equation (9) may result in a simple summation. The greater the difference between r_n and u_n, s_n and v_n, t_n and w_n, the simpler the summation on the right-hand side of equation (9).

The absolute value and the related phase factor of the I_i coefficients are fully determined by equation (9), but the overall phase factors depend on a different convention. In accordance with the extended Condon-Shortley convention for phase factors (Wybourne 1974), we take

$$I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]\\ [\lambda-1, r_n^m] & [\mu-1, s_n] & [\nu-1, t_n^m]\end{pmatrix} \geqslant 0 \tag{10}$$

where r^m and t^m are the highest-weight bases for $[\lambda]$ and $[\nu]$ respectively. The Young tableau of r^m is obtained by assigning n natural numbers successively into the Young diagram $[\lambda]$ in ascending order from left to right and from top to bottom (the natural order), and the corresponding Yamanouchi symbol $(r_n^m r_{n-1}^m \ldots r_1^m)$ of the tableau is called the greatest. Under this convention, the value and phase factor of the I_i coefficient with the form of (10) can be completely calculated, and then, taking this I_i coefficient as the normalisation factor in equation (3), the other I_i can be evaluated by (9). For example, we can calculate the I_i coefficients for $S_3 \supset S_2$ from the I_i coefficients for $S_2 \supset S_1$, e.g.

$$I_i\begin{pmatrix}[21] & [21] & [21]\\ [2] & [2] & [2]\end{pmatrix} I_i\begin{pmatrix}[21] & [21] & [21]\\ [2] & [1^2] & [1^2]\end{pmatrix}$$

$$= \tfrac{2}{3} I_i\begin{pmatrix}[2] & [2] & [2]\\ [1] & [1] & [1]\end{pmatrix} I_i\begin{pmatrix}[2] & [1^2] & [1^2]\\ [1] & [1] & [1]\end{pmatrix} D_{1,1}^{[21]}(2,3)[D_{1,2}^{[21]}(2,3)]^2 = -\tfrac{1}{4}$$

and obtain

$$I_i\begin{pmatrix}[21] & [21] & [21]\\ [2] & [2] & [2]\end{pmatrix} = \tfrac{1}{2} \qquad I_i\begin{pmatrix}[21] & [21] & [21]\\ [2] & [1^2] & [1^2]\end{pmatrix} = -\tfrac{1}{2}.$$

The I_i coefficients for groups S_3-S_6 have been calculated and tabulated by the above procedures and will be published elsewhere (Li and Zhang 1987).

The I_i coefficients have the following orthogonal properties:

$$\sum_{r_n s_n j} I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ [\lambda-1, r_n] & [\mu-1, s_n] & [\nu-1, t_n]_j\end{pmatrix} I_{i'}\begin{pmatrix}[\lambda] & [\mu] & [\nu']_{i'}\\ [\lambda-1, r_n] & [\mu-1, s_n] & [\nu-1, t_n]_j\end{pmatrix}$$

$$= \frac{f_{[\nu-1,t_n]}}{f_{[\nu]}} \delta_{ii'} \delta_{\nu\nu'} \tag{11}$$

$$\sum_{iv} \frac{f_{[\nu]}}{f_{[\nu-1,t_n]}} I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ [\lambda-1, r_n] & [\mu-1, s_n] & [\nu-1, t_n]_j\end{pmatrix}$$

$$\times I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ [\lambda-1, u_n] & [\mu-1, v_n] & [\nu-1, t_n]_{j'}\end{pmatrix}$$

$$= \delta_{jj'} \delta_{r_n u_n} \delta_{s_n v_n}. \tag{12}$$

The symmetry properties of I_i coefficients are an important problem for the symmetric group. In most cases, a permutation of the columns only causes a change in the phase of I_i and leaves its absolute value unchanged. Hamermesh (1962) has proved that when $[\lambda] \neq [\mu] \neq [\nu]$ this changed phase can be chosen to be positive or negative arbitrarily. But in the case of $[\lambda] = [\mu] \neq [\nu]$, the symmetry under odd permutations of the columns depends on whether the representation $[\nu]$ occurs in the space of a symmetric or antisymmetric square of $[\lambda]$. If we make the decomposition of the space of symmetric and antisymmetric squares of each representation and define the phase factor $(-1)^{[\nu]} = 1$ for those $[\nu] \subset [\lambda]^{[2]}$ and $(-1)^{[\nu]} = -1$ for those $[\nu] \subset [\lambda]^{[1^2]}$, then

the parity of every representation is given by a phase factor $(-1)^{[\lambda]}$ and the I_i coefficients transform as the basis of the representation [3] or $[1^3]$ under the S_3 permutation of three columns:

