# The evaluation of U(2n) matrix elements in Weyl-basis tableaux adapted to U(2) × U(n)



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# The evaluation of U(2$n$) matrix elements in Weyl-basis tableaux adapted to U(2)×U($n$)†

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**Abstract.** This paper presents simple and clear closed expressions of the generator matrix elements of U(2$n$) in Weyl-basis tableaux, symmetry adapted to U(2)×U($n$).

## 1. Introduction

In recent papers [1, 2] we have presented a Weyl graphical method for evaluating the matrix elements of U($n$) generators as well as products of generators. It is our aim in this paper to derive a closed expression of the matrix elements of U(2$n$) generators in Weyl-basis tableaux adapted to U(2)×U($n$). This expression will be applied to dealing with the spin-dependent Hamiltonians in many-electron systems.

For spin-dependent Hamiltonians, Harter and Patterson [3] have advocated the evaluation of the matrix elements in the Slater basis and transferred the results to the spin-orbit basis via their 'assembly formula'. By considering the transformation properties of the generators of U(2$n$) under commutation with the generators of U($n$)×U(2), Gould and Chandler [4] have derived the adjoint coupling coefficients and used them for calculating the matrix elements of the generators of U(2$n$) in a Paldus-basis symmetry adapted to the subgroup U($n$)×U(2) (i.e. the spin-orbit basis). Recently, a different approach was developed by Lev [5] who presented an iterative method for calculating the matrix representatives of spin-dependent operators in the symmetric-group approach to many-electron systems, by considering the Lie algebra of the totally symmetric spin-dependent operators and their generators.

In this paper we shall apply the results of [1, 2] as well as the Wigner–Eckart theorem to obtaining the closed formulae of U(2$n$) generator matrix elements in the spin-orbit basis for the three cases of $\Delta S=0$, $\pm1$. In our derivation we find it both convenient and natural to introduce an additional quantum number $P$ into the case of $\Delta S=0$. Such a procedure thereby offers a new insight and is more reasonable than that of Gould and Chandler. The closed formulae derived in this paper are simpler and clearer as well as more practical than those presented in [4, 5] and all the results are the same as those obtained by Lev's method (up to a phase factor).

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We should also note that the method developed in this paper may be extended into the evaluation of U($mn$) matrix elements in a Weyl-basis tableau, symmetry adapted to the subgroup U($m$)×U($n$), which we will undertake in the future.

This paper is organised as follows. The general theory and derivation are outlined in § 2. The specific formulae for different shifts of $\Delta S$ are then developed in § 3 and several examples are also given out in this section. Finally, the technique for obtaining the whole column of the U($2n$) generator matrix representation is presented in § 4.

## 2. General theory

Let $|W_{2n}\rangle$ be the canonical Weyl-basis tableau spanning the irreducible representation (IR) $[1^N]$ of U($2n$), where $N$ is the number of electrons in the system concerned. Let $|W_2, W_n\rangle$ be a non-canonical Weyl-basis tableau, symmetry adapted to the group chain U($2n$) ⊃ U(2)×U($n$) (i.e. spin-orbit basis), where $|W_2\rangle$ or $|W_n\rangle$ denotes the canonical Weyl-basis tableau spanning the IR $[Y_2]$ or U(2) of $[Y_n]$ or U($n$). $[Y_2]$ and $[Y_n]$ must be manually the conjugate Young diagram, namely $[Y_2]=[\tilde{Y}_n]$, by virtue of Pauli's exclusion principle. If we designate $\lambda_i$ ($i=1, 2$) as the number of boxes in the $i$th column of $[Y_n]$, or that in the $i$th row of $[Y_2]$, both $[Y_2]$ and $[Y_n]$ can be labelled by $[\lambda_1\ \lambda_2]$, and $\lambda_1$, $\lambda_2$ satisfy relations such that

$$\begin{aligned} &\lambda_1+\lambda_2=N \\ &S=(\lambda_1-\lambda_2)/2 \end{aligned} \tag{1}$$

where $S$ is the spin quantum number of the system.

By the transformation properties of the U($2n$) generators and the well known Wigner–Eckart theorem, the matrix elements of the U($2n$) generator $a_{\mu i,\nu j}$ (the Greek subscripts refer to spin orbital and the Latin subscripts refer to space orbitals) between the spin-orbit basis can be expressed in the form

$$\begin{aligned} &\left\langle \begin{matrix}[\lambda_1'\ \lambda_2']\\ W_2'\ \ W_n'\end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix}[\lambda_1\ \lambda_2]\\ W_2\ \ W_n\end{matrix}\right\rangle \\ &\qquad = \langle[\lambda_1'\ \lambda_2']\|a\|[\lambda_1\ \lambda_2]\rangle \left\langle \begin{matrix}[\lambda_1'\ \lambda_2']\\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu};\ \begin{matrix}[\lambda_1\ \lambda_2]\\ W_2\end{matrix}\right\rangle \\ &\qquad \times \left\langle \begin{matrix}[\lambda_1'\ \lambda_2']\\ W_n'\end{matrix} \middle| i\otimes\bar{j};\ \begin{matrix}[\lambda_1\ \lambda_2]\\ W_n\end{matrix}\right\rangle \qquad \mu,\ \nu=-\tfrac{1}{2}, \tfrac{1}{2} \qquad i, j=1, 2, \ldots, n \end{aligned} \tag{2}$$

where the first term on the right-hand side is the U(2)×U($n$) reduced matrix element, being independent of the weights of the IR for U(2) and U($n$). The second and third terms are the coupling coefficients for U(2) and U($n$), respectively, where $i\otimes\bar{j}$ is the unit basis tensor, in terms of Weyl tableaux, for the carried tensor product space $\Gamma\otimes\Gamma^*$ of U($n$), and $\mu\otimes\bar{\nu}$ is that of U(2). (For typographic convenience, we have omitted the squares surrounding the letters or numbers in the Weyl tableaux.) The explicit expressions for the coupling coefficients for U(2), which are completely known, are shown in the appendix. In this paper, we address the solution for the coupling coefficients for U($n$) and the reduced matrix elements in (2).

According to the reduction of product of Young diagrams, the U($2n$) matrix elements in (2) will be zero unless the IR of initial, intermediate and final states satisfy the selection rules in table 1 labelled by $\Delta S=S'-S$ and an additional quantum number

**Table 1.** The selection rules for the non-zero coupling coefficients of U(2) or U($n$).

| | $[\lambda_1' \ \lambda_2']$ | $[\lambda_1'' \ \lambda_2'']$ | $[\lambda_1 \ \lambda_2]$ |
|---|---|---|---|
| $\Delta S=-1$ | $\lambda_1-1 \ \lambda_2+1$ | $\lambda_1-1 \ \lambda_2$ | $\lambda_1 \ \lambda_2$ |
| $\Delta S=0 \ P=1$ | $\lambda_1 \ \lambda_2$ | $\lambda_1-1 \ \lambda_2$ | $\lambda_1 \ \lambda_2$ |
| $\Delta S=0 \ P=2$ | $\lambda_1 \ \lambda_2$ | $\lambda_1 \ \lambda_2-1$ | $\lambda_1 \ \lambda_2$ |
| $\Delta S=1$ | $\lambda_1+1 \ \lambda_2-1$ | $\lambda_1 \ \lambda_2-1$ | $\lambda_1 \ \lambda_2$ |

