Unitary group tensor operator algebras for many-electron systems. III. Matrix elements in $U(n_1+n_2) \supset U(n_1) \times U(n_2)$ partitioned basis

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Exploiting our earlier results [J. Math. Chem. 4 (1990) 295–353 and 13 (1993) 273–316] on the unitary group $U(n)$ Racah–Wigner algebra, specifically designed for quantum chemical calculations of molecular electronic structure, and the related tensor operator formalism that enabled us to introduce spin-free orbital equivalents of the second quantization-like creation and annihilation operators as well as higher rank symmetric, antisymmetric and adjoint tensors, we consider the problem of $U(n)$ basis partitioning that is required for group-function type approaches to the many-electron problem. Using the $U(n) \supset U(n_1) \times U(n_2)$, $n = n_1 + n_2$ adapted basis, we evaluate all required matrix elements of $U(n)$ generators and their products that arise in one- and two-body components of non-relativistic electronic Hamiltonians. The formalism employed naturally leads to a segmented form of these matrix elements, with many of the segments being identical to those of the standard unitary group approach. Relationship with similar approaches described earlier is briefly pointed out.

1. Introduction

It is well known that the molecular many-electron correlation problem quickly becomes unmanageable as the electron number and/or the dimension of the one-electron model space employed surpass certain rather modest limits. Yet, various constituting parts of such a molecular system, be they atomic substituents or larger fragments, preserve a great deal of individuality from one system to another. In the quantum chemical description based on molecular orbital (MO) or valence bond (VB) formalisms, the approximate "additivity" of the total energy as well as

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of various properties, when the molecule is assembled from chemically well characterized smaller fragments, will be reflected by an approximate separability of corresponding wave functions, particularly when we employ a one-electron basis that is well localized in the constituting parts of the total system. Although only a limited localization may be achieved, particularly when using orthonormal MOs, the electrons in larger systems may be usefully partitioned into more or less well-separated groups or shells. The symmetry constraints and/or significant energy separation between such groups, if present, will also facilitate such a partitioning.

The success of various empirical schemes that are based on approximate additivity rules stimulated numerous attempts by molecular theorists to emulate this phenomenon in actual quantum chemical computations by building many-electron wave functions from those describing smaller molecular groups, fragments, aggregates or shells. Thus, the atoms in molecular method [1,2], the separated electron group method [3], the molecules in molecules idea [4] or the method of molecular fragments [5], as well as the semi-empirical and very successful diatomics in molecules approach [6], all exploit the same basic idea of system partitioning.

Within the symmetric group spin-free approach, the idea of system partitioning was first explored by Matsen and Klein [7]. In the configuration interaction (CI) context, the advantages and feasibility of the group-function-type approach from the unitary (or general linear) group viewpoint were examined by Wormer and van der Avoird [8].

Later, Wormer [9] contemplated the feasibility of such an approach employing the unitary group formalism [10–21], while relying on graphical methods of spin algebras [22–24]. The same approach was employed by Paldus and Boyle [25] for a related partitioning problem which arises in the hole–particle formalism, providing explicit expressions for all one- and two-electron segment values that are required in addition to those needed in the standard particle-only unitary group approach (UGA) [26].

More recently, UGA was applied to general system partitioning by Gould and Paldus [27], using the Green–Gould [28–30] formalism. In these papers a complete derivation of the U(n) generator matrix elements (MEs) in a basis adapted to the subgroup $U(n_1) \times U(n_2), n = n_1 + n_2$, was given. From the viewpoint of the Clifford algebra UGA (CAUGA), the system partitioning problem was subsequently studied by Paldus et al. [31].

In this paper we shall explore the UGA paritioning relying on earlier communications in this series [#1] [32,33], where we presented the U(n) tensor operator formalism that is particularly suitable for the quantum chemical many-electron problem. The general formulation of the U(n) Racah–Wigner algebra for our purposes, together with the necessary explicit expressions for U(n) isoscalar factors

[#1] The preceding papers of this series, refs. [32] and [33], will be referred to in the following as Parts I and II, respectively. Likewise, we shall refer to eq. (x) or table x of Part I as eq. (I.x) or table I.x, respectively, and similarly for Part II. Note also the two misprints in table I.2 pointed out in footnote #1 of Part II.

or reduced Wigner coefficients and U(n) Racah coefficients for both standard and nonstandard or partitioned bases, was presented in Part I. In Part II these results were exploited in developing the tensor operator formalism that is necessary for efficient handling of one- and two-body MEs of molecular electronic Hamiltonians within the spin-adapted canonical Gel'fand–Tsetlin (GT) basis. In fact, the basic vector operators that we introduced in Part II represent spin-free or orbital analogues of spin orbital creation and annihilation operators of the standard second quantization formalism. Using these vector and contragredient vector (i.e., rank one tensor) operators, associated with a single box U(n) irreducible representation (irrep) [#2] $\langle 1\dot{0}\rangle \equiv (0,1)$ as elementary "building blocks", we constructed symmetry adapted second rank tensor operators, namely symmetric and antisymmetric tensors associated with irreps $\langle 2\dot{0}\rangle \equiv (1,0)$ and $\langle 1^2\dot{0}\rangle \equiv (0,2)$, respectively, and an adjoint tensor associated with the adjoint irrep $\langle 1\dot{0}\ -1\rangle$. Using these results we were able to derive all the segment values required for the evaluation of one- and two-body MEs within the canonical UGA basis. In this paper we shall employ the same formalism, developed in Parts I and II, to obtain the necessary segment values for the evaluation of one- and two-body MEs in partitioned bases that are adapted to the chain $\mathrm{U}(n) \supset \mathrm{U}(n_1) \times \mathrm{U}(n_2)$ with $n = n_1 + n_2$. Thus, following a brief review of our notation for the nonstandard or partitioned bases in section 2, we derive all necessary segment values for the evaluation of MEs of U(n) generators in section 3. In sections 4 and 5 we carry out similar derivations for MEs of spin-free creation and annihilation vector operators and for the two-body operators, respectively. A brief discussion and conclusions are then the subject of the last section (section 6).