$$I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ [\lambda-1] & [\mu-1] & [\nu-1]_j\end{pmatrix}=(-1)^{[\lambda]+[\mu]+[\nu]+[\lambda-1]+[\mu-1]+[\nu-1]}\theta([\lambda][\mu][\nu])_i$$
$$\times\theta([\lambda-1][\mu-1][\nu-1])_j I_i\begin{pmatrix}[\mu] & [\lambda] & [\nu]_i\\ [\mu-1] & [\lambda-1] & [\nu-1]_j\end{pmatrix} \tag{13}$$

where the factor θ is introduced to distinguish the behaviour of those $[\nu]\subset[\lambda]^{[2]}(\theta=1)$ from those $[\nu]\subset[\lambda]^{[1^2]}(\theta=-1)$ when the multiplicity of the reduction $[\lambda]\times[\lambda]\to[\nu]$ is greater than one.

A rather different and interesting property emerges when $[\lambda]=[\mu]=[\nu]$. Derome (1966) has discussed that it is not always possible to choose the coefficient such that its absolute value is invariant under every permutation of the columns. In the following description, for the purpose of generalisation we use the symbol Γ to denote an irreducible representation of an arbitrary group. Since the transformation property of $V\binom{\Gamma\ \Gamma\ \Gamma_i}{\gamma_1\ \gamma_2\ \gamma_3}$ coefficients under a permutation of columns is identical with that of the tensor product function $\phi^{\Gamma}_{\gamma_1}\phi^{\Gamma}_{\gamma_2}\phi^{\Gamma}_{\gamma_3}$ under the corresponding permutation of basis states, the V coefficients may transform as the irreducible bases of S_3. After all the tensor product functions are divided into three subspaces $\Gamma^{[\eta]}$ with definite symmetry type [3], $[1^3]$ or [21] then, if and only if the subspace contains at least one identity representation A, the reduction coupling of the corresponding subspace is possible. Otherwise the V coefficients vanish identically.

Suppose that the multiplicity of the reduction of the direct product space $\Gamma\times\Gamma\to\Gamma$ equals f and the identity representation A occurs (f_1,f_2,f_3) times in the subspace $(\Gamma^{[3]},\Gamma^{[1^3]},\Gamma^{[21]})$, which can be determined by the characters of the corresponding space given as (Boyle 1972, Ford 1972)

$$\chi(\Gamma^{[\eta]};R)=\tfrac{1}{6}\sum_{\nu}K_\nu\chi^{[\eta]}(P_\nu)[\chi^{\Gamma}(R)]^{\nu_1}[\chi^{\Gamma}(R^2)]^{\nu_2}\ldots[\chi^{\Gamma}(R^n)]^{\nu_n}. \tag{14}$$

Then f groups of V coefficients have three kinds of symmetry properties; $(f_1,f_2,2f_3)$ groups of V coefficients have symmetry type ([3], $[1^3]$, [21]) under the permutations of the columns.

The first example of a V coefficient with symmetry type [21] (mixed symmetry) is the reduction coefficient of $[321]\times[321]\to 5[321]$ for S_6, where the numbers of totally symmetric representation [6] occurring in the space $[321]^{[3]}$, $[321]^{[1^3]}$ and $[321]^{[21]}$ are 2, 1 and 1. Therefore, there are two groups of V coefficients transforming as two bases of the representation [21]. Due to this symmetry property of V coefficients, the symmetry of I_i coefficients can be easily deduced and summarised as follows: I_i coefficients may transform as any one of the irreducible bases of S_3 under the permutations of the columns:

$$\hat{P}\left[I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ [\lambda-1] & [\mu-1] & [\nu-1]_m\end{pmatrix}^{[\eta]}_{[\rho]},\ I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_j\\ [\lambda-1] & [\mu-1] & [\nu-1]_n\end{pmatrix}^{[\eta]}_{[\rho]}\right]$$
$$=\left[I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ [\lambda-1] & [\mu-1] & [\nu-1]_m\end{pmatrix}^{[\eta]}_{[\rho]},\right.$$
$$\left.I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_j\\ [\lambda-1] & [\mu-1] & [\nu-1]_n\end{pmatrix}^{[\eta]}_{[\rho]}\right]D^{[\eta]}(\hat{P})D^{[\rho]}(\hat{P}) \tag{15}$$

where $[\eta]$ and $[\rho]$ can be any one of the representations [3], [1³], [21] of S_3, and $D^{[\eta]}$ and $D^{[\rho]}$ are the related representation matrices.

