INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, VOL. XXV, 603–633 (1984)

Unitary Group Approach to the Many-Electron Problem. II. Adjoint Tensor Operators for $U(n)$

M. D. GOULD AND G. S. CHANDLER
School of Chemistry, University of Western Australia, Nedlands 6009, Western Australia

Abstract

In this paper we present a derivation of the $U(n)$ adjoint coupling coefficients for the representations appropriate to many-electron systems. Since the states of a many-fermion system are to comprise the totally antisymmetric Nth rank tensor representation of $U(2n)$, the work of this paper enables the matrix elements of the $U(2n)$ generators to be evaluated directly in the $U(n)\times U(2)$ (i.e., spin orbit) basis using their transformation properties as adjoint tensor operators. A connection between the adjoint coupling coefficients, as derived in this paper, and the matrix elements of certain (spin independent) two-body operators is also presented. This indicates that in CI calculations, one may obtain the matrix elements of spin-dependent operators from the known matrix elements of certain spin-independent two-body operators. In particular this implies a segment-level formula for the matrix elements of the $U(2n)$ generators in the spin-orbit basis.

1. Introduction

This paper is the second in a series of three directed toward an evaluation of the matrix elements of spin-dependent Hamiltonians, for many-electron systems, directly in the spin-orbit basis. In the previous paper of the series [1] (herein referred to as I) an explicit segment-level formula was obtained for the matrix elements of the group generators in the electronic Gel'fand basis. In the present paper we apply the results in I to obtain an explicit expression for the $U(n)$ adjoint coupling coefficients corresponding to the reduction of the tensor product representation $[\mathrm{Adj}]\otimes[a, b, c]$ where $[\mathrm{Adj}]$ denotes the adjoint representation of $U(n)$ and $[a, b, c]$ denotes the representation of $U(n)$ corresponding to the orbital part of an $N=(2a+b)$ electron state with total spin $S=b/2$ (and where c is given by $a+b+c=n$). Adjoint tensor operators for $U(n)$ have been discussed previously, in the general case, by Louck and Biedenharn [2].

As mentioned in I, our motivation for considering adjoint tensor operators of $U(n)$ is that the $U(2n)$ generators transform as the representation $[\mathrm{Adj}]\otimes[\mathrm{Adj}]$ of the subgroup $U(n)\times U(2)$. Now recall that the states of a many-fermion system are to comprise the totally antisymmetric Nth-rank tensor representation of $U(2n)$ (i.e., the Slater determinants) and that states of well-defined M_L, M_S and total spin S may be constructed by considering a basis symmetry adapted to the subgroup $U(n)\times U(2)$ (spin orbit). Thus we may obtain the matrix elements of the $U(2n)$ generators (and hence the matrix elements of spin-dependent Hamiltonians) directly in the spin-orbit basis using their transformation properties as adjoint tensor operators. Hence it is necessary to obtain explicit expressions for the adjoint coupling coefficients.

 CCC 0020-7608/84/030603-31$04.00

It is the aim of this paper to obtain the $U(n)$ adjoint coupling coefficients for the representations appropriate to many-electron systems. Our results are presented in terms of group generator matrix elements and hence may be evaluated using the results of I. From the viewpoint of computational applications, we note that the group generator matrix elements need to be evaluated in CI calculations anyway and it is felt that the adjoint coefficients of this paper may be calculated without too much extra computational labor. In fact, it turns out that there is a close connection between the adjoint coefficients derived in this paper and the matrix elements of two-body operators. It is shown (using two methods) in the final section of this paper that the general $U(n)$ adjoint coefficients may be obtained directly from the matrix elements of certain two-body operators and these are already known (see, e.g., Paldus and Boyle [3, 4], Drake and Schlesinger [5] and Kent and Schlesinger [6]).

We remark, in this connection, that certain relationships between the matrix elements of spin-dependent operators and two-body operators have already been noted by Drake and Schlesinger [5] using different methods.

We begin in Sect. 2 by showing that the general $U(n)$ adjoint coupling coefficients may be obtained from the $U(n)$ vector coupling coefficients and these are already known from the generator matrix element formulas. In Sect. 3 we derive the general $U(2)$ adjoint coefficients since these are needed for the spin part of the spin-orbit states. In Sect. 4 we apply the results of I to obtain explicit expressions for the $U(n)$ vector coupling coefficients, and these are used in Sect. 5 to derive the $U(n)$ adjoint coupling coefficients. In Sect. 6 the connection with the matrix elements of two-body operators is discussed.

We remark that our derivation of the $U(n)$ adjoint coefficients yields a formula which is in the form of a sum of products. However, in view of the results of Sect. 6 of this paper and Refs. 4–6, it should be possible to obtain a segment-level formula for the adjoint coupling coefficients. This simplication is best seen in the $SU(2)$-based formalism, together with the graphical methods of spin algebras (see the introduction to I), and will be discussed in a future publication.

2. Tensor Operators of $U(n)$

It was shown in I that an explicit formula can be obtained for the matrices of the $U(n)$ generators in the electronic Gel'fand basis. We consider here the more general problem of obtaining the matrix elements of unit adjoint tensor operators of $U(n)$. Throughout we adopt the notation of I.

The infinitesimal generators $E_{ij}(i, j=1, \ldots, n)$ of the Lie group $U(n)$ satisfy the commutation relations

$$[E_{ij}, E_{kl}] = \delta_{kj}E_{il} - \delta_{il}E_{kj}, \tag{1}$$

and the Hermiticity condition:

$$(E_{ij})^\dagger = E_{ji}. \tag{2}$$

The n^2-dimensional vector space spanned by the generators E_{ij} constitutes the unitary group Lie algebra which we denote simply by L.

Let V be a finite dimensional representation of $U(n)$ with basis $e_1, \ldots, e_k$ ($k = \dim V$). Since V constitutes a representation of $U(n)$ (or equivalently of L), one sees that acting on the space V the elements $x \in L$ are represented by endomorphisms $\pi(x) \in \operatorname{End} V$.

We call a collection of operators $\{T_i\}_{i=1}^k$ indexed like the basis vectors $\{e_i\}$ of V a tensor operator of rank π if the components T_i transform according to (c.f. Appendix)

$$[x, T_i] = \sum_{j=1}^{k} \pi(x)_{ji} T_j, \qquad x \in L, \tag{3}$$

where $\pi(x)$ is the matrix representing $x \in L$ in the basis $\{e_i\}$ of V. In other words, the components T_i of the tensor operator transform under commutation with the elements of L like the basis vectors e_i of the representation V. If $V = V(\boldsymbol{\lambda})$ is an irreducible representation with highest weight $\boldsymbol{\lambda}$, we call the tensor operator an irreducible tensor operator of rank $\boldsymbol{\lambda}$.

Note that our definition of tensor operator is basis dependent since the components T_i of the tensor operator, which are required to satisfy Eq. (3), will depend upon the basis $\{e_i\}$ chosen for V. We remark, however, that it is possible to give a basis-independent definition of a tensor operator using the concept of intertwining operators (c.f., e.g., with I Appendix B and [7]). A more detailed exposition on $U(n)$ tensor operators is given in the pioneering papers of Biedenharn and co-workers [8–10].

We have already seen in I a particular class of tensor operators, namely the vector operators $\{\Psi_i\}_{i=1}^n$ of $U(n)$. To see how vector operators as defined by Eq. (12) of I [denoted (I. Eq. No.) throughout] are a particular case of the more general definition (3), suppose V is the vector representation of $U(n)$ with basis $\{e_i\}_{i=1}^n$ satisfying $E_{ij} e_k = \delta_{kj} e_i$. Then for this case Eq. (3) gives the following transformation law:

$$[E_{ij}, \Psi_k] = \delta_{kj} \Psi_i, \tag{4}$$

which agrees with eq. (I.12). Similarly, if we take V to be the contragredient vector representation, then Eq. (3) yields the transformation law for contragredient vector operators

$$[E_{ij}, \Phi_k] = -\delta_{ik} \Phi_j, \tag{5}$$

which agrees with Eq. (I.17). Note that if $\{\Psi_i\}_{i=1}^n$ is a $U(n)$ vector operator, then as can be seen by taking the Hermitian conjugate of Eq. (4), the operators $\Psi_i^\dagger = (\Psi_i)^\dagger$ necessarily constitute a $U(n)$ contragredient vector operator.

Here we shall be concerned with the class of adjoint tensor operators [2] of $U(n)$ which transform like the basis vectors of the adjoint representation of $U(n)$. Recall that the adjoint representation of $U(n)$ is the n^2-dimensional representation afforded by the group generators themselves:

$$\operatorname{Adj}(x) \circ y = [x, y], \qquad x, y \in L.$$

We may choose as a basis for this representation the elementary matrices e_{ij} $(i, j = 1, \ldots, n)$ with one in the (i, j) position and zeros elsewhere. The matrix representing the generator E_{ij} in this basis is determined from [cf. Eq. (1)]:

$$E_{ij}e_{kl} = \delta_{kj}e_{il} - \delta_{il}e_{kj}.$$

We define an adjoint tensor operator, with respect to the basis $\{e_{ij}\}$, as a collection of n^2 components $\{X_{ij}\}_{i,j=1}^{n}$ which, from Eq. (3), transform according to the law:

$$[E_{ij}, X_{kl}] = \delta_{kj}X_{il} - \delta_{il}X_{kj}. \tag{6}$$

In particular, the $U(n)$ generators E_{ij} themselves transform as an adjoint tensor operator.

The motivation for considering adjoint tensor operators is that the infinitesimal generators of the group $U(2n)$ transform as the representation [Adj]⊗[Adj] under commutation with the generators of its subgroup $U(n)\times U(2)$ (outer direct product). To see this we note that the $U(2n)$ generators may be written:

$$E_{i\mu,j\nu}, \qquad i, j = 1, \ldots, n;\ \mu, \nu = 1, 2$$

and satisfy

$$[E_{i\mu,j\nu}, E_{k\rho,l\tau}] = \delta_{(k\rho),(j\nu)}E_{i\mu,l\tau} - \delta_{(i\mu),(l\tau)}E_{k\rho,j\nu}, \tag{7}$$

where $\delta_{(k\rho),(j\nu)} = \delta_{kj}\delta_{\rho\nu}$. The infinitesimal generators of the subgroup $U(n)\times U(2)$ are then given by

$$\begin{aligned} a_{ij} &= \sum_{\mu=1}^{2} E_{i\mu,j\mu}, \\ \gamma_{\mu\nu} &= \sum_{i=1}^{n} E_{i\mu,i\nu}, \end{aligned} \tag{8}$$

and satisfy $[a_{ij}, \gamma_{\mu\nu}] = 0$. The generators $E_{i\mu,j\nu}$, in view of the commutation relations (7), transform under commutation with the generators (8) as the representation [Adj]⊗[Adj]; viz.

$$\begin{aligned} [a_{ij}, E_{k\mu,l\nu}] &= \delta_{kj}E_{i\mu,l\nu} - \delta_{il}E_{k\mu,j\nu}, \\ [\gamma_{\mu\nu}, E_{i\rho,j\tau}] &= \delta_{\rho\nu}E_{i\mu,j\tau} - \delta_{\mu\tau}E_{i\rho,j\nu}. \end{aligned} \tag{9}$$

We now recall that the states of a many-fermion system are to comprise the totally antisymmetric Nth-rank tensor representation of $U(2n)$. The basis states for this representation are the Slater determinants. States of well-defined M_L, M_S and total spin S may be constructed by considering a basis for this space which is symmetry adapted to the subgroup $U(n)\times U(2)$ (herein called the spin-orbit basis). Thus we may obtain the matrix elements of the $U(2n)$ generators (which are necessary for spin-dependent operators) directly in the spin-orbit basis using their transformation properties as adjoint tensor operators.

We note that the adjoint representation of $U(n)$ is equivalent to the representation $V\otimes V^*$, where V is the fundamental vector representation of $U(n)$ and V^* is the contragredient vector representation. If $\{e_i\}_{i=1}^{n}$ (respectively, $\{\bar{e}_i\}_{i=1}^{n}$)

denotes the basis for V (respectively, V^*), then the vectors $e_i \otimes \bar{e}_j$ constitute a basis for the adjoint representation. This implies that one may construct an adjoint tensor operator X_{ij} by coupling together a $U(n)$ vector operator Ψ_i and a contragredient vector operator Φ_j; that is,

$$X_{ij} = \Psi_i \Phi_j. \tag{10}$$

However, from I Appendix B (see also Green [11] and Gould [12]), we know that the vector (respectively, contragredient vector) operator $\{\Psi_i\}$ (respectively, $\{\Phi_i\}$) may be resolved into a sum of shift components, when acting on an irreducible representation $V(\boldsymbol{\lambda})$, according to

$$\Psi_i = \sum_{r=1}^{n} \Psi[r]_i, \qquad \Phi_i = \sum_{r=1}^{n} \Phi[r]_i,$$

where $\Psi[r]$ and $\Phi[r]$ effect the following shifts on the representation labels

$$\Psi[r]: \boldsymbol{\lambda} \to \boldsymbol{\lambda} + \boldsymbol{\Delta}_r,$$

$$\Phi[r]: \boldsymbol{\lambda} \to \boldsymbol{\lambda} - \boldsymbol{\Delta}_r,$$

where $\boldsymbol{\Delta}_r$ denotes the elementary weight with one in the rth position and zeros elsewhere (see I Sec. 2).