2. Partitioning formalism

We assume that the orbital space V_n may be partitioned into a direct sum of r subspaces V_{n_i}, so that

$$V_n = \bigoplus_{i=1}^{r} V_{n_i}, \quad \sum_{i=1}^{r} n_i = n, \tag{1}$$

and that there exists an orthonormal one-electron basis set $\Omega_i \equiv \{|j\rangle\}_{j=1,2,\ldots,n_i}$ for each subspace V_{n_i}. Hence, for the total space V_n, the relevant basis set Ω is given by a disjoint union of Ω_i assuming an arbitrary but fixed ordering of subspaces V_{n_i}. To avoid any ambiguity when dealing with basis Ω for V_n, it is convenient to employ a consecutive labeling of one-electron states. We thus relabel our orthonormal orbitals $|j\rangle$ as follows $\Omega_i \equiv \{|j\rangle\}_{j=r_i+1,r_i+2,\ldots r_i+n_i}$, where $r_i = \sum_{j=1}^{i-1} n_j = r_{i-1} + n_{i-1}$ and $r_1 = 0$, so that $\Omega \equiv \{|j\rangle\}_{j=1,2,\ldots n}$. We then associate the orbital unitary group U(n_i) with each subspace V_{n_i} and U(n) with the total space V_n. For an

[#2] Recall that a U(n) two column irrep $\langle 2^a 1^b \dot{0}\rangle \equiv \langle 2^a 1^b 0^{n-(a+b)}\rangle$ is labeled as (a,b) in accordance with Paldus ABC tableau labeling [10].

N-electron system, we wish to employ the N-electron states that are symmetry adapted to the chain

$$U(n) \supset U(n_1) \times U(n_2) \times \ldots \times U(n_r)\,. \tag{2}$$

Clearly, there are many possible imbeddings of the subgroup $U(n_1) \times U(n_2) \times \ldots \times U(n_r)$ in $U(n)$, so that we have to choose a suitable "coupling scheme", similarly as in the standard angular (or spin) coupling problem. A convenient recursive scheme that builds on a simple $r = 2$ case was formulated and exploited by Gould [27b]. With such a recursive coupling, multiplicity problems are avoided, as long as we keep irrep labels arising through intermediate couplings.

In this paper, we shall consider the simplest case when $r = 2$, i.e., the partitioning of a system into two subsystems. Throughout this paper, we shall designate $U(n_1)$ orbitals by the lower case letters of the Greek alphabet α, β, γ, etc., while those associated with $U(n_2)$ by the lower case letters of the Latin alphabet i, j, k, etc. We shall also employ Paldus' labeling of $U(n)$ irreps, designating $\lambda \equiv (a, b)$, $\lambda_i \equiv (a_i, b_i), \lambda_i' \equiv (a_i', b_i')$, where $i = 1, 2$, etc.

The basis vectors adapted to the chain $U(n) \supset U(n_1) \times U(n_2)$ will then be designated as

$$\left|\lambda \quad \begin{matrix}\lambda_1 & \lambda_2\\ W_1 & W_2\end{matrix}\right\rangle \equiv \left|(a,b) \quad \begin{matrix}(a_1,b_1) & (a_2,b_2)\\ W_1 & W_2\end{matrix}\right\rangle, \tag{3}$$

following the notation used in Part I (see also eqs. (53,54) of ref. [31]), and implying that the state belongs to the irrep λ of $U(n)$ given as an outer direct product of GT basis vectors $|\lambda_i W_i\rangle \equiv |\, {}^{\lambda_i}_{W_i} \rangle$ of $U(n_i)$, $i = 1, 2$ (in the text we use linearized notation writing the irrep and Weyl tableau symbols in the same row). Since we consider at most two-column irreps and only two subsystems, no multiplicity problems arise and the notation of eq. (3) is unambiguous.

We have shown in Part I that the partitioned basis (3) may be expressed in terms of canonical $U(n)$ basis as follows [cf., eq. (I.59)]:

$$\left|(a,b) \quad \begin{matrix}(a_1,b_1) & (a_2,b_2)\\ W_1 & W_2\end{matrix}\right\rangle = \sum_W \left|\begin{matrix}(a,b)\\ W\end{matrix}\right\rangle \left\langle \begin{matrix}(a,b)\\ W\end{matrix}\right|(a,b) \quad \begin{matrix}(a_1,b_1) & (a_2,b_2)\\ W_1 & W_2\end{matrix}\Big\rangle, \tag{4}$$

defining the transformation coefficients from the partitioned basis to the $U(n)$ GT basis and vice versa. We have also shown that the transformation coefficients in eq. (4) can be factorized into a simple product of transformation isoscalar factors, referred to as I_t factors for short, and all I_t factors required for the two-column irreps were given in table I.2 [#3]. These results are extensively employed in the present paper.

[#3] Note two misprints in table I.2 (cf footnote #1 of Part II): the factor $(b + e + t + 2)$ appearing in the numerator of type C I_t (or I_s) factor should read $(b - e + t + 2)$ and, similarly, the factor $(e + 1)$ in the denominator for the type D $I_t(I_s)$ factor equals $(e + 2)$.