$P$ $(=1, 2)$ in the case of $\Delta S=0$. Therefore (2) can be rewritten as the two following subformulae:

$$\left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_2' \ \ W_n'\end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_2 \ \ W_n\end{matrix} \right\rangle_{\Delta S} = \langle[\lambda_1' \ \lambda_2']\|a\|[\lambda_1 \ \lambda_2]\rangle_{\Delta S} \left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu}; \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_2\end{matrix} \right\rangle_{\Delta S} \times \left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_n'\end{matrix} \middle| i\otimes\bar{j}; \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_n\end{matrix} \right\rangle_{\Delta S} \qquad \Delta S=\pm 1 \tag{3a}$$

$$\left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_2' \ \ W_n'\end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_2 \ \ W_n\end{matrix} \right\rangle_{\Delta S} = \sum_{P=1,2} \left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_2' \ \ W_n'\end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_2 \ \ W_n\end{matrix} \right\rangle_{\Delta S}^{P} = \sum_{P=1,2} \langle[\lambda_1' \ \lambda_2']\|a\|[\lambda_1 \ \lambda_2]\rangle_{\Delta S}^{P} \times \left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu}; \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_2\end{matrix} \right\rangle_{\Delta S}^{P} \left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_n'\end{matrix} \middle| i\otimes\bar{j}; \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_n\end{matrix} \right\rangle_{\Delta S}^{P} \qquad \Delta S=0. \tag{3b}$$

For the sake of eliminating the reduced matrix elements in (3$a$) and (3$b$), we consider the U($2n$) matrix elements between the only possible highest-weight spin-orbit basis states belonging to the IR $[\lambda_1' \ \lambda_2']$ and IR $[\lambda_1 \ \lambda_2]$, respectively. Let us assume that these matrix elements can be evaluated and expressed by the form

$$\left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_{2,m}' \ \ W_{n,m}'\end{matrix} \middle| a_{\alpha k,\beta l} \middle| \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_{2,m} \ \ W_{n,m}\end{matrix} \right\rangle_{\Delta S}^{P} = A_{\Delta S}^{P} \tag{4}$$

where the subscript $m$ refers to the maximal state and $a_{\alpha k,\beta l}$ is the appropriate U($2n$) generator making the matrix element non-zero. The subscripts $\alpha$, $\beta$, $k$, $l$ can be determined by the labels $\lambda_1$, $\lambda_2$, $\Delta S$ and $P$ (see the next section). Obviously, it is also possible to factorise, in terms of the Wigner–Eckart theorem, the matrix elements of (4) into the product of coupling coefficients for U(2) and U($n$) and the reduced matrix element, which is equal to that appearing in (3). Then, combining (3) and eliminating the reduced matrix elements, we obtain the following formulae:

$$\left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_2' \ \ W_n'\end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_2 \ \ W_n\end{matrix} \right\rangle_{\Delta S} = A_{\Delta S} \left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu}; \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_2\end{matrix} \right\rangle_{\Delta S} \left( \left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_{2,m}'\end{matrix} \middle| \alpha\otimes\bar{\beta}; \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_{2,m}\end{matrix} \right\rangle_{\Delta S} \right)^{-1} \times \left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_n'\end{matrix} \middle| i\otimes\bar{j}; \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_n\end{matrix} \right\rangle_{\Delta S} \left( \left\langle \begin{matrix}[\lambda_1' \ \lambda_2']\\ W_{n,m}'\end{matrix} \middle| k\otimes\bar{l}; \begin{matrix}[\lambda_1 \ \lambda_2]\\ W_{n,m}\end{matrix} \right\rangle_{\Delta S} \right)^{-1} \qquad \Delta S=\pm 1 \tag{5a}$$

$$\left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_2' \ \ W_n'\end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_2 \ \ W_n\end{matrix} \right\rangle_{\Delta S}$$

$$= \sum_{P=1,2} A^P_{\Delta S} \left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu}; \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_2\end{matrix} \right\rangle^P_{\Delta S} \left( \left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_{2,m}'\end{matrix} \middle| \alpha\otimes\bar{\beta}; \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_{2,m}\end{matrix} \right\rangle^P_{\Delta S} \right)^{-1}$$

$$\times \left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_n'\end{matrix} \middle| i\otimes\bar{j}; \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_n\end{matrix} \right\rangle^P_{\Delta S} \left( \left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_{n,m}'\end{matrix} \middle| k\otimes\bar{l}; \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_{n,m}\end{matrix} \right\rangle^P_{\Delta S} \right)^{-1}$$

$$\Delta S = 0. \tag{5b}$$

We now restrict our attention to the remaining problem of the ratio between two U($n$) coupling coefficients in (5). We denote by $E_{ij}$ the U($n$) generator related to the U($2n$) generators by

$$E_{ij} = \sum_{\mu=-1/2}^{1/2} a_{\mu i,\mu j} \qquad i, j = 1, 2, \ldots, n. \tag{6}$$

Using the property of $E_{i,n+1}$ ($i = 1, 2, \ldots, n$) constituting a vector operator of U($n$) and the Wigner-Eckart theorem again, we have

$$\left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_n'\end{matrix} \middle| i\otimes\bar{j}; \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_n\end{matrix} \right\rangle^P_{\Delta S} \left( \left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_{n,m}'\end{matrix} \middle| k\otimes\bar{l}; \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_{n,m}\end{matrix} \right\rangle^P_{\Delta S} \right)^{-1}$$

$$= \left\langle \begin{matrix}[Y_{n+1}] \\ [\lambda_1' \ \lambda_2'] \\ W_n'\end{matrix} \middle| E_{i,n+1} E_{n+1,j} \middle| \begin{matrix}[Y_{n+1}] \\ [\lambda_1 \ \lambda_2] \\ W_n\end{matrix} \right\rangle^P_{\Delta S} \left( \left\langle \begin{matrix}[Y_{n+1}] \\ [\lambda_1' \ \lambda_2'] \\ W_{n,m}'\end{matrix} \middle| E_{k,n+1} E_{n+1,l} \middle| \begin{matrix}[Y_{n+1}] \\ [\lambda_1 \ \lambda_2] \\ W_{n,m}\end{matrix} \right\rangle^P_{\Delta S} \right)^{-1} \tag{7}$$

where the selection of IR $[Y_{n+1}]$ of U($n+1$) should satisfy the reducing conditions as

$$\begin{aligned} &[Y_{n+1}] \supset [\lambda_1' \ \lambda_2'] && \text{i.e. } [Y_n'] \\ &[Y_{n+1}] \supset [\lambda_1'' \ \lambda_2''] && \text{i.e. } [Y_n''] \\ &[Y_{n+1}] \supset [\lambda_1 \ \lambda_2] && \text{i.e. } [Y_n]. \end{aligned} \tag{8}$$