This implies that the adjoint tensor operator X_{ij} may likewise be resolved into a sum of shift components

$$X_{ij} = X[0]_{ij} + \sum_{r \neq l} X[r, l]_{ij},$$

where the shift components $X[r, l]$ are given by

$$\begin{aligned} X[r, l]_{ij} &= \Psi[r]_i \Phi[l]_j, \quad \text{for } r \neq l, \\ X[0]_{ij} &= \sum_{r=1}^{n} \Psi[r]_i \Phi[r]_j. \end{aligned} \tag{11}$$

These shift components alter the $U(n)$ representation labels according to

$$\begin{aligned} X[r, l]&: \boldsymbol{\lambda} \to \boldsymbol{\lambda} + \boldsymbol{\Delta}_r - \boldsymbol{\Delta}_l, \\ X[0]&: \boldsymbol{\lambda} \to \boldsymbol{\lambda}, \end{aligned} \tag{12}$$

where it is understood that the shift component $X[r, l]$ necessarily vanishes if the final weight $\boldsymbol{\lambda} + \boldsymbol{\Delta}_r - \boldsymbol{\Delta}_l$ is nonlexical [see Eq. (I.3)]. An alternative proof of this result, independent of the coupling (10), is presented for general tensor operators in Ref. 12.

From the work of Louck and Biedenharn [2] we know that the zero shift component $X[0]$ of the adjoint tensor operator X_{ij} has matrix elements in the representation $V(\boldsymbol{\lambda})$ which are proportional to the matrix elements of an operator of the form $p(E)_{ij}$ for a suitable polynomial $p(x)$ (of degree $\leq n-1$) where we define polynomials in the matrix $[E_{ij}]$ according to I, Sec. 3 (hereafter Sec. I.3, etc.). Since the matrix elements of the $U(n)$ generators are known we can, in principle, determine the matrix elements of the zero shift component $X[0]_{ij}$. In fact, if $\boldsymbol{\lambda}$ has the special form of eq. I.6, then the above polynomial $p(x)$ can have, at most, degree 2 [see Eq. (I.8)]. That is, $X[0]_{ij} \equiv \gamma\delta_{ij} + \alpha E_{ij} + \beta(E^2)_{ij}$, for suitable scalars γ, α, and β, and the matrix elements of operators of this form can be obtained directly in the electronic Gel'fand basis. It turns out, moreover, that for the $U(2n)$ generators one necessarily has $\gamma = \beta = 0$ for the zero shift components of these operators regarded as tensor operators of $U(n) \times U(2)$. So we concentrate here on the nonzero shift components $X[r, l]_{ij} (r \neq l)$.

Applying the Wigner–Eckart (WE) theorem for adjoint tensor operators, we have immediately [c.f. Louck and Biedenharn [2, 8–10] and Eq. (A1)]

$$\left\langle \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \\ (\boldsymbol{\nu}') \end{matrix} \middle| X[r, l]_{ij} \middle| \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle = \langle \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \| X \| \boldsymbol{\lambda} \rangle \left\langle \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_i \otimes \bar{e}_j; \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle, \tag{13}$$

where the first term on the rhs is the reduced matrix element and the second term a $U(n)$ (adjoint) Wigner coefficient where $|{}^{\boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l}_{(\boldsymbol{\nu}')}\rangle$ and $|{}^{\boldsymbol{\lambda}}_{(\boldsymbol{\nu})}\rangle$ are two Gel'fand basis states for the spaces $V(\boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l)$ and $V(\boldsymbol{\lambda})$, respectively (see Sec. I.2). We note, moreover, that we may write

$$\left\langle \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_i \otimes \bar{e}_j; \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle = \sum_{(\boldsymbol{\tau})} \left\langle \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_i; \begin{matrix} \boldsymbol{\lambda}-\boldsymbol{\Delta}_l \\ (\boldsymbol{\tau}) \end{matrix} \right\rangle \left\langle \begin{matrix} \boldsymbol{\lambda}-\boldsymbol{\Delta}_l \\ (\boldsymbol{\tau}) \end{matrix} \middle| \bar{e}_j; \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle, \tag{14}$$

where the sum on $(\boldsymbol{\tau})$ is over all allowable Gel'fand tableaux in the space $V(\boldsymbol{\lambda}-\boldsymbol{\Delta}_l)$. The first term (under the summation) on the rhs is a $U(n)$ Wigner coefficient corresponding to the reduction $V \otimes V(\boldsymbol{\lambda}-\boldsymbol{\Delta}_l) \downarrow V(\boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l)$ where V is the vector representation (i.e., a vector coupling coefficient). The second term on the rhs is a $U(n)$ Wigner coefficient corresponding to the reduction $V^* \otimes V(\boldsymbol{\lambda}) \downarrow V(\boldsymbol{\lambda}-\boldsymbol{\Delta}_l)$, where V^* is the contragredient vector representation.

However, as pointed out by Baird and Biedenharn [8], these latter Wigner coefficients are already known from the matrix elements of the unitary group generators. To see this, consider the subgroup embedding $U(n) \subset U(n+1)$ and note that the $U(n+1)$ generators $\Psi(n)_i = E_{i\,n+1}$ $(i = 1, \ldots, n)$ (respectively, $\Psi^\dagger(n)_i = E_{n+1\,i}$) constitute a vector (respectively, contragredient vector) operator of $U(n)$. We may embed the $U(n)$ representation $V(\boldsymbol{\lambda})$ in a suitable representation $V(\hat{\boldsymbol{\lambda}})$ of $U(n+1)$, where $\hat{\boldsymbol{\lambda}}$ denotes a highest weight of $U(n+1)$. We thus have, using the WE theorem for $U(n)$,

$$\left\langle \begin{matrix} \hat{\boldsymbol{\lambda}} \\ \boldsymbol{\lambda}+\boldsymbol{\Delta}_r \\ (\boldsymbol{\nu}') \end{matrix} \middle| \Psi(n)_i \middle| \begin{matrix} \hat{\boldsymbol{\lambda}} \\ \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle = \left\langle \begin{matrix} \hat{\boldsymbol{\lambda}} \\ \boldsymbol{\lambda}+\boldsymbol{\Delta}_r \end{matrix} \middle\| \Psi(n) \middle\| \begin{matrix} \hat{\boldsymbol{\lambda}} \\ \boldsymbol{\lambda} \end{matrix} \right\rangle \left\langle \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_i; \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle, \tag{15a}$$

$$\left\langle \begin{matrix} \hat{\boldsymbol{\lambda}} \\ \boldsymbol{\lambda}-\boldsymbol{\Delta}_r \\ (\boldsymbol{\nu}') \end{matrix} \middle| \Psi^\dagger(n)_i \middle| \begin{matrix} \hat{\boldsymbol{\lambda}} \\ \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle = \left\langle \begin{matrix} \hat{\boldsymbol{\lambda}} \\ \boldsymbol{\lambda}-\boldsymbol{\Delta}_r \end{matrix} \middle\| \Psi^\dagger(n) \middle\| \begin{matrix} \hat{\boldsymbol{\lambda}} \\ \boldsymbol{\lambda} \end{matrix} \right\rangle \left\langle \begin{matrix} \boldsymbol{\lambda}-\boldsymbol{\Delta}_r \\ (\boldsymbol{\nu}') \end{matrix} \middle| \bar{e}_i; \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle. \tag{15b}$$

Since the matrix elements of the generators $E_{i\,n+1}$ and $E_{n+1\,i}$ on the lhs are known and the reduced matrix elements on the rhs are both known, one may deduce the Wigner coefficients on the rhs as required (c.f. Gould [12]). For our purposes, however, we just need to consider the special representations with highest weights of the form of Eq. (I.6) (i.e., representations corresponding to only two columns in the Weyl tableau). For these representations the Wigner coefficients may be expressed by a simple segment-level formula.

We remark that the reduced matrix element of the vector operator Ψ_i and its conjugate $\Psi_i^\dagger$ are related by (see Appendix)

$$\langle \boldsymbol{\lambda}+\boldsymbol{\Delta}_r \| \Psi \| \boldsymbol{\lambda} \rangle = \left(\frac{D[\boldsymbol{\lambda}]}{D[\boldsymbol{\lambda}+\boldsymbol{\Delta}_r]} \right)^{1/2} \langle \boldsymbol{\lambda} \| \Psi^\dagger \| \boldsymbol{\lambda}+\boldsymbol{\Delta}_r \rangle, \tag{16}$$

where $D[\boldsymbol{\lambda}] = \dim V(\boldsymbol{\lambda})$. This implies that the $U(n)$ Wigner coefficients of Eq. (15) are necessarily related by (see Appendix)

$$\left\langle \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \middle| \bar{e}_i; \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r \\ (\boldsymbol{\nu}') \end{matrix} \right\rangle = \left(\frac{D[\boldsymbol{\lambda}]}{D[\boldsymbol{\lambda}+\boldsymbol{\Delta}_r]} \right)^{1/2} \left\langle \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_i; \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle, \tag{17}$$

which is reminiscent of the well-known symmetry properties of O(3) Wigner coefficients (see, e.g., Condon and Shortley [13]). Thus, in applications, this equation implies that only the coefficients of eq. (15a) need be calculated and those of Eq. (15b) follow from the symmetry condition (17). Biedenharn, Louck and collaborators, in their extensive series of papers [8–10] have generalized the symmetry relation (17) to arbitrary (multiplicity free) tensor products of $U(n)$.

Note that if the adjoint tensor operator X_{ij} is given by Eq. (10), then we may write (in view of the WE theorem):

$$\begin{aligned} \left\langle \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \\ (\boldsymbol{\nu}') \end{matrix} \middle| X_{ij} \middle| \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle &= \left\langle \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \\ (\boldsymbol{\nu}') \end{matrix} \middle| \Psi_i \Phi_j \middle| \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle \\ &= \langle \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \| \Psi \| \boldsymbol{\lambda}-\boldsymbol{\Delta}_l \rangle \langle \boldsymbol{\lambda}-\boldsymbol{\Delta}_l \| \Phi \| \boldsymbol{\lambda} \rangle \\ &\quad \times \sum_{(\boldsymbol{\tau})} \left\langle \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_i; \begin{matrix} \boldsymbol{\lambda}-\boldsymbol{\Delta}_l \\ (\boldsymbol{\tau}) \end{matrix} \right\rangle \left\langle \begin{matrix} \boldsymbol{\lambda}-\boldsymbol{\Delta}_l \\ (\boldsymbol{\tau}) \end{matrix} \middle| \bar{e}_j; \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle. \end{aligned}$$

Comparison with Eqs. (13) and (14) shows that we have the following relationship between reduced matrix elements:

$$\langle \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \| X \| \boldsymbol{\lambda} \rangle = \langle \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \| \Psi \| \boldsymbol{\lambda}-\boldsymbol{\Delta}_l \rangle \langle \boldsymbol{\lambda}-\boldsymbol{\Delta}_l \| \Phi \| \boldsymbol{\lambda} \rangle.$$

We remark, however, that in the following we are mostly concerned with the adjoint coefficients [lhs of Eq. (14)] which reflect the transformation (i.e., geometric) properties of adjoint tensor operators. The reduced matrix element, which is independent of the geometry, depends upon the intrinsic properties of the operator concerned (i.e., the physics). So for our purposes it suffices to work with unit adjoint tensor operators whose reduced matrix elements, by definition, are unity.

Note that the symmetry relation (17) implies the following symmetry relation for adjoint Wigner coefficients:

$$\left\langle \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_i \otimes \bar{e}_j; \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle = \left(\frac{D[\boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l]}{D[\boldsymbol{\lambda}]} \right)^{1/2} \left\langle \begin{matrix} \boldsymbol{\lambda} \\ (\boldsymbol{\nu}) \end{matrix} \middle| e_j \otimes \bar{e}_i; \begin{matrix} \boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l \\ (\boldsymbol{\nu}') \end{matrix} \right\rangle. \tag{18}$$

This relation shows that only adjoint coefficients corresponding to $i \leq j$ need be calculated, the rest following from the relation (18).

Since we shall be applying these results to the representations appropriate to the orbital part of an N-electron state, we only need consider the special case where $\boldsymbol{\lambda}$ and $\boldsymbol{\lambda}+\boldsymbol{\Delta}_r-\boldsymbol{\Delta}_l$ have the form of Eq. (I.6). Note, however, that we also need to consider the general $U(2)$ adjoint coefficients since these will be needed for the spin part of the spin-orbit states. So we consider first the evaluation of the general $U(2)$ adjoint coefficients. We remark that our method of evaluation is applicable to general $U(n)$.