Clearly, MEs of U(n) operators that involve indices of only one kind, in partitioned basis (3), reduce to MEs of corresponding subgroup operators in the respective GT basis. For example for $E_{\alpha\beta}$ we simply get

$$\left\langle \lambda \begin{matrix} \lambda_1' & \lambda_2' \\ W_1' & W_2' \end{matrix} \middle| E_{\alpha\beta} \middle| \lambda \begin{matrix} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{matrix} \right\rangle = \delta_{\lambda_1'\lambda_1}\delta_{\lambda_2'\lambda_2}\delta_{W_2'W_2} \left\langle \begin{matrix} \lambda_1 \\ W_1' \end{matrix} \middle| E_{\alpha\beta} \middle| \begin{matrix} \lambda_1 \\ W_1 \end{matrix} \right\rangle , \quad (5)$$

and similarly for MEs of E_{ij}, $E_{\alpha\beta}E_{\alpha'\beta'}$, $E_{ij}E_{kl}$, etc. Thus, in the following, we only have to consider MEs of operators that contain both kinds of labels involving U(n_1) as well as U(n_2).

3. Matrix elements of generators

We consider MEs of $E_{\alpha i}$, which is hermitian conjugate of $E_{i\alpha}$. Since $E_{\alpha i}$ is a vector operator of U(n_1) and a contragredient vector operator of U(n_2),

$$[E_{\beta\gamma}, E_{\alpha i}] = \delta_{\alpha\gamma}E_{\beta i} \quad (\alpha, \beta, \gamma = 1, 2, \ldots, n_1) , \quad (6)$$

$$[E_{jk}, E_{\alpha i}] = -\delta_{ij}E_{\alpha k} \quad (i, j, k = n_1 + 1, n_1 + 2, \ldots, n_1 + n_2 = n) , \quad (7)$$

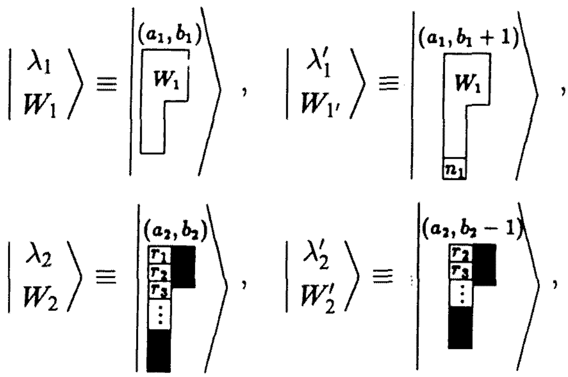
its MEs may be expressed as

$$\langle E_{\alpha i}\rangle \equiv \left\langle \lambda \begin{matrix} \lambda_1' & \lambda_2' \\ W_1' & W_2' \end{matrix} \middle| E_{\alpha i} \middle| \lambda \begin{matrix} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{matrix} \right\rangle$$

$$= \left\langle \begin{matrix} \lambda \\ \lambda_1'\lambda_2' \end{matrix} \middle\| E \middle\| \begin{matrix} \lambda \\ \lambda_1\lambda_2 \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_1 & (0,1) \\ W_1 & \alpha \end{matrix} \middle| \begin{matrix} \lambda_1' \\ W_1' \end{matrix} \right\rangle^{(s)} \left\langle \begin{matrix} \lambda_2' & (0,1) \\ W_2' & i \end{matrix} \middle| \begin{matrix} \lambda_2 \\ W_2 \end{matrix} \right\rangle^{(s)} , \quad (8)$$

where the first factor on the right-hand side is a reduced matrix element (RME) of U(n) generator in the partitioned basis depending on the irreps of U(n), U(n_1) and U(n_2). The second and third factors are the Clebsch–Gordan (CG) coefficients for vector operators. Since we employ scaled CG coefficients rather than unscaled ones, as indicated by the superscript (s), the RME in eq. (8) is in fact a scaled RME. We have shown in Part I that scaled CG coefficients are products of scaled isoscalar factors (or reduced Wigner coefficients) and all relevant isoscalar factors for vector operators may be found in table II.1. Hence, the only unknown term in eq. (8) is the RME.

There are four independent RMEs corresponding to $\lambda_1' = (a_1, b_1 + 1)$ or $(a_1 + 1, b_1 - 1)$ and $\lambda_2' = (a_2, b_2 - 1)$ or $(a_2 - 1, b_2 + 1)$. To find these RMEs, we express MEs of E_{n_1,n_1+1} in a partitioned basis in terms of MEs in the GT basis, using the transformation of eq. (4). We first choose $\lambda_1' = (a_1, b_1 + 1)$ and $\lambda_2' = (a_2, b_2 - 1)$ and let the orbitals n_1 and $(n_1 + 1)$ be singly occupied in the first column of W_1' and W_2, respectively. Moreover, we assume that the tableaux W_2 and W_2' contain a_2 doubly occupied orbitals. We can thus schematically represent these states as follows:



(9)

where $r_1 = n_1 + 1, r_2 = n_1 + 2$, etc. For simplicity's sake we assume the shaded parts of W_2 and W_2' to be identical and filled with doubly occupied orbitals, whose labels are greater than the maximum label of singly occupied orbitals. Substituting now these states, eq. (9), into eq. (8) and applying eq. (4), we can rewrite the left-hand side of eq. (8) as follows:

$$\langle E_{n_1,n_1+1}\rangle_1 = \sum_{W,W'} \left\langle (a,b) \begin{matrix} (a_1,b_1+1) \\ W_1' \end{matrix} \begin{matrix} (a_2,b_2-1) \\ W_2' \end{matrix} \middle| \begin{matrix} (a,b) \\ W' \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} (a,b) \\ W \end{matrix} \middle| (a,b) \begin{matrix} (a_1,b_1) \\ W_1 \end{matrix} \begin{matrix} (a_2,b_2) \\ W_2 \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} (a,b) \\ W' \end{matrix} \middle| E_{n_1,n_1+1} \middle| \begin{matrix} (a,b) \\ W \end{matrix} \right\rangle . \quad (10)$$