Substituting (7) into (5), we thereby obtain the general formulae for U($2n$) generator matrix elements in the spin-orbit basis as follows:

$$\left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_2' \ \ W_n'\end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_2 \ \ W_n\end{matrix} \right\rangle_{\Delta S}$$

$$= A_{\Delta S} \left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu}; \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_2\end{matrix} \right\rangle_{\Delta S} \left( \left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_{2,m}'\end{matrix} \middle| \alpha\otimes\bar{\beta}; \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_{2,m}\end{matrix} \right\rangle_{\Delta S} \right)^{-1}$$

$$\times \left\langle \begin{matrix}[Y_{n+1}] \\ [\lambda_1' \ \lambda_2'] \\ W_n'\end{matrix} \middle| E_{i,n+1} E_{n+1,j} \middle| \begin{matrix}[Y_{n+1}] \\ [\lambda_1 \ \lambda_2] \\ W_n\end{matrix} \right\rangle_{\Delta S} \left( \left\langle \begin{matrix}[Y_{n+1}] \\ [\lambda_1' \ \lambda_2'] \\ W_{n,m}'\end{matrix} \middle| E_{k,n+1} E_{n+1,l} \middle| \begin{matrix}[Y_{n+1}] \\ [\lambda_1 \ \lambda_2] \\ W_{n,m}\end{matrix} \right\rangle_{\Delta S} \right)^{-1}$$

$$\Delta S = \pm 1 \tag{9a}$$

$$\left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_2' \ \ W_n'\end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_2 \ \ W_n\end{matrix} \right\rangle_{\Delta S}$$

$$= \sum_{P=1,2} A^P_{\Delta S} \left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu}; \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_2\end{matrix} \right\rangle^P_{\Delta S} \left( \left\langle \begin{matrix}[\lambda_1' \ \lambda_2'] \\ W_{2,m}'\end{matrix} \middle| \alpha\otimes\bar{\beta}; \begin{matrix}[\lambda_1 \ \lambda_2] \\ W_{2,m}\end{matrix} \right\rangle^P_{\Delta S} \right)^{-1}$$

$$\times\left\langle\begin{matrix}[Y_{n+1}]\\ [\lambda_1'\ \lambda_2']\\ W_n'\end{matrix}\right| E_{i,n+1}E_{n+1,j}\left|\begin{matrix}[Y_{n+1}]\\ [\lambda_1\ \lambda_2]\\ W_n\end{matrix}\right\rangle_{\Delta S}^{P}\left(\left\langle\begin{matrix}[Y_{n+1}]\\ [\lambda_1'\ \lambda_2']\\ W_{n,m}'\end{matrix}\right|E_{k,n+1}E_{n+1,l}\left|\begin{matrix}[Y_{n+1}]\\ [\lambda_1\ \lambda_2]\\ W_{n,m}\end{matrix}\right\rangle_{\Delta S}^{P}\right)^{-1}$$

$$\Delta S=0. \tag{9b}$$

## 3. Specific formulae for different shifts of $\Delta S$

In this section the specific closed formulae of U($2n$) generator matrix elements in a spin–orbit basis are derived under the different shifts of $\Delta S=\pm1$, 0.

### 3.1. $\Delta S=+1$

In this case of $[\lambda_1'\ \lambda_2']=[\lambda_1+1\ \ \lambda_2-1]$ and $[\lambda_1''\ \lambda_2'']=[\lambda_1\ \ \lambda_2-1]$, the highest-weight non-canonical Weyl-basis tableaux are:

$$\left|\begin{matrix}[\lambda_1\ \lambda_2]\\ W_{2,m}\ \ W_{n,m}\end{matrix}\right\rangle = \left|\begin{array}{l}\overbrace{\uparrow\uparrow\cdots\uparrow\uparrow\cdots\uparrow\uparrow}^{\lambda_1}\\ \underbrace{\downarrow\downarrow\cdots\downarrow\downarrow}_{\lambda_2}\end{array} \otimes \begin{array}{cc}1 & 1\\ 2 & 2\\ \vdots&\vdots\\ \lambda_2&\lambda_2\\ \vdots & \\ \lambda_1 & \end{array}\right\rangle$$

and

$$\left|\begin{matrix}[\lambda_1'\ \lambda_2']\\ W_{2,m}'\ \ W_{n,m}'\end{matrix}\right\rangle = \left|\begin{array}{l}\overbrace{\uparrow\uparrow\cdots\uparrow\uparrow\cdots\uparrow\uparrow\uparrow}^{\lambda_1+1}\\ \underbrace{\downarrow\downarrow\cdots\downarrow}_{\lambda_2-1}\end{array} \otimes \begin{array}{cc}1 & 1\\ 2 & 2\\ \vdots&\vdots\\ \lambda_2-1&\lambda_2-1\\ \lambda_2 & \\ \vdots & \\ \lambda_1 & \\ \lambda_1+1 & \end{array}\right\rangle.$$

By comparison of primed and unprimed Weyl tableaux, the determination of $\alpha$, $\beta$, $k$ and $l$ is that

$$k=\lambda_1+1 \qquad l=\lambda_2 \qquad \alpha=\uparrow \qquad \beta=\downarrow.$$

The U(2) coupling coefficient between the highest-weight Weyl tableaux is evaluated below by using the formulae in the appendix:

$$\left\langle\begin{matrix}[\lambda_1'\ \lambda_2']\\ W_{2,m}'\end{matrix}\right|\alpha\otimes\bar{\beta};\ \begin{matrix}[\lambda_1\ \lambda_2]\\ W_{2,m}\end{matrix}\Bigg\rangle_{\Delta S=1}$$

$$=\left\langle\begin{array}{l}\overbrace{\uparrow\uparrow\cdots\uparrow\uparrow\cdots\uparrow\uparrow\uparrow}^{\lambda_1+1}\\ \underbrace{\downarrow\downarrow\cdots\downarrow}_{\lambda_2-1}\end{array}\right|\uparrow\otimes\bar{\downarrow};\ \begin{array}{l}\overbrace{\uparrow\uparrow\cdots\uparrow\uparrow\cdots\uparrow\uparrow}^{\lambda_1}\\ \underbrace{\downarrow\downarrow\cdots\downarrow\downarrow}_{\lambda_2}\end{array}\Bigg\rangle_{\Delta S=1}$$

$$
=\left\langle \begin{array}{l} \overbrace{\uparrow\uparrow\cdots\uparrow\uparrow\cdots\uparrow\uparrow\uparrow}^{\lambda_1+1} \\ \underbrace{\downarrow\downarrow\cdots\downarrow}_{\lambda_2-1} \end{array} \right| \uparrow ; \left. \begin{array}{l} \overbrace{\uparrow\uparrow\cdots\uparrow\uparrow\cdots\uparrow\uparrow}^{\lambda_1} \\ \underbrace{\downarrow\downarrow\cdots\downarrow}_{\lambda_2-1} \end{array} \right\rangle
$$

$$
\times\left\langle \begin{array}{l} \overbrace{\uparrow\uparrow\cdots\uparrow\uparrow\cdots\uparrow\uparrow}^{\lambda_1} \\ \underbrace{\downarrow\downarrow\cdots\downarrow}_{\lambda_2-1} \end{array} \right| \updownarrow ; \left. \begin{array}{l} \overbrace{\uparrow\uparrow\cdots\uparrow\uparrow\cdots\uparrow\uparrow}^{\lambda_1} \\ \underbrace{\downarrow\downarrow\cdots\downarrow\downarrow}_{\lambda_2} \end{array} \right\rangle
$$