3. Adjoint Tensor Operators of $U(2)$

We consider first the matrix elements of the $U(2)$ generators E_{ij} $(i, j=1, 2)$ in the Gel'fand–Tsetlin basis for the irreducible representation $V(\lambda_1, \lambda_2)$ of $U(2)$. This space is $(\lambda_1-\lambda_2+1)$-dimensional with basis $\left|\begin{smallmatrix}\lambda_1 & \lambda_2 \\ m\end{smallmatrix}\right\rangle$ where m can take integral values in the range $\lambda_1 \geq m \geq \lambda_2$. The generators E_{ii} $(i=1, 2)$ are diagonal in this basis with entries given by

$$\begin{aligned} E_{11}\left|\begin{matrix}\lambda_1 & \lambda_2 \\ m\end{matrix}\right\rangle &= m\left|\begin{matrix}\lambda_1 & \lambda_2 \\ m\end{matrix}\right\rangle, \\ E_{22}\left|\begin{matrix}\lambda_1 & \lambda_2 \\ m\end{matrix}\right\rangle &= (\lambda_1+\lambda_2-m)\left|\begin{matrix}\lambda_1 & \lambda_2 \\ m\end{matrix}\right\rangle. \end{aligned} \tag{19}$$

It remains to determine the matrix elements of the generators E_{12} and E_{21}. Using the phase convention of Baird and Biedenharn [8] (which agrees with that of Condon and Shortley [13]) we see that the matrix elements of the generator E_{12} are given by

$$E_{12}\left|\begin{matrix}\lambda_1 & \lambda_2 \\ m\end{matrix}\right\rangle = N\left|\begin{matrix}\lambda_1 & \lambda_2 \\ m+1\end{matrix}\right\rangle,$$

where

$$N = \left\langle \begin{matrix}\lambda_1 & \lambda_2 \\ m\end{matrix} \middle| E_{21}E_{12} \middle| \begin{matrix}\lambda_1 & \lambda_2 \\ m\end{matrix} \right\rangle^{1/2},$$

which, using the $U(2)$ commutation relations, may be written

$$N = \left\langle \begin{matrix}\lambda_1 & \lambda_2 \\ m\end{matrix} \middle| \tfrac{1}{2}[\sigma_2-(E_{11})^2-(E_{22})^2+E_{22}-E_{11}] \middle| \begin{matrix}\lambda_1 & \lambda_2 \\ m\end{matrix} \right\rangle^{1/2},$$

where $\sigma_2 = E_{ij}E_{ji}$ is the universal Casimir element which commutes with the $U(2)$ generators. From Schur's lemma the invariant σ_2 necessarily takes a constant value on the space $V(\lambda)$ and this eigenvalue is well known to be given by $\chi_\lambda(\sigma_2)=\lambda_1(\lambda_1+1)+\lambda_2(\lambda_2-1)$. We thereby obtain, in view of Eq. (19), the result:

$$E_{12}\left|\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right\rangle=[(\lambda_1-m)(m+1-\lambda_2)]^{1/2}\left|\begin{matrix}\lambda_1 & \lambda_2\\ & m+1\end{matrix}\right\rangle. \tag{20}$$

We similarly obtain:

$$E_{21}\left|\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right\rangle=[(m-\lambda_2)(\lambda_1+1-m)]^{1/2}\left|\begin{matrix}\lambda_1 & \lambda_2\\ & m-1\end{matrix}\right\rangle. \tag{21}$$

We now consider the direct evaluation of the adjoint and vector Wigner coefficients for $U(2)$. Acting on the irreducible representation of $U(2)$ with highest weight $\boldsymbol{\lambda}=(\lambda_1,\lambda_2)$, the $U(2)$ matrix

$$E=\begin{bmatrix}E_{11} & E_{12}\\ E_{21} & E_{22}\end{bmatrix},$$

satisfies the second-order polynomial identity (see Sec. I.3 and Appendix A):

$$(E-\lambda_1-1)(E-\lambda_2)=0. \tag{22}$$

By virtue of this identity one may construct the projection operators

$$P_1=\left(\frac{E-\lambda_2}{\lambda_1-\lambda_2+1}\right),\qquad P_2=\left(\frac{E-\lambda_1-1}{\lambda_2-\lambda_1-1}\right), \tag{23}$$

which, in view of the identity (22), satisfy the relations:

$$P_\alpha P_\beta=\delta_{\alpha\beta}P_\beta \quad\text{and}\quad [P_1]_{ij}+[P_2]_{ij}=\delta_{ij}. \tag{24}$$

Now the matrix elements of the entries of these projectors are determined by {see Eq. (I.A5) and Gould [12]}:

$$\left\langle\begin{matrix}\lambda_1 & \lambda_2\\ & m'\end{matrix}\right|[P_1]_{ij}\left|\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right\rangle=\sum_{m''}\left\langle\begin{matrix}\lambda_1 & \lambda_2\\ & m'\end{matrix};\bar{e}_i\right|\left.\begin{matrix}\lambda_1-1 & \lambda_2\\ & m''\end{matrix}\right\rangle\left\langle\begin{matrix}\lambda_1-1 & \lambda_2\\ & m''\end{matrix}\right|\left.\bar{e}_j;\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right\rangle.$$

As a particular case of this result we obtain

$$\begin{aligned}\left\langle\begin{matrix}\lambda_1-1 & \lambda_2\\ & m'\end{matrix}\right|\left.\bar{e}_i;\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right\rangle&=\left\langle\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right|[P_1]_{ii}\left|\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right\rangle^{1/2}\delta_{m',m+i-2}\\ &=\left\langle\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right|\frac{E_{ii}-\lambda_2}{\lambda_1-\lambda_2+1}\left|\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right\rangle^{1/2}\delta_{m',m+i-2},\end{aligned}$$

where we have adopted the phase convention of Baird and Biedenharn [8]. By this means we obtain:

$$\begin{aligned}\left\langle\begin{matrix}\lambda_1-1 & \lambda_2\\ & m'\end{matrix}\right|\left.\bar{e}_1;\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right\rangle&=\delta_{m',m-1}\left(\frac{m-\lambda_2}{\lambda_1-\lambda_2+1}\right)^{1/2},\\ \left\langle\begin{matrix}\lambda_1-1 & \lambda_2\\ & m'\end{matrix}\right|\left.\bar{e}_2;\begin{matrix}\lambda_1 & \lambda_2\\ & m\end{matrix}\right\rangle&=\delta_{m',m}\left(\frac{\lambda_1-m}{\lambda_1-\lambda_2+1}\right)^{1/2}.\end{aligned} \tag{25}$$

Similarly, for the matrix elements of the entries of the projector P_2 we obtain (with the phase convention of Ref. 8)

$$\left\langle \begin{matrix} \lambda_1 & \lambda_2-1 \\ & m' \end{matrix} \middle| \bar{e}_i; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle = (-1)^i \delta_{m',m-2+i} \left\langle \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \middle| [P_2]_{ii} \middle| \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle^{1/2}.$$

In this case we may use the result $[P_2]_{ii} = 1 - [P_1]_{ii}$ giving

$$\left\langle \begin{matrix} \lambda_1 & \lambda_2-1 \\ & m' \end{matrix} \middle| \bar{e}_i; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle = (-1)^i \left(1 - \left| \left\langle \begin{matrix} \lambda_1-1 & \lambda_2 \\ m' & \end{matrix} \middle| \bar{e}_i; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle \right|^2 \right)^{1/2}.$$

Thus we obtain

$$\begin{aligned} \left\langle \begin{matrix} \lambda_1 & \lambda_2-1 \\ & m' \end{matrix} \middle| \bar{e}_1; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle &= -\delta_{m',m-1} \left(\frac{\lambda_1+1-m}{\lambda_1+1-\lambda_2} \right)^{1/2}, \\ \left\langle \begin{matrix} \lambda_1 & \lambda_2-1 \\ & m' \end{matrix} \middle| \bar{e}_2; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle &= \delta_{m'm} \left(\frac{m+1-\lambda_2}{\lambda_1-\lambda_2+1} \right)^{1/2}. \end{aligned} \tag{26}$$

We may similarly evaluate the Wigner coefficients:

$$\left\langle \begin{matrix} \lambda_1+1 & \lambda_2 \\ m' & \end{matrix} \middle| e_i; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle \quad \text{and} \quad \left\langle \begin{matrix} \lambda_1 & \lambda_2+1 \\ & m' \end{matrix} \middle| e_i; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle.$$

However, in this case we may use the symmetry relation (17) which, for $U(2)$, may be written:

$$\begin{aligned} \left\langle \begin{matrix} \lambda_1+1 & \lambda_2 \\ m' & \end{matrix} \middle| e_i; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle &= \left(\frac{\lambda_1-\lambda_2+2}{\lambda_1-\lambda_2+1} \right)^{1/2} \left\langle \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \middle| \bar{e}_i; \begin{matrix} \lambda_1+1 & \lambda_2 \\ & m \end{matrix} \right\rangle, \\ \left\langle \begin{matrix} \lambda_1 & \lambda_2+1 \\ & m' \end{matrix} \middle| e_i; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle &= \left(\frac{\lambda_1-\lambda_2}{\lambda_1-\lambda_2+1} \right)^{1/2} \left\langle \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \middle| \bar{e}_i; \begin{matrix} \lambda_1 & \lambda_2+1 \\ & m' \end{matrix} \right\rangle. \end{aligned} \tag{27}$$

Thus we have obtained all $U(2)$ (vector) Wigner coefficients as required.

Our $U(2)$ adjoint coefficients, in view of Eq. (14), are thus determined by

$$\begin{aligned} &\left\langle \begin{matrix} \lambda_1+1 & \lambda_2-1 \\ m' & \end{matrix} \middle| e_i \otimes \bar{e}_j; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle \\ &= \sum_{m''} \left\langle \begin{matrix} \lambda_1+1 & \lambda_2-1 \\ m & \end{matrix} \middle| e_i; \begin{matrix} \lambda_1 & \lambda_2-1 \\ & m'' \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_1 & \lambda_2-1 \\ & m'' \end{matrix} \middle| \bar{e}_j; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle, \end{aligned}$$

which, in view of the symmetry relation (27), may be written

$$\begin{aligned} &\left\langle \begin{matrix} \lambda_1+1 & \lambda_2-1 \\ m' & \end{matrix} \middle| e_i \otimes \bar{e}_j; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle \\ &= \delta_{m'+i,m+j} \left(\frac{\lambda_1-\lambda_2+3}{\lambda_1-\lambda_2+2} \right)^{1/2} \left\langle \begin{matrix} \lambda_1 & \lambda_2-1 \\ m'-2+i & \end{matrix} \middle| \bar{e}_i; \begin{matrix} \lambda_1+1 & \lambda_2-1 \\ & m' \end{matrix} \right\rangle \\ &\quad \times \left\langle \begin{matrix} \lambda_1 & \lambda_2-1 \\ m+j-2 & \end{matrix} \middle| \bar{e}_j; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle. \end{aligned} \tag{28}$$

Using Eqs. (25) and (26) we thus obtain:

$$\left\langle \begin{matrix} \lambda_1+1 & \lambda_2-1 \\ & m' \end{matrix} \middle| e_i \otimes \bar{e}_j; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle = (-1)^j \delta_{m'm} \left(\frac{(m-\lambda_2+1)(\lambda_1+1-m)}{(\lambda_1-\lambda_2+2)(\lambda_1-\lambda_2+1)} \right)^{1/2}, \quad i=j=1 \text{ or } 2,$$

$$= \delta_{m',m+1} \left(\frac{(m-\lambda_2+1)(m+2-\lambda_2)}{(\lambda_1-\lambda_2+2)(\lambda_1-\lambda_2+1)} \right)^{1/2}, \quad i=1, j=2,$$

$$= -\delta_{m',m+1} \left(\frac{(\lambda_1+2-m)(\lambda_1+1-m)}{(\lambda_1-\lambda_2+1)(\lambda_1-\lambda_2+2)} \right)^{1/2}, \quad i=2, j=1. \tag{29}$$

The remaining $U(2)$ adjoint coefficients may then be obtained from the symmetry relation (18); viz.

$$\left\langle \begin{matrix} \lambda_1-1 & \lambda_2+1 \\ & m' \end{matrix} \middle| e_i \otimes \bar{e}_j; \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \right\rangle = \left(\frac{\lambda_1-\lambda_2-1}{\lambda_1-\lambda_2+1} \right)^{1/2} \left\langle \begin{matrix} \lambda_1 & \lambda_2 \\ & m \end{matrix} \middle| e_j \otimes \bar{e}_i; \begin{matrix} \lambda_1-1 & \lambda_2+1 \\ & m' \end{matrix} \right\rangle. \tag{30}$$

4. Vector Coefficients for $U(n)$

We derive here the vector coupling coefficients for the special irreducible representations of $U(n)$ with highest weights of the form:

$$\boldsymbol{\lambda} = 2 \sum_{r=1}^{a} \boldsymbol{\Delta}_r + \sum_{r=a+1}^{a+b} \boldsymbol{\Delta}_r. \tag{31}$$

We denote the irreducible representation with highest weight $\boldsymbol{\lambda}$ by $V(a, b, c)$ where a, b are as in Eq. (31) and c is uniquely determined by $a+b+c=n$. Our notation follows that of Sec. I.2 (see also Paldus [3]).

For convenience we assume that we are working in an irreducible representation $V(a_{n+1}, b_{n+1}, c_{n+1})$ of $U(n+1)$ with Paldus labels $[a_{n+1}, b_{n+1}, c_{n+1}]$. We adopt the Paldus representation of the Gel'fand–Tsetlin basis states in the space $V(a_{n+1}, b_{n+1}, c_{n+1})$ whose states are uniquely labeled by an $(n+1)\times 3$ Paldus tableau. We denote the Gel'fand–Paldus (GP) states in this space by (see Sec. I.2)

$$\left| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n \\ \vdots \\ \mathbf{P}_m \\ [\boldsymbol{P}] \end{matrix} \right\rangle,$$

where

$$\begin{aligned}\mathbf{P}_{n+1} &= [a_{n+1}, b_{n+1}, c_{n+1}],\\ \mathbf{P}_n &= [a_n, b_n, c_n],\\ &\vdots\\ \mathbf{P}_m &= [a_m, b_m, c_m],\end{aligned} \tag{32}$$

and where $[\mathbf{P}]$ denotes an allowable Paldus tableau for the subgroup $U(m-1)$.