Note that in eq. (10) the subtableaux of W' and W obtained by deleting boxes labelled by n_1 and $(n_1 + 1)$ must be identical lest the MEs of E_{n_1,n_1+1} vanish. This means that the position of n_1 in W' must be identical to that of $(n_1 + 1)$ in W. Under these conditions, the ME of E_{n_1,n_1+1} is equal to 1 in view of the single occupancy of the orbitals involved. Hence, the right-hand side of eq. (10) is given by a sum of products of two transformation coefficients. We recall here that these transformation coefficients may be expressed as products of I_t factors and the I_t factors for doubly occupied orbitals are simply equal to 1. Consequently, the doubly occupied parts of W_2 and W_2', eq. (9), make no contribution to the transformation coefficients and we can write

$$\langle E_{n_1,n_1+1}\rangle_1 = \sum_{\tilde{W},\tilde{W}'} \left\langle (\tilde{a},b) \begin{matrix} (a_1,b_1+1) \\ W_1' \end{matrix} \begin{matrix} (0,b_2-1) \\ \tilde{W}_2' \end{matrix} \middle| \begin{matrix} (\tilde{a},b) \\ \tilde{W}' \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} (\tilde{a},b) \\ \tilde{W} \end{matrix} \middle| (\tilde{a},b) \begin{matrix} (a_1,b_1) \\ W_1 \end{matrix} \begin{matrix} (0,b_2) \\ \tilde{W}_2 \end{matrix} \right\rangle , \quad (11)$$

where $\tilde{a} = a - a_2$ and

$$\left|\begin{matrix}(0,b_2)\\ \tilde{W}_2\end{matrix}\right\rangle \equiv \left|\begin{matrix}(0,b_2)\\ \begin{array}{|c|}\hline r_1\\ \hline r_2\\ \hline r_3\\ \hline \vdots\\ \hline\end{array}\end{matrix}\right\rangle, \quad \left|\begin{matrix}(0,b_2-1)\\ \tilde{W}_2'\end{matrix}\right\rangle \equiv \left|\begin{matrix}(0,b_2-1)\\ \begin{array}{|c|}\hline r_2\\ \hline r_3\\ \hline \vdots\\ \hline\end{array}\end{matrix}\right\rangle, \tag{12}$$

represent singly occupied parts of W_2 and W_2' in eq. (9), respectively. The $\tilde{W}$ and $\tilde{W}'$ that result by adding the boxes of $\tilde{W}_2$ and $\tilde{W}_2'$ to W_1 and W_1', respectively, must have identical subtableaux for the levels smaller than n_1 and larger than (n_1+1). This means that $\tilde{W}$ and $\tilde{W}'$ differ in only one box that contains n_1 in $\tilde{W}'$ and (n_1+1) in $\tilde{W}$, i.e.,

$$\left|\begin{matrix}(\tilde{a},b)\\ \tilde{W}\end{matrix}\right\rangle \equiv \left|\begin{matrix}(\tilde{a},b)\\ \begin{array}{|c|c|}\hline W_1 & \\ & \boxed{\omega}\\ \hline r_1 & \\ \hline \tilde{\omega} & \\ \hline\end{array}\end{matrix}\right\rangle, \quad \left|\begin{matrix}(\tilde{a},b)\\ \tilde{W}'\end{matrix}\right\rangle \equiv \left|\begin{matrix}(\tilde{a},b)\\ \begin{array}{|c|c|}\hline W_1 & \\ & \boxed{\omega}\\ \hline n_1 & \\ \hline \tilde{\omega} & \\ \hline\end{array}\end{matrix}\right\rangle. \tag{13}$$

Thus the sum in eq. (11) reduces to the sum over subtableaux ω and $\tilde{\omega}$. In view of the n-independence of isoscalar factors, the label n_1 in $\tilde{W}'$ may be replaced by $(n_1+1)=r_1$ if the W_1' is simultaneously replaced by

$$\left|\begin{matrix}(a_1,b_1+1)\\ W_1''\end{matrix}\right\rangle = \left|\begin{matrix}(a_1,b_1+1)\\ \begin{array}{|c|}\hline W_1\\ \hline r_1\\ \hline\end{array}\end{matrix}\right\rangle. \tag{14}$$

This implies that eq. (11) can be rewritten as

$$\langle E_{n_1,n_1+1}\rangle_1 = \left\langle (\tilde{a},b) \quad \begin{matrix}(a_1,b_1+1)\\ W_1''\end{matrix} \quad \begin{matrix}(0,b_2-1)\\ \tilde{W}_2'\end{matrix} \right| (\tilde{a},b) \quad \left.\begin{matrix}(a_1,b_1)\\ W_1\end{matrix} \quad \begin{matrix}(0,b_2)\\ \tilde{W}_2\end{matrix}\right\rangle. \tag{15}$$

If we introduce a basis $|(0,1)r_1\rangle$, we may interpret the bra and the ket states in (15) as arising from two different coupling sequences involving the subgroup $U(n_1)\times U(1)\times U(n_2-1)$. The bra is obtained by first coupling $|(a_1,b_1)\,W_1\rangle$ with $|(0,1)\,r_1\rangle$ to a state of (a_1,b_1+1), followed by the coupling with $|(0,b_2-1)\,\tilde{W}_2'\rangle$, while the ket results by first coupling $|(0,1)\,r_1\rangle$ with $|(0,b_2-1)\,\tilde{W}_2'\rangle$ to a state of $(0,b_2)$, followed by the coupling with $|(a_1,b_1)\,W_1\rangle$ to the final state. It thus follows that the right-hand side of eq. (11) or (15) is equal to a Racah coefficient #4 (recall the symmetry property (I.137))

$$\langle E_{n_1,n_1+1}\rangle_1 = U\{(0,b_2-1),(0,1),(\tilde{a},b),(a_1,b_1);(0,b_2),(a_1,b_1+1)\}. \tag{16}$$