For example,

$$\left[I_i\begin{pmatrix}[321] & [321] & [321]_4\\ [32] & [32] & [31^2]\end{pmatrix}, I_i\begin{pmatrix}[321] & [321] & [321]_5\\ [32] & [32] & [31^2]\end{pmatrix}\right] = [0, -\tfrac{1}{8}\sqrt{5}]$$

where 4 and 5 are the multiplicity indices. Then, from equation (15), if we take $\hat{P}$ as a transposition (2, 3) of the second and third columns, we have

$$\begin{aligned}(2,3)&\left[I_i\begin{pmatrix}[321] & [321] & [321]_4\\ [32] & [32] & [31^2]\end{pmatrix}, I_i\begin{pmatrix}[321] & [321] & [321]_5\\ [32] & [32] & [31^2]\end{pmatrix}\right]\\ &= \left[I_i\begin{pmatrix}[321] & [321] & [321]_4\\ [32] & [31^2] & [32]\end{pmatrix}, I_i\begin{pmatrix}[321] & [321] & [321]_5\\ [32] & [31^2] & [32]\end{pmatrix}\right]\\ &= [0, -\tfrac{1}{8}\sqrt{5}]\begin{bmatrix}\frac{1}{2} & -\frac{1}{2}\sqrt{3}\\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2}\end{bmatrix} = [\tfrac{1}{16}\sqrt{15}, \tfrac{1}{16}\sqrt{5}]\end{aligned}$$

where the I_i coefficients and phase factors are determined by the above procedures and taken from our other paper (Li and Zhang 1987).

Using the relation between the matrix elements of $[\lambda]$ and its conjugate $[\tilde{\lambda}]$, we have

$$\begin{aligned}&I_i\begin{pmatrix}[\tilde{\lambda}] & [\mu] & [\tilde{\nu}]_i\\ [\tilde{\lambda}-1, \tilde{r}_n] & [\mu-1, s_n] & [\tilde{\nu}-1, \tilde{t}_n]_j\end{pmatrix}\\ &\quad = \xi I_i\begin{pmatrix}[\lambda] & [\mu] & [\nu]_i\\ [\lambda-1, r_n] & [\mu-1, s_n] & [\nu-1, t_n]_j\end{pmatrix}\end{aligned} \tag{16}$$

where the phase factor $\xi = \pm 1$ depends on the conventions of the phase factor of I_i coefficients for S_n and S_{n-1}. Butler and Ford (1979) have discussed the conjugate symmetry and pointed out that both symmetry relations (13) and (16) hold simultaneously. We note when the permutation symmetry is the mixed symmetry [21], both symmetries (15) and (16) hold simultaneously unless both $[\lambda]$ and $[\nu]$ are self-conjugate representations.

3. Outer-product coupling coefficient for the symmetric group

Suppose $|[\lambda_1]r^1\rangle$ and $|[\lambda_2]r^2\rangle$ are the standard bases for S_{n_1} and S_{n_2}. We can use the so-called outer-product coupling coefficients (OPCC) to couple these bases to the standard bases for S_n $(n = n_1 + n_2)$:

$$|[\lambda]r\rangle = \sum_{r^1\omega^1}\sum_{r^2\omega^2} V\left(\begin{matrix}[\lambda_1] & [\lambda_2]\\ r^1\omega^1 & r^2\omega^2\end{matrix}\middle|\begin{matrix}[\lambda]\\ r\end{matrix}\right)|[\lambda_1]r^1\omega^1\rangle|[\lambda_2]r^2\omega^2\rangle \tag{17}$$

where $[\lambda]$ is contained in the decomposition of the outer direct product $[\lambda_1]\otimes[\lambda_2]$ given by the Littlewood rule, and $\omega^1 = \{i_1 < i_2 < \ldots < i_{n_1}\}$ and $\omega^2 = \{j_1 < j_2 < \ldots < j_{n_2}\}$ are the sets of particle indices which are selected from $\{1, 2, \ldots, n\}$. The function $|[\lambda_1]r^1\omega^1\rangle(|[\lambda_2]r^2\omega^2\rangle$ similarly) is the standard basis of $S_{n_1}(\omega^1)$, i.e. the group of permutations which operate on the n_1 objects labelled by $(i_1, i_2, \ldots, i_{n_1})$. This basis

is adapted to the subgroup chain

$$S_{n_1}(i_1 i_2, \ldots, i_{n_1-1} i_{n_1}) \supset S_{n_1-1}(i_1 i_2, \ldots, i_{n_1-1}) \supset \ldots \supset S_1(i_1) \tag{18}$$

and obtained by index replacement from the standard basis $|[\lambda_1] r^1 \omega_0^1\rangle$ of $S_{n_1}(\omega_0^1) = S_n$:

$$|[\lambda_1] r^1 \omega^1\rangle = \begin{pmatrix} 1 & 2 \ldots n_1 \\ i_1 & i_2 \ldots i_{n_1} \end{pmatrix} |[\lambda_1] r^1 \omega_0^1\rangle. \tag{19}$$