From the results of Secs. I.5–I.6, the nonvanishing matrix elements of the generator $E_{m\,n+1}$ $(m \leq n)$ are of the form:

$$\left\langle \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n + \boldsymbol{\delta}_{i_n} \\ \vdots \\ \mathbf{P}_m + \boldsymbol{\delta}_{i_m} \\ [\mathbf{P}] \end{matrix} \right| E_{m\,n+1} \left| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle, \tag{33}$$

where $i_r = 1, 2$ $(r = m, \ldots, n)$ and where the shifts $\boldsymbol{\delta}_i$ $(i = 1, 2)$ are given by

$$\boldsymbol{\delta}_1 = [0, 1, -1], \qquad \boldsymbol{\delta}_2 = [1, -1, 0]. \tag{34}$$

From Eq. (I.77), the matrix element (33) is given by

$$\begin{aligned} N\begin{pmatrix} i_n & \cdots & i_{m+1} & i_m \\ n & \cdots & m+1 & m \end{pmatrix} &= \omega\left(\frac{(4+b_m-2i_m)(1+b_n)}{(1+b_{m-1})(1+b_{n+1})}\right)^{1/2} \\ &\quad \times \prod_{r=m+1}^{n} [(1+b_r)^{1/2}]^{-1-|i_r-i_{r-1}|} \\ &\quad \times [(4+b_r-2i_r)^{1/2}]^{1-|i_r-i_{r-1}|}, \end{aligned} \tag{35}$$

where the phase $\omega = (\pm 1)$ is determined by the convention of Sec. I.7. On the other hand, using the $U(n)$ WE theorem, we see [c.f. Eq. (15a)] that the matrix element (33) may be written:

$$\left\langle \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n + \boldsymbol{\delta}_{i_n} \end{matrix} \right\| \Psi(n) \left\| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n \end{matrix} \right\rangle \left\langle \begin{matrix} \mathbf{P}_n + \boldsymbol{\delta}_{i_n} \\ \vdots \\ \mathbf{P}_m + \boldsymbol{\delta}_{i_m} \\ [\mathbf{P}] \end{matrix} \right| e_m; \left. \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle. \tag{36}$$

The reduced matrix element [first term in Eq. (36)] is determined by the operator $[R_n^{i_n}]^{1/2}$ whose eigenvalues are given by Eq. (I.43). Comparison with (35) yields the following form for the nonzero vector coupling coefficients:

$$\left\langle \begin{matrix} \mathbf{P}_n+\boldsymbol{\delta}_{i_n} \\ \vdots \\ \mathbf{P}_m+\boldsymbol{\delta}_{i_m} \\ [\mathbf{P}] \end{matrix} \middle| e_m; \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle$$

$$= \omega\left(\frac{(4+b_m-2i_m)}{U_n^{i_n}(1+b_{m-1})}\right)^{1/2} \prod_{r=m+1}^{n} [(1+b_r)^{1/2}]^{-1-|i_r-i_{r-1}|}[(4+b_r-2i_r)^{1/2}]^{1-|i_r-i_{r-1}|} \tag{37}$$

where

$$U_n^1 = n+2-c_n \quad \text{and} \quad U_n^2 = 1+a_n \tag{38}$$

and where ω is the phase of the corresponding matrix element (35).

Similarly for the contragredient vector coupling coefficients we have [see Eqs. (I.43) and (I.79)]

$$\left\langle \begin{matrix} \mathbf{P}_n-\boldsymbol{\delta}_{i_n} \\ \vdots \\ \mathbf{P}_m-\boldsymbol{\delta}_{i_m} \\ [\mathbf{P}] \end{matrix} \middle| \bar{e}_m; \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle$$

$$= \bar{\omega}\left(\frac{(b_m+2i_m-2)}{\bar{U}_n^{i_n}(1+b_{m-1})}\right)^{1/2} \prod_{r=m+1}^{n} [(1+b_r)^{1/2}]^{-1-|i_r-i_{r-1}|}[(b_r+2i_r-2)^{1/2}]^{1-|i_r-i_{r-1}|}, \tag{39}$$

where

$$\bar{U}_n^1 = (1+c_n), \qquad \bar{U}_n^2 = (n+2-a_n) \tag{40}$$

and where the phase $\bar{\omega}$ is given by the phase of the corresponding matrix element of the generator $E_{n+1\,m}$ as given in Sec. I.7.

One may check that the coefficients (37) and (39) obey the symmetry condition

$$\left\langle \begin{matrix} \mathbf{P}_n-\boldsymbol{\delta}_{i_n} \\ \vdots \\ \mathbf{P}_m-\boldsymbol{\delta}_{i_m} \\ [\mathbf{P}] \end{matrix} \middle| \bar{e}_m; \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle = \left(\frac{D[\mathbf{P}_n-\boldsymbol{\delta}_{i_n}]}{D[\mathbf{P}_n]}\right)^{1/2} \left\langle \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \middle| e_m; \begin{matrix} \mathbf{P}_n-\boldsymbol{\delta}_{i_n} \\ \vdots \\ \mathbf{P}_m-\boldsymbol{\delta}_{i_m} \\ [\mathbf{P}] \end{matrix} \right\rangle, \tag{41}$$

as required by Eq. (17).

For convenience we denote the Wigner coefficients (37) and (39) by the respective symbols

$$V\begin{pmatrix} i_n & \cdots & i_{m+1} & i_m \\ n & \cdots & m+1 & m \end{pmatrix} \quad \text{and} \quad \bar{V}\begin{pmatrix} i_n & \cdots & i_{m+1} & i_m \\ n & \cdots & m+1 & m \end{pmatrix}, \tag{42}$$

where it is understood that these coefficients, as given by Eqs. (37) and (39), are a function of the Paldus labels of the initial state (32). These coefficients are related to the matrix elements of the generators $E_{m\,n+1}$ and $E_{n+1\,m}$ [see Eqs. (I.77) and (I.79)] respectively, by

$$N\begin{pmatrix} i_n & \cdots & i_m \\ n & & m \end{pmatrix} = [R_n^{i_n}]^{1/2} V\begin{pmatrix} i_n & \cdots & i_m \\ n & & m \end{pmatrix}, \tag{43a}$$

$$\bar{N}\begin{pmatrix} i_n & \cdots & i_m \\ n & & m \end{pmatrix} = [\bar{R}_n^{i_n}]^{1/2} \bar{V}\begin{pmatrix} i_n & \cdots & i_m \\ n & & m \end{pmatrix}, \tag{43b}$$

where the operators R_n^i and $\bar{R}_n^i$ $(i=1,2)$ are determined by Eq. (I.43).

Following the notation of Sec. I.8 for indices $i=1$, 2 let us introduce the opposite index $\bar{i}$ defined by $\bar{1}=2$, $\bar{2}=1$. Then from the symmetry relation Eq. (I.84) satisfied by the matrix elements (43a) and (43b) we obtain the following relations between the vector coefficients:

$$V\begin{pmatrix} \bar{i}_n & \cdots & \bar{i}_m \\ n & & m \end{pmatrix} = (-1)^{b_n - b_m} \left(\frac{\bar{U}_n^{i_n}}{U_n^{\bar{i}_n}} \right)^{1/2} \bar{V}\begin{pmatrix} i_n & \cdots & i_m \\ n & & m \end{pmatrix}, \tag{44}$$

where U_n^i and $\bar{U}_n^j$ $(i,j=1,2)$ are as in Eqs. (38) and (40), respectively.

In the case where the Paldus labels of the groups $U(n), \ldots, U(m)$ are all altered by the same shift [i.e., $i_n = i_{n-1} = \cdots = i_m$ in Eqs. (39)–(44)] we obtain the following special vector coupling coefficients [c.f. Eqs. (I.85) and (I.86)]:

$$\begin{aligned} (-1)^{b_n - b_m} V\begin{pmatrix} 1 & \cdots & 1 & 1 \\ n & & m+1 & m \end{pmatrix} &= \left(\frac{n+2-a_n}{n+2-c_n} \right)^{1/2} \bar{V}\begin{pmatrix} 2 & \cdots & 2 & 2 \\ n & & m+1 & m \end{pmatrix} \\ &= (-1)^{a_n - a_m} \left(\frac{(2+b_m)}{(1+b_{m-1})(n+2-c_n)} \right)^{1/2} \\ &\quad \times \prod_{r=m+1}^{n} \left(\frac{b_r+2}{b_r+1} \right)^{1/2}, \end{aligned}$$

$$\begin{aligned} V\begin{pmatrix} 2 & \cdots & 2 & 2 \\ n & & m+1 & m \end{pmatrix} &= (-1)^{b_n - b_m} \left(\frac{1+c_n}{1+a_n} \right)^{1/2} \bar{V}\begin{pmatrix} 1 & \cdots & 1 & 1 \\ n & & m+1 & m \end{pmatrix} \\ &= (-1)^{a_n - a_m} \left(\frac{b_m}{(1+b_{m-1})(1+a_n)} \right)^{1/2} \prod_{r=m+1}^{n} \left(\frac{b_r}{b_r+1} \right)^{1/2}. \end{aligned}$$

We conclude this section with a decomposition law satisfied by the V coefficients (37) and (39). From the product rule Eq. (I.72a) satisfied by the W factors of I we deduce, in view of our phase convention, the following product law satisfied by the generator matrix elements:

$$\begin{aligned} & N\begin{pmatrix} i_n & \cdots & i_{m+p+1} & i' & i & \cdots & i_m \\ n & & m+p+1 & m+p & m+p-1 & & m \end{pmatrix} \\ &= \Theta_{i',i}^{(m+p)} N\begin{pmatrix} i_n & \cdots & i_{m+p+1} & i' \\ n & & m+p+1 & m+p \end{pmatrix} N\begin{pmatrix} i & \cdots & i_m \\ m+p-1 & & m \end{pmatrix}, \\ & \qquad i, i' = 1, 2, \end{aligned}$$

where

$$\Theta_{i',i}^{(m+p)} = (-1)^{[U^{i'}_{m+p}-U^{i}_{m+p-1}]} S(i-i')\{[(1+b_{m+p})(b_{m+p}+4-2i')]^{1/2}\}^{-|i-i'|}, \tag{45}$$

where $S(x) = \text{sign of } x$ with $S(0)=1$. From this relation we obtain immediately, in view of Eq. (43a), the following law satisfied by the V coefficients (37):

$$V\begin{pmatrix} i_n & \dots & i_{m+p+1} & i' & i & \dots & i_m \\ n & & m+p+1 & m+p & m+p-1 & & m \end{pmatrix}$$

$$= \Theta_{i',i}^{(m+p)} V\begin{pmatrix} i_n & \dots & i_{m+p+1} & i' \\ n & & m+p+1 & m+p \end{pmatrix} N\begin{pmatrix} i & \dots & i_m \\ m+p-1 & & m \end{pmatrix}. \tag{46}$$

We similarly obtain for the contragredient vector coefficients the result

$$\bar{V}\begin{pmatrix} i_n & \dots & i_{m+p+1} & i' & i & \dots & i_m \\ n & & m+p+1 & m+p & m+p-1 & & m \end{pmatrix}$$

$$= \bar{\Theta}_{i',i}^{(m+p)} \bar{V}\begin{pmatrix} i_n & \dots & i_{m+p+1} & i' \\ n & & m+p+1 & m+p \end{pmatrix} \bar{N}\begin{pmatrix} i & \dots & i_m \\ m+p-1 & & m \end{pmatrix}, \tag{47}$$

where

$$\bar{\Theta}_{i',i}^{(m+p)} = (-1)^{[U^{i'}_{m+p}-U^{i}_{m+p-1}]} S(i-i')\{[(1+b_{m+p})(b_{m+p}+2i'-2)]^{1/2}\}^{-|i-i'|}. \tag{48}$$

5. Adjoint Tensor Operators of $U(n)$

Following the notation of Sec. 4, we restrict ourselves to representations of $U(n)$ of the special form $V(a, b, c)$ [with highest weight given by Eq. (31)]. Thus we work in the finite dimensional Hilbert space

$$\mathcal{H} = \bigoplus_{\substack{a,b,c \\ a+b+c=n}} V(a, b, c), \tag{49}$$

where the sum is over all sets of integers (a, b, c) satisfying the requirements $a \geq 0$, $b \geq 0$, $c \geq 0$ and $a+b+c=n$.

We suppose X_{ij} is a unit $U(n)$ adjoint tensor operator acting on the Hilbert space $\mathcal{H}$:

$$X_{ij}: \mathcal{H} \to \mathcal{H}.$$

Since the adjoint tensor operator X_{ij} (by definition) is to leave the space $\mathcal{H}$ invariant, we see that acting on the representation $V(a, b, c)$ occurring in $\mathcal{H}$ that X can be resolved into three shift components (c.f. Sec. I.3)

$$X_{ij} = X_{ij}^{(0)} + X_{ij}^{(+)} + X_{ij}^{(-)},$$

which, in terms of our previous notation [see Eq. (11)] may be written [c.f. Eqs. (I.14) and (I.19)]

$$X^{(0)} = X[0], \qquad X^{(+)} = X[a+1, a+b], \qquad X^{(-)} = X[a+b+1, a].$$

These shift components thus alter the Paldus labels $[a, b, c]$ of the group $U(n)$ according to [c.f. Eq. (I.22) and preceding remarks]

$$\begin{aligned} X^{(\pm)}&:[a, b, c]\rightarrow[a, b, c]+\boldsymbol{\varepsilon}_{\pm 1},\\ X^{(0)}&:[a, b, c]\rightarrow[a, b, c]+\boldsymbol{\varepsilon}_{0}, \end{aligned} \tag{50}$$

where $\boldsymbol{\varepsilon}_i$ $(i=0, \pm 1)$ denote the shifts:

$$\boldsymbol{\varepsilon}_0=\mathbf{0}, \qquad \boldsymbol{\varepsilon}_{\pm 1}=\pm(\boldsymbol{\delta}_2-\boldsymbol{\delta}_1)=[\pm 1, \mp 2, \pm 1]. \tag{51}$$

In other words, the following must hold:

$$\begin{aligned} X_{ij}^{(+)}V(a, b, c)&\subseteq V(a+1, b-2, c+1),\\ X_{ij}^{(-)}V(a, b, c)&\subseteq V(a-1, b+2, c-1),\\ X_{ij}^{(0)}V(a, b, c)&\subseteq V(a, b, c). \end{aligned}$$

We may thus order the representations occurring in the decomposition (49) to ensure that X_{ij} is represented by a block tridiagonal matrix on the space $\mathscr{H}$.