This Racah coefficient is evaluated in the appendix so that we get

#4 For footnote see next page.

$$\langle E_{n_1,n_1+1}\rangle_1 = \frac{(-1)^{a_1+a_2+a}}{2}\left[\frac{(b_1-b_2+b+2)(b_2-b_1+b)}{b_2(b_1+1)}\right]^{1/2} . \tag{17}$$

On the other hand, using scaled isoscalar factors from table II.1, we easily evaluate the right-hand side of eq. (8) for $\alpha = n_1, i = n_1+1, \lambda_1 = (a_1, b_1)$, etc., obtaining

$$\begin{aligned}\langle E_{n_1,n_1+1}\rangle_1 =& \left\langle \begin{matrix}(a,b)\\(a_1,b_1+1)(a_2,b_2-1)\end{matrix}\right\| E \left\| \begin{matrix}(a,b)\\(a_1,b_1)(a_2,b_2)\end{matrix}\right\rangle \\ &\times \left\langle \begin{matrix}(a_1,b_1) & (0,1)\\ W_1 & n_1\end{matrix}\right|\left. \begin{matrix}(a_1,b_1+1)\\ W_1'\end{matrix}\right\rangle^{(s)} \\ &\times \left\langle \begin{matrix}(a_2,b_2-1) & (0,1)\\ W_2' & n_1+1\end{matrix}\right|\left. \begin{matrix}(a_2,b_2)\\ W_2\end{matrix}\right\rangle^{(s)} .\end{aligned} \tag{18}$$

The first CG coefficient is simply equal to a scaled isoscalar factor

$$\left\langle \begin{matrix}(a_1,b_1) & (0,1)\\ W_1 & n_1\end{matrix}\right|\left. \begin{matrix}(a_1,b_1+1)\\ W_1'\end{matrix}\right\rangle^{(s)} = \left(\begin{matrix}(a_1,b_1) & (0,1)\\ (a_1,b_1) & (0,0)\end{matrix}\right|\left. \begin{matrix}(a_1,b_1+1)\\ (a_1,b_1)\end{matrix}\right)^{(s)} = 1 , \tag{19}$$

while the second CG coefficient is given by a product of isoscalar factors from the top level n to the level (n_1+1). Since the scaled isoscalar factors equal -1 for both doubly and singly occupied orbitals, we get

$$\begin{aligned}&\left\langle \begin{matrix}(a_2,b_2-1) & (0,1)\\ W_2' & n_1+1\end{matrix}\right|\left. \begin{matrix}(a_2,b_2)\\ W_2\end{matrix}\right\rangle^{(s)} = (-1)^{a_2}\left\langle \begin{matrix}(0,b_2-1) & (0,1)\\ \tilde{W}_2' & n_1+1\end{matrix}\right|\left. \begin{matrix}(0,b_2)\\ \tilde{W}_2\end{matrix}\right\rangle^{(s)} \\ &= (-1)^{a_2}\prod_{r=1}^{b_2-1}\left(\begin{matrix}(0,b_2-r) & (0,1)\\ (0,b_2-r-1) & (0,1)\end{matrix}\right|\left. \begin{matrix}(0,b_2-r+1)\\ (0,b_2-r)\end{matrix}\right)^{(s)} \\ &\times \left(\begin{matrix}(0,0) & (0,1)\\ (0,0) & (0,0)\end{matrix}\right|\left. \begin{matrix}(0,1)\\ (0,0)\end{matrix}\right)^{(s)} = (-1)^{a_2+b_2-1} ,\end{aligned} \tag{20}$$

#4 When considering the partitioning of $U(n)$ into the three subgroups $U(n_r), r = 3$, an intermediate irrep is required in order to define uniquely the partitioned basis. Thus, either λ_1 of $U(n_1)$ and λ_2 of $U(n_2)$ are first coupled to an intermediate λ_{12}, which is then coupled with λ_3 of $U(n_3)$ to final λ, or λ_{23} resulting from the coupling of λ_2 and λ_3 is chosen as an intermediate irrep that is subsequently coupled with λ_1 to obtain λ. The relationship between the two coupling schemes is then given by

$$\left|\lambda \begin{matrix}\lambda_1 & \lambda_2 & \lambda_3\\ W_1 & W_2 & W_3\end{matrix}\right\rangle^{\lambda_{23}} = \sum_{\lambda_{12}} U\{\lambda_1\lambda_2\lambda\lambda_3;\lambda_{12}\lambda_{23}\}\left|\lambda \begin{matrix}\lambda_1 & \lambda_2 & \lambda_3\\ W_1 & W_2 & W_3\end{matrix}\right\rangle^{\lambda_{12}} .$$

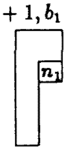
Clearly, eq. (15) easily follows, since for $\lambda_1 = (a_1,b_1), \lambda_2 = (0,1), \lambda_3 = (0,b_2-1)$ and $\lambda = (\tilde{a},b)$ we have that $\lambda_{12} = (a_1,b_1+1)$ and $\lambda_{23} = (0,b_2)$ in view of chosen occupancies. Using the relationship (I.137) we can interchange λ_1 and λ_3.