As an example, the standard basis $|[21]2\rangle$ of $S_3(2, 3, 5)$ is denoted by the tableau $\begin{array}{|c|c|}\hline 2 & 5 \\ \hline 3 \\ \cline{1-1}\end{array}$. By using the well known Racah (1965) factorisation lemma, the OPCC can be expressed as the product of an $S_n \supset S_{n-1} \otimes S_1$ outer-product isoscalar factor (I_0 coefficient for short) and the coefficient for S_{n-1}, i.e.

$$V\begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ r^1\omega^1 & r^2\omega^2 & | & r \end{pmatrix} = I_0\begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ [\lambda_1 - 1, r_n] & [\lambda_2] & | & [\lambda - 1, r_n] \end{pmatrix}$$
$$\times V\begin{pmatrix} [\lambda_1 - 1, r_n] & [\lambda_2] & | & [\lambda - 1, r_n] \\ r^1/r_n^1(\omega^1/n) & r^2\omega^2 & | & r/r_n \end{pmatrix} \tag{20}$$

when the index n is contained in the set of ω^1, where r/r_n denotes the Young tableau obtained by removing the square for index n from the Young tableau $|[\lambda]r\rangle$. On the other hand, when the index n is in the ω^2, we have

$$V\begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ r^1\omega^1 & r^2\omega^2 & | & r \end{pmatrix} = I_0\begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ [\lambda_1] & [\lambda_2 - 1, r_n^2] & | & [\lambda - 1, r_n] \end{pmatrix}$$
$$\times V\begin{pmatrix} [\lambda_1] & [\lambda_2 - 1, r_n^2] & | & [\lambda - 1, r_n] \\ r^1\omega^1 & r^2/r_n^2(\omega^2/n) & | & r/r_n \end{pmatrix}. \tag{21}$$

For example, we have

$$V\left(\begin{array}{|c|c|}\hline 2 & 5 \\ \hline 3 \\ \cline{1-1}\end{array}\ \begin{array}{|c|}\hline 1 \\ \hline 4 \\ \cline{1-1}\end{array}\ \middle|\ \begin{array}{|c|c|c|}\hline 1 & 2 & 5 \\ \hline 3 & 4 \\ \cline{1-2}\end{array}\right) = I_0\begin{pmatrix} [21] & [1^2] & | & [32] \\ [1^2] & [1^2] & | & [2^2] \end{pmatrix} V\left(\begin{array}{|c|}\hline 2 \\ \hline 3 \\ \cline{1-1}\end{array}\ \begin{array}{|c|}\hline 1 \\ \hline 4 \\ \cline{1-1}\end{array}\ \middle|\ \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \cline{1-2}\end{array}\right).$$

Then any OPCC can be obtained by successive products of the corresponding I_0 coefficients.

Now we seek an equation with which the double coset technique can be used. From equation (3), take $\omega^1 = \omega_0^1 = \{1, 2, \ldots, n_1\}$, $\omega^2 = \omega_0^2 = \{n_1 + 1, n_1 + 2, \ldots, n\}$, we have

$$V\begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ r^1\omega_0^1 & r^2\omega_0^2 & | & r^1\rho^2 \end{pmatrix} V\begin{pmatrix} [\lambda_1] & [\lambda_2] & | & [\lambda] \\ t^1\omega_0^1 & t^2\omega_0^2 & | & t^1\eta^2 \end{pmatrix}$$
$$= \frac{n_1! f_{[\lambda]}}{n! f_{[\lambda_1]}} \sum_{\hat{P}_2} \langle [\lambda_2] t^2 | \hat{P}_2 | [\lambda_2] r^2 \rangle \langle [\lambda] r^1 \eta^2 | \hat{P}_2 | [\lambda] r^1 \rho^2 \rangle \tag{22}$$

where $|[\lambda]r^1\rho^2\rangle$ is the standard basis for S_n. The symbol r^1 shows that the partial Young tableau of $|[\lambda]r^1\rho^2\rangle$, which is occupied by particles $\{1, 2, \ldots, n_1\}$, is identical with the Young tableau $|[\lambda_1]r^1\rangle$ for S_{n_1}. But the remaining part of the tableau occupied by particles $\{n_1 + 1, n_1 + 2, \ldots, n\}$, which is usually not a possible standard tableau, is denoted by ρ^2. By using a double coset decomposition of S_{n_2} with respect to