We may classify the components X_{ij} into three classes: X_{ii} (diagonal), X_{ij}, $i<j$ (raising), and X_{ij}, $i>j$ (lowering). We consider first the diagonal operators X_{ii} $(i=1, \ldots, n)$. Now for each positive integer $k<n$, the components X_{ij} $(i, j=1, \ldots, k)$ transform as an adjoint tensor operator for the subgroup $U(k)$. Thus any given diagonal component X_{mm} transforms as a component of an adjoint tensor operator with respect to the subgroups $U(m)$, $U(m+1), \ldots, U(n)$. It follows, therefore, that the diagonal operators X_{mm} may be resolved into a sum of simultaneous shift components which shift the Paldus labels of the subgroups $U(m)$, $U(m+1), \ldots, U(n)$ while leaving the Paldus labels of the subgroups $U(m-1), \ldots, U(1)$ unchanged. Since we are only concerned with those components which alter the Paldus labels of the group $U(n)$, we consider the simultaneous shift components of the operators $X_{mm}^{(\pm)}$. We have the resolution

$$X_{mm}^{(\pm)}=\sum_{k_i} X\begin{pmatrix} \pm 1 & k_{n-1} & \cdots & k_m\\ n & n-1 & \cdots & m \end{pmatrix}, \tag{52}$$

where the summation symbol is shorthand for:

$$\sum_{k_{n-1}=-1}^{1} \cdots \sum_{k_m=-1}^{1}.$$

The simultaneous shift component

$$X\begin{pmatrix} k_n & k_{n-1} & \cdots & k_m\\ n & n-1 & \cdots & m \end{pmatrix}, \quad \text{where } k_n=\pm 1,$$

leaves the Paldus labels of the group $U(m-1)$ and its subgroups unchanged and shifts the Paldus labels of the subgroups $U(m), \ldots, U(n)$ according to

$$[a_r, b_r, c_r]\rightarrow[a_r, b_r, c_r]+\boldsymbol{\varepsilon}_{k_r}, \qquad r=m, \ldots, n,$$

where the shifts $\boldsymbol{\varepsilon}_i$ $(i=0, \pm 1)$ are given by Eq. (51).

We remark that in order to preserve the lexicality of the Paldus tableaux, it suffices to consider only those simultaneous shift components which satisfy

$$|k_i - k_{i+1}| \leq 1, \qquad i = m, \ldots, n-1 \tag{53}$$

(i.e., $k_{i+1} = k_i$ or $k_i \pm 1$). A simultaneous shift component not satisfying Eq. (53) necessarily vanishes.

We have shown then that the nonvanishing diagonal adjoint coefficients are of the form (using our previous notation):

$$\left\langle \begin{matrix} \mathbf{P}'_n \\ \mathbf{P}'_{n-1} \\ \vdots \\ \mathbf{P}'_m \\ [\mathbf{P}] \end{matrix} \middle| e_m \otimes \bar{e}_m; \begin{matrix} \mathbf{P}_n \\ \mathbf{P}_{n-1} \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle, \tag{54}$$

where the final tableau labels $\mathbf{P}'_n, \ldots, \mathbf{P}'_m$ are related to the initial tableau labels by

$$\mathbf{P}'_r = \mathbf{P}_r + \boldsymbol{\varepsilon}_{k_r}, \qquad r = m, \ldots, n, \tag{55}$$

where k_r obey the triangular condition (53) and can take on values 0, ± 1 (except that $k_n \neq 0$) and where the shifts $\boldsymbol{\varepsilon}_i$ $(i = 0, \pm 1)$ are given by Eq. (51). We denote the adjoint coefficient (54) by

$$\mathscr{A}\begin{pmatrix} k_n & k_{n-1} & \cdots & k_m \\ n & n-1 & & m \end{pmatrix}, \tag{56}$$

which is a function of the Paldus labels of the initial and final states.

From Eq. (14) we see that the adjoint coefficient (56) may be expressed in terms of vector coupling coefficients according to

$$\mathscr{A}\begin{pmatrix} k_n & \cdots & k_m \\ n & & m \end{pmatrix} = \sum_{j_r=1}^{2} \left\langle \begin{matrix} \mathbf{P}'_n \\ \vdots \\ \mathbf{P}'_m \\ [\mathbf{P}] \end{matrix} \middle| e_m; \begin{matrix} \mathbf{P}_n - \boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_m - \boldsymbol{\delta}_{j_m} \\ [\mathbf{P}] \end{matrix} \right\rangle \left\langle \begin{matrix} \mathbf{P}_n - \boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_m - \boldsymbol{\delta}_{j_m} \\ [\mathbf{P}] \end{matrix} \middle| \bar{e}_m; \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_n \\ [\mathbf{P}] \end{matrix} \right\rangle, \tag{57}$$

where the shifts $\boldsymbol{\delta}_i$ $(i = 1, 2)$ are given by Eq. (34) and the summation symbol is shorthand notation for:

$$\sum_{j_n=1}^{2} \cdots \sum_{j_m=1}^{2}.$$

It is useful to introduce the following coefficients which, for simplicity, we refer to as preadjoint coefficients:

$$
\begin{aligned}
&A\left(\begin{matrix} i_n & \cdots & i_m \\ n & & m \end{matrix}\middle|\begin{matrix} j_n & \cdots & j_m \\ n & & m \end{matrix}\right) \\
&= \left\langle \begin{matrix} \mathbf{P}'_n \\ \vdots \\ \mathbf{P}'_m \\ [\mathbf{P}] \end{matrix} \middle| e_m ; \begin{matrix} \mathbf{P}_n - \boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_m - \boldsymbol{\delta}_{j_m} \\ [\mathbf{P}] \end{matrix} \right\rangle \left\langle \begin{matrix} \mathbf{P}_n - \boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_m - \boldsymbol{\delta}_{j_m} \\ [\mathbf{P}] \end{matrix} \middle| \bar{e}_m ; \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle \\
&= \left(\frac{D[\mathbf{P}'_n]}{D[\mathbf{P}_n - \boldsymbol{\delta}_{j_n}]} \right)^{1/2} \left\langle \begin{matrix} \mathbf{P}_n - \boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_m - \boldsymbol{\delta}_{j_m} \\ [\mathbf{P}] \end{matrix} \middle| \bar{e}_m ; \begin{matrix} \mathbf{P}'_n \\ \vdots \\ \mathbf{P}'_m \\ [\mathbf{P}] \end{matrix} \right\rangle \left\langle \begin{matrix} \mathbf{P}_n - \boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_m - \boldsymbol{\delta}_{j_m} \\ [\mathbf{P}] \end{matrix} \middle| \bar{e}_m ; \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle,
\end{aligned}
$$

where we have used the symmetry relation (41) and where the final Paldus labels $\mathbf{P}'_r$ are given by [cf. Eq. (55)] $\mathbf{P}'_r = \mathbf{P}_r + \boldsymbol{\delta}_{i_r} - \boldsymbol{\delta}_{j_r}$ [i.e., i_r is uniquely specified by $k_r = i_r - j_r$ with k_r as in Eq. (56)]. If the Paldus tableau

$$
\begin{pmatrix} \mathbf{P}_n - \boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_m - \boldsymbol{\delta}_{j_m} \\ [\mathbf{P}] \end{pmatrix}
$$

is nonlexical, the above coefficient necessarily vanishes. Otherwise, it may be expressed in terms of vector coupling coefficients according to

$$
\begin{aligned}
&A\left(\begin{matrix} i_n & \cdots & i_m \\ n & & m \end{matrix}\middle|\begin{matrix} j_n & \cdots & j_m \\ n & & m \end{matrix}\right) \\
&= \left(\frac{D[\mathbf{P}'_n]}{D[\mathbf{P}_n - \boldsymbol{\delta}_{j_n}]} \right)^{1/2} \bar{V}\begin{pmatrix} i_n & \cdots & i_m \\ n & \cdots & m \end{pmatrix}' \bar{V}\begin{pmatrix} j_n & \cdots & j_m \\ n & \cdots & m \end{pmatrix},
\end{aligned} \tag{58}
$$

where the second vector coupling coefficient on the rhs is given by Eq. (39) and the first (primed) vector coupling coefficient is given by Eq. (39), but in terms of the Paldus labels of the final state (i.e., primed labels). The phase of the preadjoint coefficient (58) is given by (in view of the phase convention of Sec. I.7)

$$
\omega = \prod_{r+1}^{n} S(i_r - i_{r-1}) S(j_r - j_{r-1}) (-1)^{[\sigma_{r-1}^{j_r-1} + \sigma_{r-1}'^{\,i_r-1}]}, \tag{59}
$$

where

$$
\begin{aligned}
\sigma_{r-1}^{1} &= 1 + c_{r-1} - c_r, \qquad & \sigma_{r-1}^{2} &= a_r - a_{r-1}, \\
\sigma_{r-1}'^{1} &= 1 + c'_{r-1} - c'_r, \qquad & \sigma_{r-1}'^{2} &= a'_r - a'_{r-1},
\end{aligned}
$$

and where $S(x)$ denotes the sign of x with $S(0) = 1$. Using the Paldus dimension formula [see Eq. (I.41)] together with Eq. (39) we may thus evaluate the preadjoint coefficients (58) (in terms of the Paldus labels of the initial and final states) as required. The full diagonal adjoint coefficients (56) are given in terms of preadjoint coefficients according to [see Eq. (57)]

$$\mathscr{A}\begin{pmatrix} k_n & \cdots & k_m \\ n & & m \end{pmatrix} = \sum_{\substack{i_r, j_r \\ k_r = i_r - j_r}}' A\left(\begin{matrix} i_n & \cdots & i_m \\ n & & m \end{matrix}\middle| \begin{matrix} j_n & \cdots & j_m \\ n & & m \end{matrix}\right), \tag{60}$$

where the prime indicates the only preadjoint coefficients on the rhs, such that the Paldus tableau

$$\begin{pmatrix} \mathbf{P}_n - \boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_m - \boldsymbol{\delta}_{j_m} \\ [\mathbf{P}] \end{pmatrix}$$

is lexical, contribute.

For future reference, we give the explicit form of the preadjoint coefficients below

$$\begin{aligned} &A\left(\begin{matrix} 2 & i_{n-1} & \cdots & i_m \\ n & n-1 & & m \end{matrix}\middle| \begin{matrix} 1 & j_{n-1} & \cdots & j_m \\ n & n-1 & & m \end{matrix}\right) \\ &\quad = \frac{\omega}{1+b_{m-1}} \left(\frac{(b_n-1)(b'_m+2i_m-2)(b_m+2j_m-2)}{b_n(1+c_n)(1+a_n)}\right)^{1/2} \\ &\quad \times \prod_{r=m+1}^{n} [(1+b'_r)^{1/2}]^{-1-|i_r-i_{r-1}|}[(1+b_r)^{1/2}]^{-1-|j_r-j_{r-1}|} \\ &\quad \times [(b'_r+2i_r-2)^{1/2}]^{1-|i_r-i_{r-1}|}[(b_r+2j_r-2)^{1/2}]^{1-|j_r-j_{r-1}|} \end{aligned} \tag{61a}$$

(where $i_n = 2$, $j_n = 1$)

$$\begin{aligned} &A\left(\begin{matrix} 1 & i_{n-1} & \cdots & i_m \\ n & n-1 & & m \end{matrix}\middle| \begin{matrix} 2 & j_{n-1} & \cdots & j_m \\ n & n-1 & & m \end{matrix}\right) \\ &\quad = \frac{\omega'}{1+b_{m-1}} \left(\frac{(b_n+3)(b'_m+2i_m-2)(b_m+2j_m-2)}{(b_n+2)(n+2-c_n)(n+2-a_n)}\right)^{1/2} \\ &\quad \times \prod_{r=m+1}^{n} [(1+b'_r)^{1/2}]^{-1-|i_r-i_{r-1}|}[(1+b_r)^{1/2}]^{-1-|j_r-j_{r-1}|} \\ &\quad \times [(b'_r+2i_r-2)^{1/2}]^{1-|i_r-i_{r-1}|}[(b_r+2j_r-2)^{1/2}]^{1-|j_r-j_{r-1}|} \end{aligned} \tag{61b}$$

(where $i_n = 1, j_n = 2$), where the primed labels indicate the Paldus labels of the final state. The phases ω, $\omega' = \pm 1$ may be determined from Eq. (59).

As a particular case of the above we consider the special adjoint coefficients where the shifts on the subgroup labels are the same [i.e., $k_n = k_{n-1} = \cdots = k_m = \pm 1$ in Eq. (60)]. In this case the preadjoint coefficients and full adjoint coefficients coincide [i.e., there is only a single term on the rhs of Eq. (60)]. We obtain the results:

$$\mathscr{A}\begin{pmatrix} 1 & 1 & \cdots & 1 \\ n & n-1 & \cdots & m \end{pmatrix} = A\left(\begin{matrix} 2 & 2 & \cdots & 2 \\ n & n-1 & \cdots & m \end{matrix}\right|\left.\begin{matrix} 1 & 1 & \cdots & 1 \\ n & n-1 & \cdots & m \end{matrix}\right)$$

$$= \frac{(-1)^{b_n - b_m}}{1+b_{m-1}} \left(\frac{(b_n - 1)(b_m)^2}{b_n(1+c_n)(1+a_n)} \right)^{1/2} \prod_{r=m+1}^{n} \left(\frac{b_r^2}{(b_r - 1)(b_r + 1)} \right)^{1/2}$$

$$= \frac{(-1)^{b_n - b_m}}{1+b_{m-1}} \left(\frac{(b_n - 1)(b_m + 1)(b_m - 1)}{b_n(1+c_n)(1+a_n)} \right)^{1/2} \prod_{r=m}^{n} \left(\frac{b_r^2}{(b_r - 1)(b_r + 1)} \right)^{1/2}, \tag{62a}$$

$$\mathscr{A}\begin{pmatrix} -1 & -1 & \cdots & -1 \\ n & n-1 & \cdots & m \end{pmatrix} = A\left(\begin{matrix} 1 & 1 & \cdots & 1 \\ n & n-1 & \cdots & m \end{matrix}\right|\left.\begin{matrix} 2 & 2 & \cdots & 2 \\ n & n-1 & \cdots & m \end{matrix}\right)$$

$$= \frac{(-1)^{b_n - b_m}}{1+b_{m-1}} \left(\frac{(b_n + 3)(b_m + 2)^2}{(b_n + 2)(n+2-c_n)(n+2-a_n)} \right)^{1/2} \prod_{r=m+1}^{n} \left(\frac{(b_r + 2)^2}{(1+b_r)(3+b_r)} \right)^{1/2}$$

$$= \frac{(-1)^{b_n - b_m}}{1+b_{m-1}} \left(\frac{(b_n + 3)(b_m + 1)(b_m + 3)}{(b_n + 2)(n+2-c_n)(n+2-a_n)} \right)^{1/2} \prod_{r=m}^{n} \left(\frac{(b_r + 2)^2}{(1+b_r)(3+b_r)} \right)^{1/2} \tag{62b}$$

Note that in Eq. (62a) and (62b) we have expressed the adjoint coefficients as a function of the Paldus labels of the initial state only. We may similarly express the general preadjoint coefficients (61a) and (61b) solely in terms of the Paldus labels of the initial state by noting that the final Paldus labels b'_r are related to the initial Paldus labels b_r by the equation:

$$b'_r = b_r + (-1)^{i_r} - (-1)^{j_r}, \qquad r = m, \ldots, n. \tag{63}$$

By this means we obtain a segment-level formula for the preadjoint coefficients solely in terms of the Paldus labels of the initial state.