the last isoscalar factor being again equal to 1. Therefore, the first RME is given by

$$\left\langle \begin{matrix} (a,b) \\ (a_1,b_1+1)(a_2,b_2-1) \end{matrix} \middle\| E \middle\| \begin{matrix} (a,b) \\ (a_1,b_1)(a_2,b_2) \end{matrix} \right\rangle = (-1)^{a_1+b_2+a+1}\,\frac{1}{2}\left[\frac{(b_1-b_2+b+2)(b_2-b_1+b)}{b_2(b_1+1)}\right]^{1/2} . \tag{21}$$

The remaining three RMEs may be derived in a similar way. For example, to obtain the RME corresponding to the irreps $(a'_1,b'_1)=(a_1+1,b_1-1)$ and $(a'_2,b'_2)=(a_2,b_2-1)$, we choose W_1, W_2 and W'_2 as before, but W'_1 as follows:

$$\left| \begin{matrix} \lambda'_1 \\ W'_1 \end{matrix} \right\rangle \equiv \left| \begin{matrix} (a_1+1,b_1-1) \end{matrix} \right. \tag{22}$$



i.e., the orbital n_1 is now singly occupied in the second column. Then, the left-hand side of eq. (8) equals the Racah coefficient (cf., eq. (A.13))

$$\begin{aligned} \langle E_{n_1,n_1+1}\rangle_2 &= U\{(0,b_2-1),(0,1),(\tilde{a},b),(a_1,b_1);(0,b_2),(a_1+1,b_1-1)\} \\ &= \frac{1}{2}\left[\frac{(b_1+b_2-b)(b_1+b_2+b+2)}{b_2(b_1+1)}\right]^{1/2}, \end{aligned} \tag{23}$$

and the right-hand side is given by

$$\langle E_{n_1,n_1+1}\rangle_2 = (-1)^{a_2+b_2+1}\left\langle \begin{matrix} (a,b) \\ (a_1+1,b_1-1)(a_2,b_2-1) \end{matrix} \middle\| E \middle\| \begin{matrix} (a,b) \\ (a_1,b_1)(a_2,b_2) \end{matrix} \right\rangle . \tag{24}$$

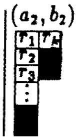
The resulting RME is given in table 1.

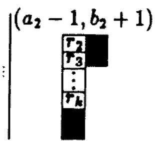
Table 1
The RMEs of U(n) generators in a partitioned basis (3).

(a'_1,b'_1)	(a'_2,b'_2)	$\left\langle \begin{matrix} (a,b) \\ (a'_1,b'_1)(a'_2,b'_2) \end{matrix} \middle\| E \middle\| \begin{matrix} (a,b) \\ (a_1,b_1)(a_2,b_2) \end{matrix} \right\rangle$
(a_1,b_1+1)	(a_2,b_2-1)	$\frac{(-1)^{a_1+a+b_2+1}}{2}\left[\frac{(b_2-b_1+b)(b_1-b_2+b+2)}{(b_1+1)b_2}\right]^{1/2}$
(a_1+1,b_1-1)	(a_2,b_2-1)	$\frac{(-1)^{a_2+b_2+1}}{2}\left[\frac{(b_1+b_2-b)(b_1+b_2+b+2)}{(b_1+1)b_2}\right]^{1/2}$
(a_1,b_1+1)	(a_2-1,b_2+1)	$\frac{(-1)^{a_2+1}}{2}\left[\frac{(b_1+b_2-b+2)(b_1+b_2+b+4)}{(b_1+1)(b_2+2)}\right]^{1/2}$
(a_1+1,b_1-1)	(a_2-1,b_2+1)	$\frac{(-1)^{a_1+a+1}}{2}\left[\frac{(b_1-b_2+b)(b_2-b_1+b+2)}{(b_1+1)(b_2+2)}\right]^{1/2}$

In order to calculate the RMEs for $(a_2', b_2') = (a_2 - 1, b_2 + 1)$, we must choose W_2 in such a way that at least one singly occupied orbital appears in the second column, i.e.,

$$\left| \begin{matrix} \lambda_2 \\ W_2 \end{matrix} \right\rangle \equiv \left| \begin{matrix} (a_2, b_2) \end{matrix} \right\rangle , \quad \left| \begin{matrix} \lambda_2' \\ W_2' \end{matrix} \right\rangle \equiv \left| \begin{matrix} (a_2 - 1, b_2 + 1) \end{matrix} \right\rangle , \tag{25}$$





where now $r_1 = n_1 + 1, r_2 = n_1 + 2, \ldots$, and $r_k = n_1 + k$ with $r_2, \ldots, r_k$ singly occupied in both W_2 and W_2' and r_1 occupied in W_2 but not in W_2'. Note that r_1 must be in the first column for W_2 to be lexical, so that another singly occupied orbital (which is convenient to choose as having the maximal label, i.e. r_k) must appear in the second column since only then the elimination of r_1 takes us from (a_2, b_2) to $(a_2 - 1, b_2 + 1)$, i.e. we eliminate a box in the second column. Again, the shaded parts are identical and filled with $(a_2 - 1)$ doubly occupied orbitals, whose labels, for the sake of convenience, are assumed to be greater than r_k. With these assumptions, consider first the case $(a_1', b_1') = (a_1, b_1 + 1)$. We can again first eliminate all doubly occupied orbitals as we did in eq. (11). However, in contrast to eq. (11), it is now impossible to completely eliminate the second column. Instead, we get

$$\begin{aligned} \langle E_{n_1, n_1+1} \rangle_3 = \sum_{\tilde{W}, \tilde{W}'} & \left\langle (\tilde{a}, b) \quad \begin{matrix} (a_1, b_1 + 1) \\ W_1' \end{matrix} \quad \begin{matrix} (0, b_2 + 1) \\ \tilde{W}_2' \end{matrix} \middle| \begin{matrix} (\tilde{a}, b) \\ \tilde{W}' \end{matrix} \right\rangle \\ \times & \left\langle \begin{matrix} (\tilde{a}, b) \\ \tilde{W} \end{matrix} \middle| (\tilde{a}, b) \quad \begin{matrix} (a_1, b_1) \\ W_1 \end{matrix} \quad \begin{matrix} (1, b_2) \\ \tilde{W}_2 \end{matrix} \right\rangle , \end{aligned} \tag{26}$$