$S_{n_2-1}\backslash/S_{n_2-1}$, a recursion formula for the I_0 coefficients which is formally similar to that for I_i may be obtained:

$$\sum_i I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]_i\\ [\lambda_1] & [\lambda_2-1, r_n^2] & | & [\lambda-1, \rho_n^2]_j\end{pmatrix} I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]_i\\ [\lambda_1] & [\lambda_2-1, t_n^2] & | & [\lambda-1, \eta_n^2]_m\end{pmatrix}$$
$$= \frac{f_{[\lambda]}}{nf_{[\lambda-1,\rho_n^2]}}\delta_{r_n^2 t_n^2}\delta_{\rho_n^2\eta_n^2}\delta_{jm} + \frac{(n-1)f_{[\lambda]}}{nf_{[\lambda-1,\rho_n^2]}f_{[\lambda-1,\eta_n^2]}}\sum_{\tilde{r}_{n-1}^2}\sum_{\tilde{t}_{n-1}^2}\sum_{\rho_{n-1}^2}\sum_{\eta_{n-1}^2}\sum_p f_{[\lambda-2,\rho_n^2\rho_{n-1}^2]}$$
$$\times I_0\begin{pmatrix}[\lambda_1] & [\lambda_2-1, r_n^2] & | & [\lambda-1, \rho_n^2]_j\\ [\lambda_1] & [\lambda_2-2, r_n^2 r_{n-1}^2] & | & [\lambda-2, \rho_n^2\rho_{n-1}^2]_p\end{pmatrix}$$
$$\times I_0\begin{pmatrix}[\lambda_1] & [\lambda_2-1, t_n^2] & | & [\lambda-1, \eta_n^2]_m\\ [\lambda_1] & [\lambda_2-2, t_n^2 t_{n-1}^2] & | & [\lambda-2, \eta_n^2\eta_{n-1}^2]_p\end{pmatrix}$$
$$\times\langle[\lambda_2]r_n^2 r_{n-1}^2|(n-1,n)|[\lambda_2]t_n^2 t_{n-1}^2\rangle$$
$$\times\langle[\lambda]\rho_n^2\rho_{n-1}^2|(n-1,n)|[\lambda]\eta_n^2\eta_{n-1}^2\rangle. \tag{23}$$

The properties of I_0 are briefly discussed here. I_0 coefficients satisfy the following orthogonal relations:

$$\sum_{\mu_1\mu_2 j} I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]_i\\ [\mu_1] & [\mu_2] & | & [\mu]_j\end{pmatrix} I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda']_{i'}\\ [\mu_1] & [\mu_2] & | & [\mu]_j\end{pmatrix} = \delta_{ii'}\delta_{[\lambda][\lambda']} \tag{24}$$

$$\sum_{\lambda i} I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]_i\\ [\mu_1] & [\mu_2] & | & [\mu]_n\end{pmatrix} I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]_i\\ [\nu_1] & [\nu_2] & | & [\mu]_m\end{pmatrix} = \delta_{nm}\delta_{[\mu_1][\nu_1]}\delta_{[\mu_2][\nu_2]}. \tag{25}$$

These relations are valid not only for the one-particle I_0, but also for many-particle I_0 which is the product of several one-particle I_0. The absolute value of I_0 remains unchanged under the permutation of the first two columns. The symmetry relation is formally similar to equation (13), but the phase factors $(-1)^{[\lambda]}$ and θ are different. The I_0 coefficients of mutual conjugate representations have the relation, similar to equation (16),

$$I_0\begin{pmatrix}[\tilde{\lambda}_1] & [\tilde{\lambda}_2] & | & [\tilde{\lambda}]_i\\ [\tilde{\lambda}_1] & [\tilde{\lambda}_2-1, \tilde{r}_n^2] & | & [\tilde{\lambda}-1, \tilde{\rho}_n^2]_j\end{pmatrix}$$
$$= \xi I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]_i\\ [\lambda_1] & [\lambda_2-1, \tilde{r}_n^2] & | & [\lambda-1, \tilde{\rho}_n^2]_j\end{pmatrix}. \tag{26}$$

Equation (23) is convenient and powerful for the evaluation of I_0 coefficients. In fact, it is even easier than the evaluation of I_i. The tabulation of I_0 is achieved by the following steps.

(i) We first calculate the I_0 for the reduction of the outer product $S_{n-1}\otimes S_1$, which are given as

$$I_0\begin{pmatrix}[\lambda_1] & [1] & | & [\lambda]\\ [\lambda_1] & [0] & | & [\lambda_1]\end{pmatrix} = f_{[\lambda]}/nf_{[\lambda_1]} \tag{27}$$

and the I_0 for $S_{n-2}\otimes S_2$ are given as

$$I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]\\ [\lambda_1] & [1] & | & [\lambda-1, \rho_n^2]\end{pmatrix} = [(\tau+\delta_{[\lambda_2]})f_{[\lambda]}/n\tau f_{[\lambda-1,\rho_n^2]}]^{1/2} \tag{28}$$

$$I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] & | & [\lambda]\\ [\lambda_1] & [1] & | & [\lambda-1, \eta_n^2]\end{pmatrix} = \delta_{[\lambda_2]}[(\tau-\delta_{[\lambda_2]})f_{[\lambda]}/n\tau f_{[\lambda-1,\eta_n^2]}]^{1/2} \tag{29}$$

where $[\lambda]$ is the representation of S_n obtained by adding two squares to the Young diagram $[\lambda_1]$ of S_{n-2}, τ is the hook length from the square η_n^2 to the square ρ_n^2 which are the two new added squares and two possible locations for filling the index n, but the length index is defined as $\rho_n^2 \geqslant \eta_n^2$. $\delta_{[\lambda_2]} = 1$ or -1 for $[\lambda_2] = [2]$ or $[1^2]$.