$$
=1\times 1=1. \tag{10a}
$$

For this case the $[Y_{n+1}]$ of $\mathrm{U}(n+1)$ satisfying (8) should be $[\lambda_1+1\ \ \lambda_2]$ and the positions of the boxes entered by the number $n+1$ in the final, intermediate and initial Weyl tableaux of $\mathrm{U}(n+1)$ are shown in figure 1. Thus, the matrix element of the two-body operator $E_{k,n+1}E_{n+1,l}$ appearing in the denominator in (5$a$) can easily be evaluated by virtue of the method presented in [1] as

$$
\left\langle \begin{array}{c} [Y_{n+1}] \\ [\lambda_1+1\ \ \lambda_2-1] \\ W'_{n,m} \end{array} \right| E_{k,n+1}E_{n+1,l} \left| \begin{array}{c} [Y_{n+1}] \\ [\lambda_1\ \ \lambda_2] \\ W_{n,m} \end{array} \right\rangle_{\Delta S=1}
$$

$$
=\left\langle \begin{array}{ll} 1 & 1 \\ \vdots & \vdots \\ \lambda_2-1 & \lambda_2-1 \\ \lambda_2 & n+1 \\ \vdots & \\ \lambda_1 & \\ \lambda_1+1 & \end{array} \right| E_{\lambda_1+1,n+1}E_{n+1,\lambda_2} \left| \begin{array}{ll} 1 & 1 \\ \vdots & \vdots \\ \lambda_2-1 & \lambda_2-1 \\ \lambda_2 & \lambda_2 \\ \vdots & \\ \lambda_1 & \\ n+1 & \end{array} \right\rangle
$$

$$
=\left\langle \begin{array}{ll} 1 & 1 \\ \vdots & \vdots \\ \lambda_2-1 & \lambda_2-1 \\ \lambda_2 & n+1 \\ \vdots & \\ \lambda_1 & \\ \lambda_1+1 & \end{array} \right| E_{\lambda_1+1,n+1} \left| \begin{array}{ll} 1 & 1 \\ \vdots & \vdots \\ \lambda_2-1 & \lambda_2-1 \\ \lambda_2 & n+1 \\ \vdots & \\ \lambda_1 & \\ n+1 & \end{array} \right\rangle
$$

$$
\times\left\langle \begin{array}{ll} 1 & 1 \\ \vdots & \vdots \\ \lambda_2-1 & \lambda_2-1 \\ \lambda_2 & n+1 \\ \vdots & \\ \lambda_1 & \\ n+1 & \end{array} \right| E_{n+1,\lambda_2} \left| \begin{array}{ll} 1 & 1 \\ \vdots & \vdots \\ \lambda_2-1 & \lambda_2-1 \\ \lambda_2 & \lambda_2 \\ \vdots & \\ \lambda_1 & \\ n+1 & \end{array} \right\rangle
$$

$$
=\left(\frac{d+2}{d+1}\right)^{1/2} \qquad d=\lambda_1-\lambda_2+1. \tag{10b}
$$

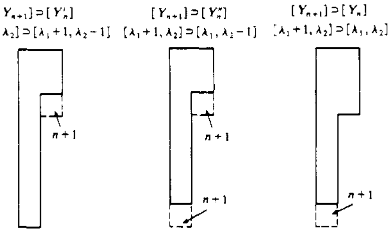


**Figure 1.** The positions of the number $n+1$ in the final, intermediate and initial Weyl tableaux of $\mathrm{U}(n+1)$ for the case of $\Delta S=1$.

Finally, the value of $A_{\Delta S=1}$ in $(5a)$ is determined by

$$A_{\Delta S=1}=\left\langle \begin{matrix} [\lambda'_1\ \lambda'_2] \\ W'_{2,m}\ \ W'_{n,m}\end{matrix} \middle| a_{\alpha k;\beta l} \middle| \begin{matrix} [\lambda_1\ \lambda_2] \\ W_{2,m}\ \ W_{n,m}\end{matrix}\right\rangle_{\Delta S=1}$$

$$=\left\langle \begin{matrix} \overbrace{\uparrow\uparrow\cdots\uparrow\uparrow\cdots\uparrow\uparrow\uparrow}^{\lambda_1+1} \\ \underbrace{\downarrow\downarrow\cdots\downarrow}_{\lambda_2-1} \end{matrix} \otimes \begin{matrix} 1 & 1 \\ \vdots & \vdots \\ \lambda_2-1 & \lambda_2-1 \\ \lambda_2 & \\ \vdots & \\ \lambda_1 & \\ \lambda_1+1 & \end{matrix} \middle| a_{\uparrow,\lambda_1+1;\downarrow\lambda_2} \middle| \begin{matrix} \overbrace{\uparrow\uparrow\cdots\uparrow\uparrow\cdots\uparrow\uparrow}^{\lambda_1} \\ \underbrace{\downarrow\downarrow\cdots\downarrow\downarrow}_{\lambda_2} \end{matrix} \otimes \begin{matrix} 1 & 1 \\ \vdots & \vdots \\ \lambda_2-1 & \lambda_2-1 \\ \lambda_2 & \lambda_2 \\ \vdots & \\ \lambda_1 & \end{matrix} \right\rangle$$

$$=\left\langle \begin{matrix} 1 \\ 2 \\ \vdots \\ 2\lambda_2-2 \\ 2\lambda_2-1 \\ 2\lambda_2+1 \\ \vdots \\ 2\lambda_1-1 \\ 2\lambda_1+1 \end{matrix} \middle| a_{2\lambda_1+1,2\lambda_2} \middle| \begin{matrix} 1 \\ 2 \\ \vdots \\ 2\lambda_2-2 \\ 2\lambda_2-1 \\ 2\lambda_2 \\ 2\lambda_2+1 \\ \vdots \\ 2\lambda_1-1 \end{matrix} \right\rangle =(-1)^{d+1} \tag{10c}$$

where we have used the property of the transformation coefficients from the maximal non-canonical Weyl tableaux of $\mathrm{U}(2n)$

$$\left| \begin{matrix} [\lambda'_1\ \lambda'_2] \\ W'_{2,m}\ \ W'_{n,m}\end{matrix} \right\rangle \qquad \text{and} \qquad \left| \begin{matrix} [\lambda_1\ \lambda_2] \\ W_{2,m}\ \ W_{n,m}\end{matrix} \right\rangle$$

to their corresponding canonical Weyl tableaux being value one, and the single index $\eta$ $(\eta=1,2,\ldots,2n)$ for the $\mathrm{U}(2n)$ generators in the expression of matrix elements between canonical Weyl tableaux. The single index $\eta$ is associated with the index pair $(\mu i)$ by

$$\eta = 2i-1 \qquad \text{for } \mu = \tfrac{1}{2}$$
$$\eta = 2i \qquad \text{for } \mu = -\tfrac{1}{2}.$$