We remark that the occurrence of more than one preadjoint coefficient contributing to the sum on the rhs of Eq. (60) is because some subgroup Paldus labels may be the same for the initial and final states. If the index $k_r = 0$ (corresponding to the zero shift $\boldsymbol{\varepsilon}_0 = \mathbf{0}$), for $n-1 \geq r \geq m$, then we see that there are two possible choices for the indices i_r, j_r: namely, $i_r = j_r = 1$ and $i_r = j_r = 2$. On the other hand, if $k_r = 1$ (respectively, -1), then we see that there is only one possible choice for the indices i_r and j_r: namely, $i_r = 2$, $j_r = 1$ (respectively, $i_r = 1$, $j_r = 2$). If l denotes the number of indices $k_m, \ldots, k_n$ equal to zero, we see that there can be at most 2^l terms occurring on the rhs of Eq. (60).

We now consider the matrix elements of the operators $X_{ij}^{(\pm)}$ with $i < j$. The operators $X_{m\,m+p}^{(\pm)}$ transform as an adjoint tensor operator with respect to the subgroups $U(m+p), \ldots, U(n)$ as before, but transform as a vector operator with respect to the subgroups $U(m), \ldots, U(m+p-1)$. Thus in this case we obtain the following resolution into simultaneous shift components:

$$X^{(\pm)}_{m\,m+p} = \sum_{k_r=-1}^{+1} \sum_{l_r=1}^{2} X\begin{pmatrix} \pm 1 & \cdots & k_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & \cdots & m+p & \vdots & m+p-1 & \cdots & m \end{pmatrix}, \tag{64}$$

where the summation symbol is shorthand notation for:

$$\sum_{k_{n-1}=-1}^{+1} \cdots \sum_{k_{m+p}=-1}^{+1} \sum_{l_{m+p-1}=1}^{2} \cdots \sum_{l_m=1}^{2}.$$

The simultaneous shift component

$$X\begin{pmatrix} k_n & \cdots & k_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & \cdots & m+p & \vdots & m+p-1 & \cdots & m \end{pmatrix} \qquad (k_n = \pm 1)$$

leaves the Paldus labels of the group $U(m-1)$ and its subgroups unchanged but alters the Paldus labels of the subgroups $U(m), \ldots, U(n)$ according to

$$[a_r, b_r, c_r] \to [a_r, b_r, c_r] + \boldsymbol{\varepsilon}_{k_r} \qquad (r = m+p, \ldots, m),$$
$$[a_q, b_q, c_q] \to [a_q, b_q, c_q] + \boldsymbol{\delta}_{l_q} \qquad (q = m, \ldots, m+p-1),$$

where k_r can take on the values $0, \pm 1$ [subject to the triangular conditions of Eq. (53)] and where l_r can take on values 1, 2. The shifts $\boldsymbol{\delta}_i$ $(i = 1, 2)$ and $\boldsymbol{\varepsilon}_i$ $(i = 0, \pm 1)$ are given by Eqs. (34) and (51), respectively.

This shows that the nonvanishing (raising) adjoint coefficients are of the form (using our previous notation):

$$\left\langle \begin{matrix} \mathbf{P}'_n \\ \vdots \\ \mathbf{P}'_m \\ [\mathbf{P}] \end{matrix} \middle| e_m \otimes \bar{e}_{m+p}; \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle, \tag{65}$$

where the Paldus labels of the final state are related to the Paldus labels of the initial state by

$$\begin{aligned} \mathbf{P}'_r &= \mathbf{P}_r + \boldsymbol{\varepsilon}_{k_r}, \qquad & r &= m+p, \ldots, n, \\ \mathbf{P}'_q &= \mathbf{P}_q + \boldsymbol{\delta}_{l_q}, \qquad & q &= m, \ldots, m+p-1, \end{aligned} \tag{66}$$

where $k_r = 0, \pm 1$ (except that $k_n = \pm 1$) and $l_q = 1, 2$. We denote the adjoint coefficient (65) by

$$\mathscr{A}\begin{pmatrix} k_n & \cdots & k_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & \cdots & m+p & \vdots & m+p-1 & \cdots & m \end{pmatrix}. \tag{67}$$

In this case we introduce the preadjoint coefficients [c.f. Eq. (58) and preceding remarks]

$$
\begin{aligned}
&A\begin{pmatrix} i_n & \cdots & i_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{pmatrix.} \Bigg| \begin{matrix} j_n & \cdots & j_{m+p} \\ n & & m+p \end{matrix}\Bigg) \\
&= \left\langle \begin{matrix} \mathbf{P}'_n \\ \vdots \\ \mathbf{P}'_{m+p} \\ \mathbf{P}'_{m+p-1} \\ \vdots \\ \mathbf{P}'_m \\ [\mathbf{P}] \end{matrix} \;\middle|\; e_m;\; \begin{matrix} \mathbf{P}_n-\boldsymbol{\delta}_{j_m} \\ \vdots \\ \mathbf{P}_{m+p}-\boldsymbol{\delta}_{j_{m+p}} \\ \mathbf{P}_{m+p-1} \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle \left\langle \begin{matrix} \mathbf{P}_n-\boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_{m+p}-\boldsymbol{\delta}_{j_{m+p}} \\ \mathbf{P}_{m+p-1} \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \;\middle|\; \bar{e}_{m+p};\; \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_{m+p} \\ \mathbf{P}_{m+p-1} \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{matrix} \right\rangle \\
&= \left(\frac{D[\mathbf{P}'_n]}{D[\mathbf{P}_n-\boldsymbol{\delta}_{j_n}]}\right)^{1/2} \bar{V}\begin{pmatrix} i_n & \cdots & i_{m+p} & l_{m+p-1} & \cdots & l_m \\ n & & m+p & m+p-1 & & m \end{pmatrix}' \\
&\quad \times \bar{V}\begin{pmatrix} j_n & \cdots & j_{m+p} \\ n & & m+p \end{pmatrix},
\end{aligned}
\tag{68}
$$

where the Paldus labels of the final state are determined by

$$
\begin{aligned}
\mathbf{P}'_r &= \mathbf{P}_r+\boldsymbol{\delta}_{i_r}-\boldsymbol{\delta}_{j_r}, \qquad & r &= m+p, \ldots, n \\
\mathbf{P}'_r &= \mathbf{P}_r+\boldsymbol{\delta}_{l_r} & r &= m, \ldots, m+p-1,
\end{aligned}
$$

and where i_r, j_r and l_r can take values one or two and where the shifts $\boldsymbol{\delta}_i$ ($i=1$, 2) are given by Eq. (34). The $\bar{V}$ coefficients in Eq. (68) are given by Eq. (39) where we note that the first $\bar{V}$ coefficient on the rhs is given as a function of the Paldus labels of the final state (i.e., primed labels) which are determined by Eq. (66). Note that the preadjoint coefficient (68) necessarily vanishes unless the intermediate Paldus tableau

$$
\begin{pmatrix} \mathbf{P}_n-\boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_{m+p}-\boldsymbol{\delta}_{j_{m+p}} \\ \mathbf{P}_{m+p-1} \\ \vdots \\ \mathbf{P}_m \\ [\mathbf{P}] \end{pmatrix}
\tag{69}
$$

is lexical.

In view of Eq. (14), the full adjoint coefficient (67) may be expressed in terms of the preadjoint coefficients (68) according to

$$\mathscr{A}\begin{pmatrix} k_n & \cdots & k_{m+p} \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p \vdots & m+p-1 & & m \end{pmatrix}$$

$$= \sum_{\substack{i_r, j_r \\ k_r = i_r - j_r}}{}' A\left(\begin{matrix} i_n & \cdots & i_{m+p} \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p \vdots & m+p-1 & & m \end{matrix}\middle| \begin{matrix} j_n & \cdots & j_{m+p} \\ n & & m+p \end{matrix}\right), \tag{70}$$

where the prime indicates that only preadjoint coefficients whose intermediate pattern (69) is lexical contribute to the sum in Eq. (70). We remark also that the adjoint coefficient (67) [and the coefficient (56)] necessarily vanishes if the final Paldus tableau is nonlexical.

Now from Eq. (68) we obtain, in view of the composition law (48) for $\bar{V}$-coefficients the following result for the preadjoint coefficients (68):

$$A\left(\begin{matrix} i_n & \cdots & i_{m+p} \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p \vdots & m+p-1 & & m \end{matrix}\middle| \begin{matrix} j_n & \cdots & j_{m+p} \\ n & & m+p \end{matrix}\right)$$

$$= \left(\frac{D[\mathbf{P}_n']}{D[\mathbf{P}_n - \boldsymbol{\delta}_{j_n}]}\right)^{1/2} \bar{\Theta}^{(m+p)'}_{i_{m+p}, l_{m+p-1}} \bar{V}\begin{pmatrix} i_n & \cdots & i_{m+p} \\ n & & m+p \end{pmatrix}'$$

$$\times \bar{V}\begin{pmatrix} j_n & \cdots & j_{m+p} \\ n & & m+p \end{pmatrix} \bar{N}\begin{pmatrix} l_{m+p-1} & \cdots & l_m \\ m+p-1 & & m \end{pmatrix}', \tag{71}$$

where $\bar{\Theta}^{(m+p)}_{i,j}$ is given by Eq. (48) and where the primed terms are given as before but as a function of the Paldus labels of the final state. From Eq. (58) we see that the rhs of Eq. (71) may be expressed in terms of the (diagonal) preadjoint coefficients (58) according to

$$\left(\frac{1+b_{m+p-1}}{1+b'_{m+p-1}}\right)^{1/2} \bar{\Theta}^{(m+p)'}_{i_{m+p}, l_{m+p-1}} \bar{N}\begin{pmatrix} l_{m+p-1} & \cdots & l_m \\ m+p-1 & & m \end{pmatrix}'$$

$$\times A\left(\begin{matrix} i_n & \cdots & i_{m+p} \\ n & & m+p \end{matrix}\middle| \begin{matrix} j_n & \cdots & j_{m+p} \\ n & & m+p \end{matrix}\right), \tag{72}$$

where

$$\bar{\Theta}^{(m+p)'}_{i,j} = (-1)^{[(U^i_{m+p})' - (U^j_{m+p-1})']} S(j-i)\{[(1+b'_{m+p})(b'_{m+p}+2i-2)]^{1/2}\}^{-|i-j|} \tag{73}$$

and where $(U^i_{m+p})'(i=1,2)$ is given by Eq. (38) but in terms of the Paldus labels (i.e., primed labels) of the final state [see Eqs. (63) and (66)]. We remark that the occurrence of the term $[(1+b_{m+p-1})/(1+b'_{m+p-1})]^{1/2}$ in Eq. (72) is because the (diagonal) adjoint coefficient of Eq. (72) depends on the label b_{m+p-1} [see Eq. (61)] and this label is different for the initial and final states of Eq. (68). As before, everything may be expressed in terms of the Paldus labels of the initial state using the relation [c.f. Eq. (63)]:

$$\begin{aligned} b'_r &= b_r + (-1)^{i_r} - (-1)^{j_r}, \qquad && r = m+p, \ldots, n, \\ b'_r &= b_r + (-1)^{l_r}, && r = m, \ldots, m+p-1. \end{aligned} \tag{74}$$

Equation (72) demonstrates that the general matrix elements of the operators $X_{ij}^{(\pm)}$ $(i<j)$ may be obtained from the matrix elements of the diagonal operators $X_{ii}^{(\pm)}$ together with a knowledge of the generator matrix elements.