(ii) Next we calculate the I_0 coefficients for the outer product $S_{n_1} \otimes S_{n_2}$ $(n_2 = 3, 4, \ldots)$ by equation (23) from the known I_0 coefficients and the extended Condon-Shortley convention

$$I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] \\ [\lambda_1] & [\lambda_2 - 1]\end{pmatrix}\begin{vmatrix}[\lambda] \\ [\lambda - 1, (\rho_n^2)^m]\end{vmatrix} \geqslant 0. \tag{30}$$

This convention determines the choice of phase of the normalisation factor (see equation (4)) of I_0.

(iii) By the above procedures we obtain all the I_0 coefficients with the form of

$$I_0\begin{pmatrix}[\lambda_1] & [\lambda_2] \\ [\lambda_1] & [\lambda_2 - 1]\end{pmatrix}\begin{vmatrix}[\lambda] \\ [\lambda - 1]\end{pmatrix} \qquad I_0\begin{pmatrix}[\lambda_2] & [\lambda_1] \\ [\lambda_2] & [\lambda_1 - 1]\end{pmatrix}\begin{vmatrix}[\lambda] \\ [\lambda - 1]\end{pmatrix}.$$

When the phase factors $(-1)^{[\lambda]}$ have been evaluated, the tabulation of I_0 is completed. We use the orthogonal relation (24) and take $(-1)^{[n]} = 1$ for the determination of the phase factors $(-1)^{[\lambda]}$.

It is interesting that the evaluated phase factors $(-1)^{[\lambda]}$ satisfy the following rule. If the phase factor $(-1)^{[\lambda]}$ of some representation of S_n is known, the phase factor $(-1)^{[\lambda+1, r_{n+1}]}$ of the representation $[\lambda + 1, r_{n+1}]$, which is obtained by adding one square to the r_{n+1}th row of $[\lambda]$, is given by

$$(-1)^{[\lambda+1, r_{n+1}]} = (-1)^{[\lambda] + r_{n+1} + 1}. \tag{31}$$

By using this rule the phase factor $(-1)^{[\lambda]}$ can be given by

$$(-1)^{[\lambda]} = (-1)^{r_1 + r_2 + \ldots + r_n + n} = (-1)^{\sum_r (r-1)\lambda_r}. \tag{32}$$

The I_0 coefficients of S_3–S_6 are calculated and tabulated, which will be reported elsewhere.

4. CG coefficient for the unitary group

Based on the duality between the symmetric and unitary groups, it was shown that the irreducible basis for $U(N)$ can be achieved by the projection operator of the symmetric group. Weyl (1946) used an idempotent Young operator to construct his Weyl basis. The canonical basis for the unitary group is the so-called Gelfand basis which is adapted to the subgroup chain $U(N) \supset U(N-1) \supset \ldots \supset U(1)$ and denoted by the Gelfand symbol $|\langle\lambda\rangle m\rangle$ or Weyl tableau $|\langle\lambda\rangle U\rangle$.

CG coefficients for the unitary group discussed in this paper are defined as the coupling of the Gelfand bases

$$|\langle\nu\rangle W\rangle = \sum_{UV} V\begin{pmatrix}\langle\lambda\rangle & \langle\mu\rangle \\ U & V\end{pmatrix}\begin{vmatrix}\langle\nu\rangle \\ W\end{pmatrix}|\langle\lambda\rangle U\rangle|\langle\mu\rangle V\rangle. \tag{33}$$

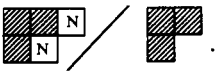
Many authors (Kaplan 1974, Lezuo 1972, Patterson and Harter 1976a, b, Sarma and Sahasrabudhe 1980, Dinesha *et al* 1981) have shown that the construction of the Gelfand basis can be carried out by using the standard projection operators of the symmetric group. It was proved (Chen *et al* 1977) that the quasistandard basis of

the state permutation groups is identical with the Gelfand basis of the unitary group. Then it was shown (Chen *et al* 1978, 1984a, b) that the outer-product coupling coefficient is the coupling coefficient for the $U(m+n) \supset U(m) \times U(n)$ irreducible bases and the CG coefficient for the Gelfand basis of $SU(n)$. Since CG coefficients can be expressed by successive products of the isoscalar factors of the unitary group (I_u for short) due to the Racah factorisation lemma, we only need the formula for I_u and its relation to I_0 coefficients for the state permutation groups. The I_0 for the state permutation groups are numerically identical with I_0 for the particle permutation groups, but the particle indices are replaced by the state indices.