From 9$(a)$, $(10a)$, $(10b)$ and $(10c)$, the expression of U$(2n)$ matrix elements in the spin-orbit basis for the shift $\Delta S = 1$ is obtained as

$$\left\langle \begin{matrix}[\lambda_1+1\ \ \lambda_2-1]\\ W_2'\ \ W_n'\end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix}[\lambda_1\ \ \lambda_2]\\ W_2\ \ W_n\end{matrix}\right\rangle_{\Delta S=1}$$
$$= (-1)^{d+1}\left(\frac{d+1}{d+2}\right)^{1/2} \left\langle \begin{matrix}(\lambda_1+1\ \ \lambda_2-1]\\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu};\ \begin{matrix}[\lambda_1\ \ \lambda_2]\\ W_2\end{matrix}\right\rangle_{\Delta S}$$
$$\times \left\langle \begin{matrix}[\lambda_1+1\ \ \lambda_2]\\ [\lambda_1+1\ \ \lambda_2-1]\\ W_n'\end{matrix} \middle| E_{i,n+1}\,E_{n+1,j} \middle| \begin{matrix}[\lambda_1+1\ \ \lambda_2]\\ [\lambda_1\ \ \lambda_2]\\ W_n\end{matrix}\right\rangle_{\Delta S} \qquad \Delta S = 1. \tag{11}$$

It is necessary to mention that, in using (11), the calculation of the matrix elements of the two-body operator $E_{i,n+1}\,E_{n+1,j}$ must be parallel to that of $E_{k,n+1}\,E_{n+1,l}$ in $(10b)$. In other words, the positions of $n+1$ in the final, intermediate and initial Weyl tableaux must be identical to those shown in figure 1.

### *3.2. $\Delta S = -1$*

In this case, we have

$$[\lambda_1'\ \ \lambda_2'] = [\lambda_1-1\ \ \lambda_2+1] \qquad [\lambda_1''\ \ \lambda_2''] = [\lambda_1-1\ \ \lambda_2].$$

In the same way as above we can take

$$k = \lambda_2+1 \qquad l = \lambda_1 \qquad \alpha = \downarrow \qquad \beta = \uparrow.$$

The $[Y_{n+1}]$ of U$(n+1)$ should be $[\lambda_1\ \ \lambda_2+1]$ and figure 2 shows the positions of the number $n+1$ in the final, intermediate and initial Weyl tableaux of U$(n+1)$. Thus the factors in $(9a)$ can be evaluated as

$$\left\langle \begin{matrix}[\lambda_1'\ \ \lambda_2']\\ W_{2,m}'\end{matrix} \middle| \alpha\otimes\bar{\beta};\ \begin{matrix}[\lambda_1\ \ \lambda_2]\\ W_{2,m}\end{matrix}\right\rangle_{\Delta S=-1} = \left(\frac{d-2}{d}\right)^{1/2}$$

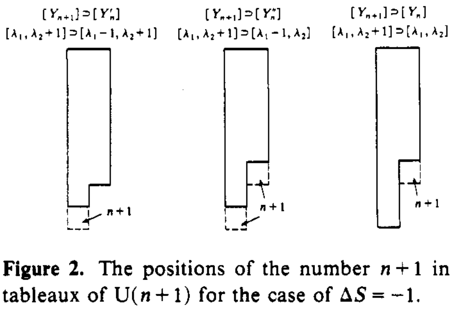


**Figure 2.** The positions of the number $n+1$ in the final, intermediate and initial Weyl tableaux of U$(n+1)$ for the case of $\Delta S = -1$.

$$\left\langle \begin{matrix} [Y_{n+1}] \\ [\lambda_1' \ \lambda_2'] \\ W'_{n,m} \end{matrix} \middle| E_{k,n+1} E_{n+1,l} \middle| \begin{matrix} [Y_{n+1}] \\ [\lambda_1 \ \lambda_2] \\ W_{n,m} \end{matrix} \right\rangle_{\Delta S=-1} = \left(\frac{d}{d-1}\right)^{1/2} \tag{12}$$

$$A_{\Delta S=-1} = (-1)^{d-1}.$$

Substituting (12) into (9*a*), we, finally, obtain the expression of U(2$n$) matrix elements in the spin-orbit basis for the shift $\Delta S=-1$ as follows:

$$\left\langle \begin{matrix} [\lambda_1-1 \ \lambda_2+1] \\ W_2' \ W_n' \end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2 \ W_n \end{matrix} \right\rangle_{\Delta S}$$

$$= (-1)^{d-1}\left(\frac{d-1}{d-2}\right)^{-1/2} \left\langle \begin{matrix} [\lambda_1-1 \ \lambda_2+1] \\ W_2' \end{matrix} \middle| \mu\otimes\bar{\nu}; \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2 \end{matrix} \right\rangle_{\Delta S}$$

$$\times \left\langle \begin{matrix} [\lambda_1 \ \lambda_2+1] \\ [\lambda_1-1 \ \lambda_2+1] \\ W_n' \end{matrix} \middle| E_{i,n+1} E_{n+1,j} \middle| \begin{matrix} [\lambda_1 \ \lambda_2+1] \\ [\lambda_1 \ \lambda_2] \\ W_n \end{matrix} \right\rangle_{\Delta S} \qquad \Delta S=-1. \tag{13}$$

### 3.3. $\Delta S=0$

The case is somewhat complicated because two intermediate IR, $[\lambda_1-1 \ \lambda_2]$ and $[\lambda_1 \ \lambda_2-1]$, are involved. An additional quantum number $P$ is introduced to solve this problem. That is, all the intermediate states which appeared in the calculation must belong to the indicated IR of U(2) or U($n$) for each given $P$. The detailed derivation is as below:

*P = 1.* From table 1 we have in this subcase

$$[\lambda_1' \ \lambda_2'] = [\lambda_1 \ \lambda_2] \qquad \text{and} \qquad [\lambda_1'' \ \lambda_2''] = [\lambda_1-1 \ \lambda_2].$$

It is natural to take $k=\lambda_1$, $l=\lambda_1$, $\alpha=\uparrow$ and $\beta=\uparrow$. The $[Y_{n+1}]$ of U($n+1$) is chosen as $[\lambda_1 \ \lambda_2]$. Figure 3 shows the positions of the number $n+1$ in the final, intermediate and initial Weyl tableaux of U($n+1$). Similarly, we have

$$\left\langle \begin{matrix} [\lambda_1' \ \lambda_2'] \\ W'_{2,m} \end{matrix} \middle| \alpha\otimes\bar{\beta}; \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_{2,m} \end{matrix} \right\rangle^{P=1}_{\Delta S=0} = \left(\frac{d-1}{d}\right)^{1/2}$$

$$\left\langle \begin{matrix} [Y_{n+1}] \\ [\lambda_1' \ \lambda_2'] \\ W'_{n,m} \end{matrix} \middle| E_{k,n+1} E_{n+1,l} \middle| \begin{matrix} [Y_{n+1}] \\ [\lambda_1 \ \lambda_2] \\ W_{n,m} \end{matrix} \right\rangle^{P=1}_{\Delta S=0} = 1 \tag{14}$$

$$A^{P=1}_{\Delta S=0} = 1.$$

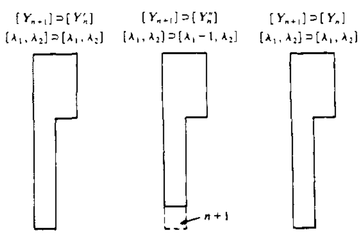


**Figure 3.** The positions of the number $n+1$ in the final, intermediate and initial Weyl tableaux of U($n+1$) for the case of $\Delta S=0$ and $P=1$.