We may similarly obtain a corresponding expression for the matrix elements of the lowering operators $X_{ij}^{(\pm)}$ $(i>j)$. In this case we consider the adjoint coefficients

$$\bar{\mathscr{A}}\begin{pmatrix} k_n & \cdots & k_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{pmatrix} = \left\langle \begin{matrix} \mathbf{P}'_n \\ \vdots \\ \mathbf{P}'_n \\ [\mathbf{P}] \end{matrix} \middle| e_{m+p} \otimes \bar{e}_m ; \begin{matrix} \mathbf{P}_n \\ \vdots \\ \mathbf{P}_n \\ [\mathbf{P}] \end{matrix} \right\rangle, \tag{75}$$

where the Paldus labels of the final state are given by

$$\begin{aligned} \mathbf{P}'_r &= \mathbf{P}_r - \boldsymbol{\varepsilon}_{k_r}, \qquad & r &= m+p, \ldots, n, \\ \mathbf{P}'_r &= \mathbf{P}_r - \boldsymbol{\delta}_{l_r}, \qquad & r &= m, \ldots, m+p-1, \end{aligned} \tag{76}$$

where k_r can take values $k_r = 0, \pm 1$ [subject to the triangular rule of Eq. (53)] and l_r can take on values $l_r = 1, 2$ and where the shifts $\boldsymbol{\varepsilon}_i$ $(i = 0, \pm 1)$ and $\boldsymbol{\delta}_j$ $(j = 1, 2)$ are given as before. In this case we introduce the preadjoint coefficients [c.f. Eq. (68)]:

$$\begin{aligned} &\bar{A}\left(\begin{matrix} i_n & \cdots & i_{m+p} \\ n & & m+p \end{matrix} \middle| \begin{matrix} j_n & \cdots & j_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{matrix}\right) \\ &\quad = \left(\frac{D[\mathbf{P}'_n]}{D[\mathbf{P}_n - \boldsymbol{\delta}_{j_n}]}\right)^{1/2} \bar{V}\begin{pmatrix} i_n & \cdots & i_{m+p} \\ n & & m+p \end{pmatrix}' \\ &\quad \times \bar{V}\begin{pmatrix} j_n & \cdots & j_{m+p} & l_{m+p-1} & \cdots & l_m \\ n & & m+p & m+p-1 & & m \end{pmatrix}. \end{aligned}$$

Using the decomposition law (47) satisfied by $\bar{V}$ coefficients we thus obtain

$$\begin{aligned} &\bar{A}\left(\begin{matrix} i_n & \cdots & i_{m+p} \\ n & & m+p \end{matrix} \middle| \begin{matrix} j_n & \cdots & j_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{matrix}\right) \\ &\quad = \left(\frac{1+b_{m+p-1}}{1+b'_{m+p-1}}\right)^{1/2} \bar{\Theta}^{(m+p)}_{j_{m+p}, l_{m+p-1}} \bar{N}\begin{pmatrix} l_{m+p-1} & \cdots & l_m \\ m+p-1 & & m \end{pmatrix} \\ &\quad \times A\left(\begin{matrix} i_n & \cdots & i_{m+p} \\ n & & m+p \end{matrix} \middle| \begin{matrix} j_n & \cdots & j_{m+p} \\ n & & m+p \end{matrix}\right), \end{aligned} \tag{77}$$

where $\bar{\Theta}^{(m+p)}_{i,j}$ is given by Eq. (48) and the last term on the rhs of (77) is the diagonal adjoint coefficient which is given by Eq. (61) as before.

The full adjoint coefficient (75) is given as a sum of preadjoint coefficients according to

$$\mathscr{A}\begin{pmatrix} k_n & \cdots & k_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{pmatrix}$$

$$= \sum_{\substack{i_r, j_r \\ k_r = j_r - i_r}}' \bar{A}\left(\begin{matrix} i_n & \cdots & i_{m+p} \\ n & & m+p \end{matrix}\middle| \begin{matrix} j_n & \cdots & j_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{matrix}\right), \quad (78)$$

where the prime indicates that only those coefficients on the rhs whose intermediate Paldus tableau

$$\begin{pmatrix} \mathbf{P}_n - \boldsymbol{\delta}_{j_n} \\ \vdots \\ \mathbf{P}_{m+p} - \boldsymbol{\delta}_{j_{m+p}} \\ \mathbf{P}_{m+p-1} - \boldsymbol{\delta}_{l_{m+p-1}} \\ \vdots \\ \mathbf{P}_m - \boldsymbol{\delta}_{l_m} \\ [\mathbf{P}] \end{pmatrix}$$

is lexical contribute.

Thus we have evaluated all (nonzero shift) adjoint coefficients as required. A close inspection of the preadjoint formulas (72) and (77) shows that the full adjoint coefficients (67) and (75) are related by

$$\mathscr{A}\begin{pmatrix} k_n & \cdots & k_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{pmatrix}$$

$$= \left(\frac{D[\mathbf{P}'_n]}{D[\mathbf{P}_n]}\right)^{1/2} \bar{\mathscr{A}}\begin{pmatrix} k_n & \cdots & k_{m+p} & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{pmatrix}',$$

where $\mathbf{P}'_n = \mathbf{P}_n + \boldsymbol{\varepsilon}_{k_n}$ ($k_n = \pm 1$) and where the prime on the rhs indicates the adjoint coefficient (75) as a function of the labels of the final Paldus tableau [i.e., the primed labels which are determined by Eq. (76)]. This result agrees with the symmetry relations (18) as we require.

We conclude by considering two special cases for the adjoint coefficients (67) and (75). In the case where the Paldus labels of the subgroups $U(m+p), \ldots, U(n)$ are shifted in the same way [i.e., $k_n = k_{n-1} = \cdots = k_{m+p} = \pm 1$ in Eqs. (67) and (75)], the preadjoint coefficients coincide with the full adjoint coefficients [i.e., there is only one term on the rhs of Eq. (70) and (78)]. We obtain the following special cases:

$$\mathscr{A}\begin{pmatrix} 1 & \cdots & 1 & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{pmatrix}$$
$$= A\left(\begin{matrix} 2 & \cdots & 2 & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{matrix}\middle|\begin{matrix} 1 & \cdots & 1 \\ n & & m+p \end{matrix}\right)$$
$$= \bar{\Theta}^{(m+p)'}_{2,l_{m+p-1}}\left(\frac{1+b_{m+p-1}}{1+b'_{m+p-1}}\right)^{1/2}\bar{N}\begin{pmatrix} l_{m+p-1} & \cdots & l_m \\ m+p-1 & & m \end{pmatrix}'$$
$$\times A\left(\begin{matrix} 2 & \cdots & 2 \\ n & & m+p \end{matrix}\middle|\begin{matrix} 1 & \cdots & 1 \\ n & & m+p \end{matrix}\right), \tag{79a}$$

$$\mathscr{A}\begin{pmatrix} -1 & \cdots & -1 & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{pmatrix}$$
$$= A\left(\begin{matrix} 1 & \cdots & 1 & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{matrix}\middle|\begin{matrix} 2 & \cdots & 2 \\ n & & m+p \end{matrix}\right)$$
$$= \left(\frac{1+b_{m+p-1}}{1+b'_{m+p-1}}\right)^{1/2}\bar{\Theta}^{(m+p)'}_{1,l_{m+p-1}}\bar{N}\begin{pmatrix} l_{m+p-1} & \cdots & l_m \\ m+p-1 & & m \end{pmatrix}'$$
$$\times A\left(\begin{matrix} 1 & \cdots & 1 \\ n & & m+p \end{matrix}\middle|\begin{matrix} 2 & \cdots & 2 \\ n & & m+p \end{matrix}\right), \tag{79b}$$

$$\bar{\mathscr{A}}\begin{pmatrix} -1 & \cdots & -1 & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{pmatrix}$$
$$= \bar{A}\left(\begin{matrix} 2 & \cdots & 2 \\ n & & m+p \end{matrix}\middle|\begin{matrix} 1 & \cdots & 1 & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{matrix}\right)$$
$$= \left(\frac{1+b_{m+p-1}}{1+b'_{m+p-1}}\right)^{1/2}\bar{\Theta}^{(m+p)}_{1,l_{m+p-1}}\bar{N}\begin{pmatrix} l_{m+p-1} & \cdots & l_m \\ m+p-1 & & m \end{pmatrix}$$
$$\times A\left(\begin{matrix} 2 & \cdots & 2 \\ n & & m+p \end{matrix}\middle|\begin{matrix} 1 & \cdots & 1 \\ n & & m+p \end{matrix}\right), \tag{80a}$$

$$\bar{\mathscr{A}}\begin{pmatrix} 1 & \cdots & 1 & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{pmatrix}$$
$$= \bar{A}\left(\begin{matrix} 1 & \cdots & 1 \\ n & & m+p \end{matrix}\middle|\begin{matrix} 2 & \cdots & 2 & \vdots & l_{m+p-1} & \cdots & l_m \\ n & & m+p & & m+p-1 & & m \end{matrix}\right)$$
$$= \left(\frac{1+b_{m+p-1}}{1+b'_{m+p-1}}\right)^{1/2}\bar{\Theta}^{(m+p)}_{2,l_{m+p-1}}\bar{N}\begin{pmatrix} l_{m+p-1} & \cdots & l_m \\ m+p-1 & & m \end{pmatrix}$$
$$\times A\left(\begin{matrix} 1 & \cdots & 1 \\ n & & m+p \end{matrix}\middle|\begin{matrix} 2 & \cdots & 2 \\ n & & m+p \end{matrix}\right). \tag{80b}$$

We may make the formulas above fully explicit using the known formulas for the generator matrix elements [see Eq. (I.77) and (I.79)] and the adjoint coefficient formulas (62). We record here two special cases of the above formulas which will be needed in the next paper of the present series

$$\begin{aligned}
&\mathscr{A}\begin{pmatrix} 1 & \cdots & 1 \vdots 2 & \cdots & 2 \\ n & & m+p \vdots m+p-1 & & m \end{pmatrix} \\
&\quad = A\begin{pmatrix} 2 & \cdots & 2 \vdots 2 & \cdots & 2 & 1 & \cdots & 1 \\ n & & m+p \vdots m+p-1 & & m & n & & m+p \end{pmatrix} \\
&\quad = (-1)^{a_{m+p}-a_{m+p-1}}\left(\frac{1+b_{m+p-1}}{b_{m+p-1}}\right)^{1/2} \bar{N}\begin{pmatrix} 2 & \cdots & 2 \\ m+p-1 & & m \end{pmatrix}' \\
&\quad\quad \times A\begin{pmatrix} 2 & \cdots & 2 & 1 & \cdots & 1 \\ n & & m+p & n & & m+p \end{pmatrix},
\end{aligned} \tag{81a}$$

$$\begin{aligned}
&\bar{\mathscr{A}}\begin{pmatrix} 1 & \cdots & 1 \vdots 2 & \cdots & 2 \\ n & & m+p \vdots m+p-1 & & m \end{pmatrix} \\
&\quad = \bar{A}\begin{pmatrix} 1 & \cdots & 1 & 2 & \cdots & 2 \vdots 2 & \cdots & 2 \\ n & & m+p & n & & m+p \vdots m+p-1 & & m \end{pmatrix} \\
&\quad = (-1)^{a_{m+p}-a_{m+p-1}}\left(\frac{1+b_{m+p-1}}{2+b_{m+p-1}}\right)^{1/2} \bar{N}\begin{pmatrix} 2 & \cdots & 2 \\ m+p-1 & & m \end{pmatrix} \\
&\quad\quad \times A\begin{pmatrix} 1 & \cdots & 1 & 2 & \cdots & 2 \\ n & & m+p & n & & m+p \end{pmatrix},
\end{aligned} \tag{81b}$$

which may be evaluated using Eq. (62) and (I.85)–(I.96).

6. Simplifications and Connection with the Two-Body Operators

It was pointed out by Drake and Schlesinger [5] that there appears to be a close relationship between the matrix elements of spin-dependent operators and the matrix elements of (spin-independent) two-body operators. We demonstrate here that the matrix elements of unit adjoint tensor operators may be obtained from the known matrix elements of two body operators. This implies that in determining the adjoint coefficients of this paper (and ultimately the matrix elements of spin-dependent operators), one only need calculate the matrix elements of two-body operators (and these are needed in CI calculations anyway).

We present two different approaches, one being recursive and the other using the subgroup embedding $U(n) \subset U(n+1)$. We begin by considering the group $U(n)$ as a subgroup of $U(n+1)$. We then note that the operators [c.f. Eq. (10)]

$$Y_{ij} = E_{i\,n+1} E_{n+1\,j}$$

transform as an adjoint tensor operator of $U(n)$. Hence applying the $U(n)$ WE theorem [see Eq. (13)], we obtain

$$\left\langle \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}'_n \end{matrix} \middle\| Y \middle\| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n \end{matrix} \right\rangle \left\langle \begin{matrix} \mathbf{P}'_n \\ [\mathbf{P}'] \end{matrix} \middle| e_i \otimes \bar{e}_j ; \begin{matrix} \mathbf{P}_n \\ [\mathbf{P}] \end{matrix} \right\rangle = \left\langle \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}'_n \\ [\mathbf{P}'] \end{matrix} \middle| E_{i\,n+1} E_{n+1\,j} \middle| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n \\ [\mathbf{P}] \end{matrix} \right\rangle,$$

where $[\mathbf{P}]$ and $[\mathbf{P}']$ are Paldus tableaux for the subgroup $U(n-1)$. The lhs of the above equation may be written

$$\left\langle \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n + \boldsymbol{\delta}_2 - \boldsymbol{\delta}_1 \end{matrix} \middle\| \Psi \middle\| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n - \boldsymbol{\delta}_1 \end{matrix} \right\rangle \left\langle \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n - \boldsymbol{\delta}_1 \end{matrix} \middle\| \Psi^\dagger \middle\| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n \end{matrix} \right\rangle \times \left\langle \begin{matrix} \mathbf{P}_n + \boldsymbol{\delta}_2 - \boldsymbol{\delta}_1 \\ [\mathbf{P}'] \end{matrix} \middle| e_i \otimes \bar{e}_j ; \begin{matrix} \mathbf{P}_n \\ [\mathbf{P}] \end{matrix} \right\rangle,$$

where the first two terms are the reduced matrix elements of the vector (respectively, contragredient vector) operator $\Psi_i = E_{i\,n+1}$ (respectively, $\Psi_i^\dagger = E_{n+1\,i}$) which may be evaluated from Eq. (I.43), viz.

$$\left\langle \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n + \boldsymbol{\delta}_2 - \boldsymbol{\delta}_1 \end{matrix} \middle\| \Psi \middle\| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n - \boldsymbol{\delta}_1 \end{matrix} \right\rangle = \left(\frac{(1+a_n)b_n}{1+b_{n+1}} \right)^{1/2},$$

$$\left\langle \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n - \boldsymbol{\delta}_1 \end{matrix} \middle\| \Psi^\dagger \middle\| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n \end{matrix} \right\rangle = \left(\frac{(1+c_n)(1+b_n)}{1+b_{n+1}} \right)^{1/2}.$$

Thus we obtain the result:

$$\left\langle \begin{matrix} \mathbf{P}_n + \boldsymbol{\delta}_2 - \boldsymbol{\delta}_1 \\ [\mathbf{P}'] \end{matrix} \middle| e_i \otimes \bar{e}_j ; \begin{matrix} \mathbf{P}_n \\ [\mathbf{P}] \end{matrix} \right\rangle$$

$$= \frac{1+b_{n+1}}{[(1+c_n)(1+a_n)b_n(1+b_n)]^{1/2}} \left\langle \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n + \boldsymbol{\delta}_2 - \boldsymbol{\delta}_1 \\ [\mathbf{P}'] \end{matrix} \middle| E_{i\,n+1} E_{n+1\,j} \middle| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n \\ [\mathbf{P}] \end{matrix} \right\rangle. \tag{82}$$

We similarly obtain

$$\left\langle \begin{matrix} \mathbf{P}_n + \boldsymbol{\delta}_1 - \boldsymbol{\delta}_2 \\ [\mathbf{P}'] \end{matrix} \middle| e_i \otimes \bar{e}_j ; \begin{matrix} \mathbf{P}_n \\ [\mathbf{P}] \end{matrix} \right\rangle$$

$$= \frac{1+b_{n+1}}{[(n+2-c_n)(n+2-a_n)(1+b_n)(2+b_n)]^{1/2}} \left\langle \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n + \boldsymbol{\delta}_1 - \boldsymbol{\delta}_2 \\ [\mathbf{P}'] \end{matrix} \middle| E_{i\,n+1} E_{n+1\,j} \middle| \begin{matrix} \mathbf{P}_{n+1} \\ \mathbf{P}_n \\ [\mathbf{P}] \end{matrix} \right\rangle. \tag{83}$$

Equations (82) and (83) show how the general (nonzero shift) $U(n)$ adjoint coefficients follow from the known matrix elements of the $U(n+1)$ generators. Thus our (independent) derivation of the $U(n)$ adjoint coefficients is closely related to the problem of finding the matrix elements of two-body operators. This suggests that the approach of this paper may be extended to obtain the matrix elements of two-body operators.