The canonical bases for $U(N)$ are generated by using the standard projection operator $\hat{\omega}_{rt}^{[\lambda]}$ to the primitive function

$$\hat{\omega}_{rt}^{[\lambda]} = \frac{f_{[\lambda]}}{n!} \sum_{\hat{P}} D_{rt}^{[\lambda]}(\hat{P}) \hat{P} \tag{34}$$

where $D_{rt}^{[\lambda]}(\hat{P})$ is a standard Young-Yamanouchi representation matrix element and $\hat{P}$ is the permutation operating on a state index. The I_u coefficient is independent of the Weyl tableau of $U(N-1)$, i.e. the shaded part of the Weyl tableau

$I_u(U(N) \supset U(N-1)) =$ 

Then we can choose the primitive function so that the state ϕ_N can appear several times but the other states appear only once. When the state ϕ_N appears f times, the canonical basis $|\langle\lambda\rangle W\rangle$ is expressed by

$$\begin{aligned} |\langle\lambda\rangle W\rangle &= \frac{f_{[\lambda]}}{n!} \sum_{\hat{P}} D_{rt}^{[\lambda]}(\hat{P}) \hat{P}[\phi_1(1) \ldots \phi_N(n-f+1)\phi_N(n-f+2) \ldots \phi_N(n)] \\ &= [N([\nu]\xi^2)]^{-1} |[\nu] t^1 \xi^2\rangle \end{aligned} \tag{35}$$

where

$$N([\nu]\xi^2) = \left(\frac{f_{[\nu_1]} n!}{f_{[\nu]} g!}\right)^{1/2} I_0\begin{pmatrix} [\nu_1] & [f] \\ [\nu_1] & [0] \end{pmatrix} \begin{matrix} [\nu] \\ [\nu - f, \xi^2] \end{matrix}. \tag{36}$$

$|[\nu] t^1 \xi^2\rangle$ is the standard basis for the state permutation group, in which the state ϕ_N appears f times in the partial part ξ^2 of the tableau. Then we obtain the following formula for the calculation of I_u by I_0 coefficients of the symmetric group:

$$\begin{aligned} I_u\begin{pmatrix} \langle\lambda\rangle & \langle\mu\rangle \\ \langle\lambda_1\rangle & \langle\mu_1\rangle \end{pmatrix} \begin{matrix} \langle\nu\rangle \\ \langle\nu_1\rangle \end{matrix} &= \left[\frac{f_{[\nu]} f_{[\lambda_1]} f_{[\mu_1]} n_1! n_2! g!}{f_{[\lambda]} f_{[\mu]} f_{[\nu_1]} n! g_1! g_2!}\right]^{1/2} I_0\begin{pmatrix} [\nu_1] & [f] \\ [\nu_1] & [0] \end{pmatrix} \begin{matrix} [\nu] \\ [\nu - f, \xi^2] \end{matrix}^{-1} \\ &\times \sum_{\rho^2(\omega^1)} \sum_{\eta^2(\omega^2)} I_0\begin{pmatrix} [\lambda_1] & [f_1] \\ [\lambda_1] & [0] \end{pmatrix} \begin{matrix} [\lambda] \\ [\lambda - f_1, \rho^2(\omega^1)] \end{matrix} \\ &\times I_0\begin{pmatrix} [\mu_1] & [f_2] \\ [\mu_1] & [0] \end{pmatrix} \begin{matrix} [\mu] \\ [\mu - f_2, \eta^2(\omega^2)] \end{matrix} \\ &\times I_0\begin{pmatrix} [\lambda] & [\mu] \\ [\lambda - f_1, \rho^2(\omega^1)] & [\mu - f_2, \eta^2(\omega^2)] \end{pmatrix} \begin{matrix} [\nu] \\ [\nu - f, \xi^2] \end{matrix}. \end{aligned} \tag{37}$$