$P=2$. In this subcase, $[\lambda_1' \ \lambda_2']=[\lambda_1 \ \lambda_2]$ and $[\lambda_1'' \ \lambda_2'']=[\lambda_1 \ \lambda_2-1]$. It is natural to take $k=\lambda_2$, $l=\lambda_2$, $\alpha=\downarrow$ and $\beta=\downarrow$. The $[Y_{n+1}]$ of $\mathrm{U}(n+1)$ is chosen as $[\lambda_1 \ \lambda_2]$. Figure 4 shows the positions of the number $n+1$ in the final, intermediate and initial Weyl tableaux of $\mathrm{U}(n+1)$ under the above choice. Thus, we have

$$\left\langle \begin{matrix} [\lambda_1' \ \lambda_2'] \\ W_{2,m}' \end{matrix} \middle| \alpha \otimes \bar{\beta}; \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_{2,m} \end{matrix} \right\rangle^{P=2}_{\Delta S=0} = \left(\frac{d}{d+1}\right)^{1/2}$$

$$\left\langle \begin{matrix} [Y_{n+1}] \\ [\lambda_1' \ \lambda_2'] \\ W_{n,m}' \end{matrix} \middle| E_{k,n+1} E_{n+1,l} \middle| \begin{matrix} [Y_{n+1}] \\ [\lambda_1 \ \lambda_2] \\ W_{n,m} \end{matrix} \right\rangle^{P=2}_{\Delta S=0} = \frac{d+1}{d} \tag{15}$$

$$A^{P=2}_{\Delta S=0}=1.$$

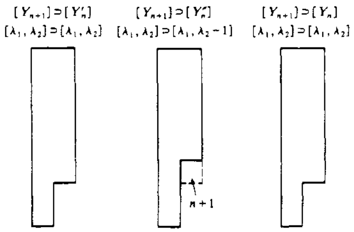


**Figure 4.** The positions of the number $n+1$ in the final, intermediate and initial Weyl tableaux of $\mathrm{U}(n+1)$ for the case of $\Delta S=0$ and $P=2$.

Substituting (14) and (15) into (9*b*), the final expression for $\Delta S=0$ is obtained as

$$\begin{aligned} &\left\langle \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2' \ \ W_n' \end{matrix} \middle| a_{\mu i,\nu j} \middle| \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2 \ \ W_n \end{matrix} \right\rangle_{\Delta S=0} \\ &\quad = \left(\frac{d}{d-1}\right)^{1/2} \left\langle \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2' \end{matrix} \middle| \mu \otimes \bar{\nu}; \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2 \end{matrix} \right\rangle^{P=1}_{\Delta S=0} \\ &\quad \times \left\langle \begin{matrix} [\lambda_1 \ \lambda_2] \\ [\lambda_1 \ \lambda_2] \\ W_n' \end{matrix} \middle| E_{i,n+1} E_{n+1,j} \middle| \begin{matrix} [\lambda_1 \ \lambda_2] \\ [\lambda_1 \ \lambda_2] \\ W_n \end{matrix} \right\rangle^{P=1}_{\Delta S=0} \\ &\quad + \left(\frac{d}{d+1}\right)^{1/2} \left\langle \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2' \end{matrix} \middle| \mu \otimes \bar{\nu}; \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2 \end{matrix} \right\rangle^{P=2}_{\Delta S=0} \\ &\quad \times \left\langle \begin{matrix} [\lambda_1 \ \lambda_2] \\ [\lambda_1 \ \lambda_2] \\ W_n' \end{matrix} \middle| E_{i,n+1} E_{n+1,j} \middle| \begin{matrix} [\lambda_1 \ \lambda_2] \\ [\lambda_1 \ \lambda_2] \\ W_n \end{matrix} \right\rangle^{P=2}_{\Delta S=0} \qquad \Delta S=0. \end{aligned} \tag{16}$$

Some examples will be given to demonstrate the use of equations (13) and (16). Before doing so, we emphasise again that, in the application of these formulae the positions of the number $n+1$ in the Weyl tableaux of $\mathrm{U}(n+1)$ must be the same as those in the corresponding figures 1-4.

*Example 1.* For $n=8$, $d=4$, $\Delta S=-1$:

$$\left\langle \begin{array}{l}\uparrow\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\downarrow\end{array} \otimes \begin{array}{cc}1&2\\2&4\\5&6\\7&7\\8&\end{array} \right| a_{\downarrow 6;\uparrow 3} \left| \begin{array}{l}\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\end{array} \otimes \begin{array}{cc}1&2\\2&3\\4&7\\5&\\7&\\8&\end{array} \right\rangle$$

$$=(-1)^3\left(\frac{4-1}{4-2}\right)^{1/2}\left\langle \begin{array}{l}\uparrow\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\downarrow\end{array}\right| \downarrow\otimes\bar{\uparrow};\ \left.\begin{array}{l}\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\end{array}\right\rangle \left\langle \begin{array}{cc}1&2\\2&4\\5&6\\7&7\\8&\\9&\end{array} \right| E_{69}E_{93} \left| \begin{array}{cc}1&2\\2&3\\4&7\\5&9\\7&\\8&\end{array} \right\rangle$$

$$=(-1)^3\left(\frac{3}{2}\right)^{1/2}\left[\left(\frac{1}{3}\right)^{1/2}\left(\frac{2}{4}\right)^{1/2}\right] \left\langle \begin{array}{cc}1&2\\2&4\\5&6\\7&7\\8&\\9&\end{array} \right| E_{69} \left| \begin{array}{cc}1&2\\2&4\\5&7\\7&9\\8&\\9&\end{array} \right\rangle \left\langle \begin{array}{cc}1&2\\2&4\\5&7\\7&9\\8&\\9&\end{array} \right| E_{93} \left| \begin{array}{cc}1&2\\2&3\\4&7\\5&9\\7&\\8&\end{array} \right\rangle$$

$$=(-1)\sqrt{\frac{3}{2}}\sqrt{\frac{1}{3}}\sqrt{\frac{2}{4}}\left(-\sqrt{\frac{1}{2}}\right)\sqrt{\frac{1}{3}}=\frac{1}{12}\sqrt{6}.$$