Finally we note an alternative (recursive) method for obtaining the $U(n)$ adjoint coefficients. If X_{ij} is a unit $U(n)$ adjoint tensor operator, we have

$$X_{ij}=[E_{ij}, X_{jj}], \qquad i\neq j \tag{84}$$

showing that the matrix elements of the nondiagonal operators X_{ij} $(i\neq j)$ may be obtained from those of the diagonal operators X_{jj} and the known matrix elements of the $U(n)$ generators. Thus it suffices, in principle, to determine only the diagonal unit adjoint tensor operators [see Eqs. (57)–(61)]. This fact was implicitly used in our derivation of the general adjoint coefficients, but it may be computationally advantageous to use Eq. (84) directly.

In fact, it suffices, in principle, to determine the matrix elements of the single component X_{nn}. For this simple case we have [see Eqs. (61) for the case $m=n$]

$$\left\langle \begin{matrix}\mathbf{P}_n+\boldsymbol{\delta}_2-\boldsymbol{\delta}_1\\ [\mathbf{P}']\end{matrix}\right| X_{nn} \left|\begin{matrix}\mathbf{P}_n\\ [\mathbf{P}]\end{matrix}\right\rangle = \left\langle \begin{matrix}\mathbf{P}_n+\boldsymbol{\delta}_2-\boldsymbol{\delta}_1\\ [\mathbf{P}']\end{matrix}\right| e_n\otimes\bar{e}_n; \left.\begin{matrix}\mathbf{P}_n\\ [\mathbf{P}]\end{matrix}\right\rangle$$

$$= \delta_{[\mathbf{P}'],[\mathbf{P}]}\frac{1}{1+b_{n-1}}\left(\frac{b_n(b_n-1)}{(1+c_n)(1+a_n)}\right)^{1/2}, \tag{85}$$

$$\left\langle \begin{matrix}\mathbf{P}_n+\boldsymbol{\delta}_1-\boldsymbol{\delta}_2\\ [\mathbf{P}]\end{matrix}\right| X_{nn} \left|\begin{matrix}\mathbf{P}_n\\ [\mathbf{P}]\end{matrix}\right\rangle = \left\langle \begin{matrix}\mathbf{P}_n+\boldsymbol{\delta}_1-\boldsymbol{\delta}_2\\ [\mathbf{P}']\end{matrix}\right| e_n\otimes\bar{e}_n; \left.\begin{matrix}\mathbf{P}_n\\ [\mathbf{P}]\end{matrix}\right\rangle$$

$$= \delta_{[\mathbf{P}'],[\mathbf{P}]}\frac{1}{1+b_{n-1}}\left(\frac{(b_n+3)(b_n+2)}{(n+2-a_n)(n+2-c_n)}\right)^{1/2}, \tag{86}$$

where $[\mathbf{P}']$ and $[\mathbf{P}]$ are two Paldus tableaux for the subgroup $U(n-1)$. Using Eqs. (85) and (86) we may obtain the matrix elements of the operators X_{in} and X_{ni} using the relation:

$$X_{in}=[E_{in}, X_{nn}], \qquad X_{ni}=[E_{ni}, X_{nn}], \qquad i<n.$$

The matrix elements of the general operator X_{ij} are then given by

$$X_{ij}=[E_{nj}, X_{in}]=[E_{nj},[E_{in}, X_{nn}]], \qquad i\neq j<n,$$

$$X_{ii}=X_{nn}-[E_{ni}, X_{in}]=X_{nn}-[E_{ni},[E_{in}, X_{nn}]], \qquad i<n.$$

Thus using Eqs. (85) and (86) together with the matrix elements of two-body operators, the above relations show that one may obtain the general $U(n)$ adjoint coefficients as required.

Since a segment-level formula may be obtained for the matrix elements of products of two generators (see Refs. 4 and 5), Eqs. (82) and (83) suggest that a segment-level formula is obtainable for the $U(n)$ adjoint coefficients. We shall consider this aspect of the problem in a future publication.

Appendix

We derive here certain symmetry relations satisfied by $U(n)$ Clebsch–Gordon coefficients which were used in Sec. 2. Our approach follows that of Louck and co-workers [8–10] (also see Refs. 7–12).

Let $V(\boldsymbol{\lambda})$ be an irreducible (finite dimensional) representation of $U(n)$ with highest weight $\boldsymbol{\lambda}$. Then we may choose an orthonormal basis $e_1, \ldots, e_d$ [$d = \dim V(\boldsymbol{\lambda})$] consisting of weight vectors (see Sect. I.2 for definitions). We assume the basis vector e_i has weight $\boldsymbol{\lambda}_i$ [where $\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_d$ are the weights occurring in $V(\boldsymbol{\lambda})$]. Suppose $\{T_i\}_{i=1}^{d}$ is an irreducible tensor operator of rank $\boldsymbol{\lambda}$ (with respect to the basis $\{e_i\}$) and let

$$T_i^\dagger = (T_i)^\dagger$$

be the Hermitian conjugate of T.

Now let $V(\boldsymbol{\mu})$ be an irreducible representation of $U(n)$ with highest weight $\boldsymbol{\mu}$. Then the irreducible representations occurring in the tensor product $V(\boldsymbol{\lambda}) \otimes V(\boldsymbol{\mu})$ have highest weights of the form $\boldsymbol{\mu} + \boldsymbol{\lambda}_i$ $(i = 1, \ldots, d)$ and where the representation $V(\boldsymbol{\mu} + \boldsymbol{\lambda}_i)$ may possibly occur with multiplicities (see, e.g., Edwards and Gould [7]). If the representation $V(\boldsymbol{\mu} + \boldsymbol{\lambda}_i)$ occurs with unit multiplicity in the space $V(\boldsymbol{\lambda}) \otimes V(\boldsymbol{\mu})$, we obtain, using the $U(n)$ WE theorem, the result

$$\left\langle \begin{matrix} \boldsymbol{\mu}+\boldsymbol{\lambda}_i \\ (\boldsymbol{\nu}') \end{matrix} \middle| T_j \middle| \begin{matrix} \boldsymbol{\mu} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle = \langle \boldsymbol{\mu}+\boldsymbol{\lambda}_i \| T \| \boldsymbol{\mu} \rangle \left\langle \begin{matrix} \boldsymbol{\mu}+\boldsymbol{\lambda}_i \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_j;\ \begin{matrix} \boldsymbol{\mu} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle, \tag{A1}$$

where $\left| \begin{smallmatrix} \boldsymbol{\mu} \\ (\boldsymbol{\nu}) \end{smallmatrix} \right\rangle$ and $\left| \begin{smallmatrix} \boldsymbol{\mu}+\boldsymbol{\lambda}_i \\ (\boldsymbol{\nu}') \end{smallmatrix} \right\rangle$ are two Gel'fand basis states for the spaces $V(\boldsymbol{\mu})$ and $V(\boldsymbol{\mu} + \boldsymbol{\lambda}_i)$, respectively. Taking the Hermitian conjugate of Eq. (A1) we obtain the relations

$$\begin{aligned} \left\langle \begin{matrix} \boldsymbol{\mu} \\ (\boldsymbol{\nu}) \end{matrix} \middle| T_j^\dagger \middle| \begin{matrix} \boldsymbol{\mu}+\boldsymbol{\lambda}_i \\ (\boldsymbol{\nu}') \end{matrix} \right\rangle &= \langle \boldsymbol{\mu} \| T^\dagger \| \boldsymbol{\mu}+\boldsymbol{\lambda}_i \rangle \left\langle \begin{matrix} \boldsymbol{\mu} \\ (\boldsymbol{\nu}) \end{matrix} \middle| \bar{e}_j;\ \begin{matrix} \boldsymbol{\mu}+\boldsymbol{\lambda}_i \\ (\boldsymbol{\nu}') \end{matrix} \right\rangle \\ &= \langle \boldsymbol{\mu}+\boldsymbol{\lambda}_i \| T \| \boldsymbol{\mu} \rangle^* \left\langle \begin{matrix} \boldsymbol{\mu}+\boldsymbol{\lambda}_i \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_j;\ \begin{matrix} \boldsymbol{\mu} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle^*, \end{aligned} \tag{A2}$$

where $\bar{e}_j$ denotes the dual basis for the contragredient representation $V^*(\boldsymbol{\lambda})$ of $V(\boldsymbol{\lambda})$. However, for $U(n)$ the phases for the Clebsch–Gordon coefficients may be chosen real. Moreover, the reduced matrix elements are independent of the labels j, $(\boldsymbol{\nu})$, and $(\boldsymbol{\nu}')$, from which it follows that we may write

$$\left\langle \begin{matrix} \boldsymbol{\mu} \\ (\boldsymbol{\nu}) \end{matrix} \middle| \bar{e}_j;\ \begin{matrix} \boldsymbol{\mu}+\boldsymbol{\lambda}_i \\ (\boldsymbol{\nu}') \end{matrix} \right\rangle = \eta \left\langle \begin{matrix} \boldsymbol{\mu}+\boldsymbol{\lambda}_i \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_j;\ \begin{matrix} \boldsymbol{\mu} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle,$$

where η is a constant independent of $(\boldsymbol{\nu})$, $(\boldsymbol{\nu}')$, and j.

Taking the modulus squared of both sides of this relation and summing on $(\boldsymbol{\nu})$, $(\boldsymbol{\nu}')$, and j, we obtain the result

$$\eta = \pm (D[\boldsymbol{\mu}]/D[\boldsymbol{\mu}+\boldsymbol{\lambda}_i])^{1/2}. \tag{A3}$$

However, Baird and Biedenharn [8, 9] have shown that the maximal Wigner coefficients may be chosen to have a positive real phase from which we deduce that η in Eq. (A3) can be chosen positive. Thus we obtain the relation:

$$\left\langle \begin{matrix} \boldsymbol{\mu} \\ (\boldsymbol{\nu}) \end{matrix} \middle| \bar{e}_j; \begin{matrix} \boldsymbol{\mu}+\boldsymbol{\lambda}_i \\ (\boldsymbol{\nu}') \end{matrix} \right\rangle = \left(\frac{D[\boldsymbol{\mu}]}{D[\boldsymbol{\mu}+\boldsymbol{\lambda}_i]} \right)^{1/2} \left\langle \begin{matrix} \boldsymbol{\mu}+\boldsymbol{\lambda}_i \\ (\boldsymbol{\nu}') \end{matrix} \middle| e_j; \begin{matrix} \boldsymbol{\mu} \\ (\boldsymbol{\nu}) \end{matrix} \right\rangle. \tag{A4}$$

From Eq. (A2) we also obtain the result:

$$\langle \boldsymbol{\mu}+\boldsymbol{\lambda}_i \| T \| \boldsymbol{\mu} \rangle^* = \left(\frac{D[\boldsymbol{\mu}]}{D[\boldsymbol{\mu}+\boldsymbol{\lambda}_i]} \right)^{1/2} \langle \boldsymbol{\mu} \| T^\dagger \| \boldsymbol{\mu}+\boldsymbol{\lambda}_i \rangle.$$

If the reduced matrix elements are real, we thus obtain:

$$\langle \boldsymbol{\mu}+\boldsymbol{\lambda}_i \| T \| \boldsymbol{\mu} \rangle = \left(\frac{D(\boldsymbol{\mu}]}{D[\boldsymbol{\mu}+\boldsymbol{\lambda}_i]} \right)^{1/2} \langle \boldsymbol{\mu} \| T^\dagger \| \boldsymbol{\mu}+\boldsymbol{\lambda}_i \rangle. \tag{A5}$$

Equations (16)–(18) of Sect. 2 are a special case of Eqs. (A4) and (A5).

Acknowledgments

The authors would like to express their appreciation for the referees' invaluable comments which have helped improve the paper in several places. They also acknowledge helpful discussions with Dr. R. Glass. This work was carried out under support from the Australian Research Grants Scheme.

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Received January 10, 1983
Accepted for publication July 5, 1983