The meaning of each symbol is as follows. $(|[\lambda]r^1\rho^2\rangle, |[\mu]s^1\eta^2\rangle, |[\nu]t^1\xi^2\rangle)$ are the Young tableaux for the groups (S_{n_1}, S_{n_2}, S_n). $I_0\left(\begin{smallmatrix}[\lambda] & [\mu] \\ [\lambda_1] & [\mu_1]\end{smallmatrix}\middle|[\nu]_{[\nu_1]}\right)$ is f-state I_0 coefficient, which is equal to the product of f one-state I_0 coefficients, for example

$$I_0\left(\begin{array}{|c|c|}\hline 6 & 5 \\ \hline 4 \\ \cline{1-1} \end{array}\middle|\begin{array}{|c|c|}\hline 4 \\ \hline 5 \\ \hline 6 \\ \cline{1-1} \end{array}\right) = I_0\begin{pmatrix}[21] & [21] \\ [2] & [21]\end{pmatrix}\middle|\begin{matrix}[321] \\ [32]\end{matrix}\Bigg) I_0\begin{pmatrix}[2] & [21] \\ [2] & [1^2]\end{pmatrix}\middle|\begin{matrix}[32] \\ [31]\end{matrix}\Bigg)$$

$$\times I_0\begin{pmatrix}[2] & [1^2] \\ [2] & [1]\end{pmatrix}\middle|\begin{matrix}[31] \\ [21]\end{matrix}\Bigg).$$

$([\lambda_1], [\mu_1], [\nu_1])$ are the representations for the groups (S_{g_1}, S_{g_2}, S_g) and obtained by detaching (f_1, f_2, f) squares from the Young diagrams $([\lambda], [\mu], [\nu])$ in the order from the greater to smaller state index which is denoted by $(\rho^2(\omega^1), \eta^2(\omega^2), \xi^2)$, where $g_1 = n_1 - f_1$, $g_2 = n_2 - f_2$, $g = n - f$, ω^1 is the set of f_1 indices selected from n, $n-1, \ldots, n-f+1$ and ω^2 is the set of remaining indices.

The orthogonal relations and symmetry properties of I_u are formally similar to those of I_0. Another property of I_u, which should be pointed out, is that I_u coefficients calculated by equation (37) are independent of the rank of the unitary group and are available for arbitrary N.

A simple example is illustrated here. We calculate a I_u coefficient where the state ϕ_N is doubly occupied. By (27)-(29) and (37), we have

$$I_u\begin{pmatrix}\langle 21\rangle & \langle 2\rangle \\ \langle 1^2\rangle & \langle 1\rangle\end{pmatrix}\middle|\begin{matrix}\langle 2^21\rangle \\ \langle 21\rangle\end{matrix}\Bigg) = \sqrt{\tfrac{2}{3}}\Bigg[I_0\begin{pmatrix}[21] & [2] \\ [21] & [1]\end{pmatrix}\middle|\begin{matrix}[2^21] \\ [21^2]\end{matrix}\Bigg) I_0\begin{pmatrix}[21] & [1] \\ [1^2] & [1]\end{pmatrix}\middle|\begin{matrix}[21^2] \\ [21]\end{matrix}\Bigg)$$

$$+ I_0\begin{pmatrix}[21] & [2] \\ [1^2] & [2]\end{pmatrix}\middle|\begin{matrix}[2^21] \\ [21^2]\end{matrix}\Bigg) I_0\begin{pmatrix}[1^2] & [2] \\ [1^2] & [1]\end{pmatrix}\middle|\begin{matrix}[21^2] \\ [21]\end{matrix}\Bigg)\Bigg]$$

$$= \sqrt{\tfrac{2}{3}}[\tfrac{1}{2}\sqrt{2}(-\tfrac{1}{4}) + (-\tfrac{1}{2}\sqrt{2})\tfrac{1}{2}] = -\tfrac{1}{4}\sqrt{3}.$$

5. Conclusion

The present discussion on the inner-product coupling coefficient (IPCC) largely based on Hamermesh's K coefficient (the isoscalar factor). One notes that the idea of the K coefficient is rather powerful, but the computation method provided by Hamermesh needs algebra equations to be solved which is a tedious procedure, as pointed out by Hamermesh himself. We introduced the double coset technique to improve the computation method and gave a recursion formula for the isoscalar factor. Although this formula is formally complicated by notation, the practical calculation is very simple and easy.

Many authors have paid great attention to the importance of IPCC, and a number of contributions have been presented on the subject. However, people do not pay enough attention to the outer-product coupling coefficient (OPCC) for S_n. By virtue of the duality between the outer-product reduction of S_n and the Kronecker product reduction of $U(N)$, the OPCC may play an important role in group representation theory. On the other hand, the OPCC are used extensively in physics and chemistry.

In the present paper, we have discussed how to exploit the DC technique to deduce a direct computation formula for I_0 coefficients, and then we calculated the OPCC. By the duality of the basis of S_n and $U(N)$, the isoscalar factor for $U(N) \supset U(N-1)$ is related to I_0 coefficients.

We have outlined some of our major results on the coupling coefficients for S_n and $U(N)$. The present method has been used to make practical calculations for S_n and $U(N)$. Some distinct formulae for the coupling of many-electron Gelfand bases were found. Based on our results, we obtain a new formulation for the matrix element of a spin-dependent operator. This and other aspects of our work will be developed in other work, to appear subsequently.

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