*Example 2.* For $n=7$, $d=3$, $\Delta S=0$:

$$\left\langle \begin{array}{l}\uparrow\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\end{array} \otimes \begin{array}{cc}1&1\\2&2\\3&7\\4&\\6&\end{array} \right| a_{\uparrow 1;\downarrow 5} \left| \begin{array}{l}\uparrow\uparrow\uparrow\downarrow\downarrow\\ \downarrow\downarrow\downarrow\end{array} \otimes \begin{array}{cc}1&2\\2&3\\4&5\\6&\\7&\end{array} \right\rangle$$

$$=\left(\frac{3}{3-1}\right)^{1/2}\left\langle \begin{array}{l}\uparrow\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\end{array}\right| \uparrow\otimes\bar{\downarrow};\ \left.\begin{array}{l}\uparrow\uparrow\uparrow\downarrow\downarrow\\ \downarrow\downarrow\downarrow\end{array}\right\rangle^{P=1} \left\langle \begin{array}{cc}1&1\\2&2\\3&7\\4&\\6&\end{array} \right| E_{18}E_{85} \left| \begin{array}{cc}1&2\\2&3\\4&5\\6&\\7&\end{array} \right\rangle^{P=1}$$

$$+\left(\frac{3}{3+1}\right)^{1/2}\left\langle \begin{array}{l}\uparrow\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\end{array}\right| \uparrow\otimes\bar{\downarrow};\ \left.\begin{array}{l}\uparrow\uparrow\uparrow\downarrow\downarrow\\ \downarrow\downarrow\downarrow\end{array}\right\rangle^{P=2} \left\langle \begin{array}{cc}1&1\\2&2\\3&7\\4&\\6&\end{array} \right| E_{18}E_{85} \left| \begin{array}{cc}1&2\\2&3\\4&5\\6&\\7&\end{array} \right\rangle^{P=2}$$

$$
=\left(\frac{3}{2}\right)^{1/2}\left\langle\begin{matrix}\uparrow\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\end{matrix}\middle|\uparrow;\ \begin{matrix}\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\end{matrix}\right\rangle\left\langle\begin{matrix}\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\end{matrix}\middle|\bar{\downarrow};\ \begin{matrix}\uparrow\uparrow\uparrow\downarrow\downarrow\\ \downarrow\downarrow\downarrow\end{matrix}\right\rangle
$$

$$
\times\left\{\left\langle\begin{matrix}1&1\\2&2\\3&7\\4&\\6&\end{matrix}\middle| E_{18}\middle|\begin{matrix}1&2\\2&3\\4&6\\7&\\8&\end{matrix}\right\rangle\left\langle\begin{matrix}1&2\\2&3\\4&6\\7&\\8&\end{matrix}\middle| E_{85}\middle|\begin{matrix}1&2\\2&3\\4&5\\6&\\7&\end{matrix}\right\rangle\right.
$$

$$
\left.+\left\langle\begin{matrix}1&1\\2&2\\3&7\\4&\\6&\end{matrix}\middle| E_{18}\middle|\begin{matrix}1&2\\2&3\\4&7\\6&\\8&\end{matrix}\right\rangle\left\langle\begin{matrix}1&2\\2&3\\4&7\\6&\\8&\end{matrix}\middle| E_{85}\middle|\begin{matrix}1&2\\2&3\\4&5\\6&\\7&\end{matrix}\right\rangle\right\}
$$

$$
+\left(\frac{3}{4}\right)^{1/2}\left\langle\begin{matrix}\uparrow\uparrow\uparrow\uparrow\downarrow\\ \downarrow\downarrow\downarrow\end{matrix}\middle|\uparrow;\ \begin{matrix}\uparrow\uparrow\uparrow\downarrow\downarrow\\ \downarrow\downarrow\end{matrix}\right\rangle\left\langle\begin{matrix}\uparrow\uparrow\uparrow\downarrow\downarrow\\ \downarrow\downarrow\end{matrix}\middle|\bar{\downarrow};\ \begin{matrix}\uparrow\uparrow\uparrow\downarrow\downarrow\\ \downarrow\downarrow\downarrow\end{matrix}\right\rangle
$$

$$
\times\left\{\left\langle\begin{matrix}1&1\\2&2\\3&7\\4&\\6&\end{matrix}\middle| E_{18}\middle|\begin{matrix}1&2\\2&3\\4&8\\6&\\7&\end{matrix}\right\rangle\left\langle\begin{matrix}1&2\\2&3\\4&8\\6&\\7&\end{matrix}\middle| E_{85}\middle|\begin{matrix}1&2\\2&3\\4&5\\6&\\7&\end{matrix}\right\rangle\right\}
$$

$$
=\sqrt{\frac{3}{2}}\sqrt{\frac{1}{2}}\sqrt{\frac{2}{3}}\left[(0)\left(\frac{1}{2}\right)+\left(\frac{2}{3}\right)\left(-\frac{1}{6}\sqrt{3}\right)\right]
$$

$$
+\sqrt{\frac{3}{4}}\left(-\sqrt{\frac{2}{4}}\right)\sqrt{\frac{1}{3}\frac{1}{6}}\sqrt{2}\sqrt{\frac{2}{3}}
$$

$$
=-\frac{1}{12}\sqrt{6}.
$$

These results are the same as evaluated by using the method of Lev [5].

## 4. The matrix representation

In this section we will discuss briefly the matrix representation of the U($2n$) generator. It is clear that, for a given $\Delta S$ and $P$, the U(2) coupling coefficients are identical for all the U($2n$) matrix elements with the same generator $a_{\mu i,\nu j}$ and the same initial Weyl tableau $\left|\begin{matrix}[\lambda_1 & \lambda_2]\\ W_2 & W_n\end{matrix}\right\rangle$. So, the whole column of the U($2n$) generator matrix representation may be related to the following formula:

$$
(-1)^{d+1}\left(\frac{d+1}{d+2}\right)^{1/2}\left\langle\begin{matrix}[\lambda_1+1 & \lambda_2-1]\\ & W_2'\end{matrix}\middle|\mu\otimes\bar{\nu};\ \begin{matrix}[\lambda_1 & \lambda_2]\\ & W_2\end{matrix}\right\rangle_{\Delta S=1}
$$

$$\times \left| E_{i,n+1}E_{n+1,j} \middle| \begin{matrix}[\lambda_1+1\ \ \lambda_2]\\ [\lambda_1\ \ \lambda_2]\\ W_n\end{matrix}\right\rangle_{\Delta S=1}$$

$$+(-1)^{d-1}\left(\frac{d-1}{d-2}\right)^{1/2}\left\langle \begin{matrix}[\lambda_1-1\ \ \lambda_2+1]\\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu};\ \begin{matrix}[\lambda_1\ \ \lambda_2]\\ W_2\end{matrix}\right\rangle_{\Delta S=-1}$$

$$\times \left| E_{i,n+1}E_{n+1,j} \middle| \begin{matrix}[\lambda_1\ \ \lambda_2+1]\\ [\lambda_1\ \ \lambda_2]\\ W_n\end{matrix}\right\rangle_{\Delta S=-1}$$

$$+\left(\frac{d}{d-1}\right)^{1/2}\left\langle \begin{matrix}[\lambda_1\ \ \lambda_2]\\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu};\ \begin{matrix}[\lambda_1\ \ \lambda_2]\\ W_2\end{matrix}\right\rangle^{P=1}_{\Delta S=0}$$

$$\times \left| E_{i,n+1}E_{n+1,j} \middle| \begin{matrix}[\lambda_1\ \ \lambda_2]\\ [\lambda_1\ \ \lambda_2]\\ W_n\end{matrix}\right\rangle^{P=1}_{\Delta S=0}$$

$$+\left(\frac{d}{d+1}\right)^{1/2}\left\langle \begin{matrix}[\lambda_1\ \ \lambda_2]\\ W_2'\end{matrix} \middle| \mu\otimes\bar{\nu};\ \begin{matrix}[\lambda_1\ \ \lambda_2]\\ W_2\end{matrix}\right\rangle^{P=2}_{\Delta S=0}$$

$$\times \left| E_{i,n+1}E_{n+1,j} \middle| \begin{matrix}[\lambda_1\ \ \lambda_2]\\ [\lambda_1\ \ \lambda_2]\\ W_n\end{matrix}\right\rangle^{P=2}_{\Delta S=0} \tag{17}$$

where the $|W_2'\rangle$, for a given $\Delta S$, can easily be determined by the generator $a_{\mu i,\nu j}$ and $|W_2\rangle$. So, the required matrix representation may be produced by removing all the boxes entered by $n+1$ from those Weyl tableaux obtained by (17).

## Appendix

Let us denote by $d$ the axial distance between the last box of each column in canonical Weyl basis tableaux spanning the IR $[\lambda_1\ \ \lambda_2]$ of U(2), i.e. $d=\lambda_1-\lambda_2+1$. Let $d_1$ and $d_2$ be the number of boxes in $|W_2\rangle$ shown in the following figure:

$$\left|\begin{matrix}\uparrow\cdots\uparrow\uparrow\overbrace{\uparrow\cdots\uparrow\uparrow}^{d_1}\underbrace{\downarrow\cdots\downarrow\downarrow}_{d_2}\\ \downarrow\cdots\downarrow\downarrow\end{matrix}\right\rangle.$$

Thus, the expressions of the vector coupling coefficients of U(2) are as follows:

$$\left\langle \begin{matrix}\overbrace{\uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\uparrow\downarrow\cdots\downarrow\downarrow}^{\lambda_1+1}\\ \downarrow\cdots\downarrow\downarrow\end{matrix} \middle| \uparrow;\ \begin{matrix}\overbrace{\uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow}^{\lambda_1}\\ \underbrace{\downarrow\cdots\downarrow\downarrow}_{\lambda_2}\end{matrix}\right\rangle=\left(\frac{d_1+1}{d}\right)^{1/2} \tag{A1}$$

$$\left\langle \begin{matrix} \overbrace{\uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow\downarrow}^{\lambda_1+1} \\ \downarrow\cdots\downarrow\downarrow \end{matrix} \middle| \downarrow;\ \begin{matrix} \overbrace{\uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow}^{\lambda_1} \\ \downarrow\cdots\downarrow\downarrow \end{matrix} \right\rangle = \left(\frac{d_2+1}{d}\right)^{1/2} \tag{A2}$$

$$\left\langle \begin{matrix} \uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\uparrow\downarrow\cdots\downarrow \\ \underbrace{\downarrow\cdots\downarrow\downarrow\downarrow}_{\lambda_2+1} \end{matrix} \middle| \uparrow;\ \begin{matrix} \uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow \\ \underbrace{\downarrow\cdots\downarrow\downarrow}_{\lambda_2} \end{matrix} \right\rangle = -\left(\frac{d_2}{d}\right)^{1/2} \tag{A3}$$

$$\left\langle \begin{matrix} \uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow \\ \underbrace{\downarrow\cdots\downarrow\downarrow\downarrow}_{\lambda_2+1} \end{matrix} \middle| \downarrow;\ \begin{matrix} \uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow \\ \underbrace{\downarrow\cdots\downarrow\downarrow}_{\lambda_2} \end{matrix} \right\rangle = \left(\frac{d_1}{d}\right)^{1/2} \tag{A4}$$

and the expressions of the contragradient vector coupling coefficients of U(2) are given by

$$\left\langle \begin{matrix} \overbrace{\uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\downarrow\cdots\downarrow\downarrow}^{\lambda_1-1} \\ \downarrow\cdots\downarrow\downarrow \end{matrix} \middle| \bar{\uparrow};\ \begin{matrix} \overbrace{\uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow}^{\lambda_1} \\ \downarrow\cdots\downarrow\downarrow \end{matrix} \right\rangle = \left(\frac{d_1}{d}\right)^{1/2} \tag{A5}$$

$$\left\langle \begin{matrix} \overbrace{\uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow}^{\lambda_1-1} \\ \downarrow\cdots\downarrow\downarrow \end{matrix} \middle| \bar{\downarrow};\ \begin{matrix} \overbrace{\uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow}^{\lambda_1} \\ \downarrow\cdots\downarrow\downarrow \end{matrix} \right\rangle = \left(\frac{d_2}{d}\right)^{1/2} \tag{A6}$$

$$\left\langle \begin{matrix} \uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\downarrow\cdots\downarrow\downarrow\downarrow \\ \underbrace{\downarrow\cdots\downarrow}_{\lambda_2-1} \end{matrix} \middle| \bar{\uparrow};\ \begin{matrix} \uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow \\ \underbrace{\downarrow\cdots\downarrow\downarrow}_{\lambda_2} \end{matrix} \right\rangle = -\left(\frac{d_2+1}{d}\right)^{1/2} \tag{A7}$$

$$\left\langle \begin{matrix} \uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow \\ \underbrace{\downarrow\cdots\downarrow}_{\lambda_2-1} \end{matrix} \middle| \bar{\downarrow};\ \begin{matrix} \uparrow\cdots\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\downarrow\cdots\downarrow\downarrow \\ \underbrace{\downarrow\cdots\downarrow\downarrow}_{\lambda_2} \end{matrix} \right\rangle = \left(\frac{d_1+1}{d}\right)^{1/2}. \tag{A8}$$

In the above formulae all the parameters $d_1$, $d_2$ and $d$ refer to the initial Weyl tableaux.

The coupling coefficients

$$\left\langle \begin{matrix} [\lambda_1' \ \lambda_2'] \\ W_2' \end{matrix} \middle| \mu \otimes \bar{\nu};\ \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2 \end{matrix} \right\rangle_{\Delta S}^{P}$$

can be obtained by the relation:

$$\left\langle \begin{matrix} [\lambda_1' \ \lambda_2'] \\ W_2' \end{matrix} \middle| \mu \otimes \bar{\nu};\ \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2 \end{matrix} \right\rangle_{\Delta S}^{P} = \sum_{W_2''} \left\langle \begin{matrix} [\lambda_1' \ \lambda_2'] \\ W_2' \end{matrix} \middle| \mu;\ \begin{matrix} [\lambda_1'' \ \lambda_2''] \\ W_2'' \end{matrix} \right\rangle \left\langle \begin{matrix} [\lambda_1'' \ \lambda_2''] \\ W_2'' \end{matrix} \middle| \bar{\nu};\ \begin{matrix} [\lambda_1 \ \lambda_2] \\ W_2 \end{matrix} \right\rangle \tag{A9}$$

where the IR $[\lambda_1'' \ \lambda_2'']$ should be determined by the selection rules of table 1 for the given $\Delta S$ and $P$.

## References

[1] Lin H-L and Cao Y-F 1987 *J. Chem. Phys.* **86** 6325
[2] Lin H-L and Cao Y-F 1988 *J. Chem. Phys.* **89** 3079
[3] Harter W G 1973 *Phys. Rev.* A **8** 2819
Harter W G and Patterson C W 1976 *A Unitary Calculus for Atomic Orbitals* (*Lecture Notes in Physics* **49**) (Berlin: Springer)
[4] Gould M D and Chandler G S 1984 *Int. J. Quantum Chem.* **25** 553, **25** 603, **25** 1089, **26** 441; 1985 *Int. J. Quantum. Chem.* **27** 787
[5] Lev A 1986 *Phys. Rev.* A **34** 2674