where $\tilde{a} = a - a_2 + 1$ and $\tilde{W}_2$ and $\tilde{W}_2'$ are singly occupied subtableaux of W_2 and W_2', respectively. The largest orbital label in eq. (26) is now r_k. We can thus express the transformation coefficients in eq. (26) in terms of products of I_t factors for $U(r_k) \supset U(r_k - 1)$ and the transformation coefficients for $U(r_k - 1)$, so that the orbital label r_k can be eliminated from the second column of $\tilde{W}_2$. Since the orbital r_k may appear in the first or the second column of both $\tilde{W}$ and $\tilde{W}'$, eq. (26) reduces to

$$\begin{aligned} \langle E_{n_1, n_1+1} \rangle_3 = \sum_{\tau} & I_t \begin{pmatrix} (a_1, b_1 + 1) & (0, b_2 + 1) & (\tilde{a}, b) \\ (a_1, b_1 + 1) & (0, b_2) & (\tilde{a}, b) - \tau \end{pmatrix} \\ \times & I_t \begin{pmatrix} (a_1, b_1) & (1, b_2) & (\tilde{a}, b) \\ (a_1, b_1) & (0, b_2 + 1) & (\tilde{a}, b) - \tau \end{pmatrix} \\ \times & \sum_{U, U'} \left\langle (\tilde{a}, b) - \tau \quad \begin{matrix} (a_1, b_1 + 1) \\ W_1' \end{matrix} \quad \begin{matrix} (0, b_2) \\ V_2' \end{matrix} \middle| \begin{matrix} (\tilde{a}, b) - \tau \\ U' \end{matrix} \right\rangle \end{aligned}$$

$$\times \left\langle \begin{matrix} (\tilde{a},b)-\tau \\ U \end{matrix} \middle| \begin{matrix} (\tilde{a},b)-\tau \end{matrix} \begin{matrix} (a_1,b_1) \\ W_1 \end{matrix} \begin{matrix} (0,b_2+1) \\ V_2 \end{matrix} \right\rangle, \tag{27}$$

where $(\tilde{a},b)-\tau=(\tilde{a},b-1)$ when $\tau=1$ and $(\tilde{a},b)-\tau=(\tilde{a}-1,b+1)$ when $\tau=2$ are the intermediate irreps. The V_2' and V_2 are obtained by removing a box labeled with r_k from $\tilde{W}_2'$ and $\tilde{W}_2$, respectively, and, similarly, U' and U result from $\tilde{W}'$ and W, respectively. Notice that the sums of products of two transformation coefficients over U and U' have the same form as those in eq. (11) and are thus equal to the Racah coefficients appearing on the right-hand side of eq. (16). We thus get

$$\begin{aligned}\langle E_{n_1,n_1+1}\rangle_3 = \sum_{\tau=1}^{2} & I_t\begin{pmatrix} (a_1,b_1+1) & (0,b_2+1) & (\tilde{a},b) \\ (a_1,b_1+1) & (0,b_2) & (\tilde{a},b)-\tau \end{pmatrix} \\ & \times I_t\begin{pmatrix} (a_1,b_1) & (1,b_2) & (\tilde{a},b) \\ (a_1,b_1) & (0,b_2+1) & (\tilde{a},b)-\tau \end{pmatrix} \\ & \times U\{(0,b_2),(0,1),[(\tilde{a},b)-\tau],(a_1,b_1);(0,b_2+1),(a_1,b_1+1)\}\,. \end{aligned} \tag{28}$$

Both the I_t factors (see table I.2) and the Racah coefficients (eq. (A.7) and (17)) appearing in the above expression are known. On the other hand, the right-hand side of eq. (8) is in this case easily found to be

$$\langle E_{n_1,n_1+1}\rangle_3 = \frac{(-1)^{a_2+b_2+1}}{b_2+1}\left\langle \begin{matrix} (a,b) \\ (a_1,b_1+1)(a_2-1,b_2+1) \end{matrix} \middle\| E \middle\| \begin{matrix} (a,b) \\ (a_1,b_1)(a_2,b_2) \end{matrix} \right\rangle. \tag{29}$$

Comparing eqs. (28) and (29) we find the desired explicit form for the third RME in table 1. Finally, we find similarly the last RME for $(a_1',b_1')=(a_1+1,b_1-1)$. All four possible RMEs are given in table 1. Thus, using eqs. (5) and (8) we may find any generator ME in the partitioned basis (3).

It should be recalled that, similarly as in the standard UGA, the RMEs appearing in eq. (8) are associated with raising generators, since clearly $\alpha<i$ [cf., eqs. (II.39, 39′ and 39″)]. In view of the hermitian property of U(n) generators, the MEs of $E_{i\alpha}$ are easily found in an analogous way as those for the raising generators $E_{\alpha i}$, eq. (8). The corresponding RMEs satisfy again the following symmetry properties:

$$\begin{aligned}\left\langle \begin{matrix} \lambda \\ \lambda_1'\lambda_2' \end{matrix} \middle\| E^R \middle\| \begin{matrix} \lambda \\ \lambda_1\lambda_2 \end{matrix} \right\rangle &= (-1)^{\lambda_1+\lambda_1'+\lambda_2+\lambda_2'}\left\langle \begin{matrix} \lambda \\ \lambda_2\lambda_1 \end{matrix} \middle\| E^R \middle\| \begin{matrix} \lambda \\ \lambda_2'\lambda_1' \end{matrix} \right\rangle \\ &= \left\langle \begin{matrix} \lambda \\ \lambda_1\lambda_2 \end{matrix} \middle\| E^L \middle\| \begin{matrix} \lambda \\ \lambda_1'\lambda_2' \end{matrix} \right\rangle = (-1)^{\lambda_1+\lambda_1'+\lambda_2+\lambda_2'}\left\langle \begin{matrix} \lambda \\ \lambda_2'\lambda_1' \end{matrix} \middle\| E^L \middle\| \begin{matrix} \lambda \\ \lambda_2\lambda_1 \end{matrix} \right\rangle, \end{aligned} \tag{30}$$

where the phase factors may be evaluated using eq. (I.121) and the superscripts R and L imply raising and lowering generators, respectively (cf., eqs. (II.39′, 39″)). Clearly, the last two RMEs in eq. (30) are associated with the subgroup chain $U(n) \supset U(n_2) \times U(n_1)$. Since the raising or lowering character is implied by the irreps involved, we can drop the superscripts R and L for RMEs. We can thus write in analogy to eq. (8) that

$$\left\langle \lambda \begin{array}{cc} \lambda_1' & \lambda_2' \\ W_1' & W_2' \end{array} \middle| E_{i\alpha} \middle| \lambda \begin{array}{cc} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{array} \right\rangle = \left\langle \begin{array}{c} \lambda \\ \lambda_1'\lambda_2' \end{array} \middle\| E \middle\| \begin{array}{c} \lambda \\ \lambda_1\lambda_2 \end{array} \right\rangle \times \left\langle \begin{array}{cc} \lambda_1' & (0,1) \\ W_1' & \alpha \end{array} \middle| \begin{array}{c} \lambda_1 \\ W_1 \end{array} \right\rangle^{(s)} \left\langle \begin{array}{cc} \lambda_2 & (0,1) \\ W_2 & i \end{array} \middle| \begin{array}{c} \lambda_2' \\ W_2' \end{array} \right\rangle^{(s)} . \tag{8′}$$

4. Matrix elements of spin-free creation and annihilation operators

We recall that the $U(n)$ creation ($C^\dagger$) and annihilation (C) operators play the key role in our tensor algebra formalism. Their importance stems from the fact that the $U(n)$ generators E_{rs} and two-body operators $e_{rs;r's'}$ may be expressed in terms of these operators in a similar way as in the standard spin orbital based second quantization formalism, namely (cf., Part II)

$$E_{rs} = \sum_{\tau=1}^{2} C_r^{\tau\dagger} C_s^{\tau} , \tag{31}$$

$$e_{rs;r's'} \equiv E_{rs}E_{r's'} - \delta_{r's}E_{rs'} = \sum_{\tau,\sigma=1}^{2} C_{r'}^{\sigma\dagger} C_r^{\tau\dagger} C_s^{\tau} C_{s'}^{\sigma} , \tag{32}$$

where r, s, r', s', etc., are either $U(n_1)$ or $U(n_2)$ labels. Although we did not use eq. (31) in evaluating the generator MEs in the preceding section, eq. (32) is essential for the evaluation of two-body MEs. We thus have to derive first the MEs of operators $C^\dagger$ and C in a partitioned basis.

We have seen in Part II that the MEs of $C_r^{\sigma\dagger}$ and C_s^{σ} operators in a canonical $U(n)$ GT basis are given by scaled CG coefficients (cf., eqs. (II.25′ and 25″)). Designating the $U(n_1)$ and $U(n_2)$ counterparts of these operators as $\tilde{C}_\alpha^{\tau\dagger}$, $\tilde{C}_\alpha^{\tau}$, $\tilde{C}_i^{\tau\dagger}$ and $\tilde{C}_i^{\tau}$, their MEs in standard GT bases of $U(n_1)$ and $U(n_2)$ are again given by scaled $U(n_1)$ and $U(n_2)$ CG coefficients. However the $U(n)$ operators, say $C_\alpha^{\tau\dagger}$ or $C_i^{\tau\dagger}$, do not represent unit tensor operators with respect to subgroups $U(n_1)$ and $U(n_2)$. Thus, while these $U(n)$ operators induce a unique shift on $U(n)$ irreps, i.e., $\lambda \rightarrow \lambda - \tau$, this is not the case with respect to either $U(n_1)$ or $U(n_2)$. In other words, the resulting $U(n_1)$ and $U(n_2)$ irreps are not unique. Consequently, the MEs of $U(n)$ operators $C_r^{\tau\dagger}$ or C_r^{τ}, $r = \alpha$ or i, in the $U(n) \supset U(n_1) \times U(n_2)$ partitioned basis are not simply given by CG coefficients. Nonetheless, since $C_\alpha^{\tau\dagger}$ and $C_i^{\tau\dagger}$ are vector operators with respect to U(n_1) and U(n_2), respectively, we can apply the Wigner–Eckart theorem and obtain

$$\left\langle \lambda \begin{array}{cc} \lambda_1' & \lambda_2' \\ W_1' & W_2' \end{array} \middle| C_\alpha^{\sigma\dagger} \middle| \lambda - \tau \begin{array}{cc} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{array} \right\rangle$$
$$= \delta_{\sigma\tau}\delta_{\lambda_2'\lambda_2}\delta_{W_2'W_2} \left\langle \begin{array}{c} \lambda \\ \lambda_1'\lambda_2 \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1\lambda_2 \end{array} \right\rangle \left\langle \begin{array}{c} \lambda_1 \\ W_1 \end{array} \begin{array}{c} (0,1) \\ \alpha \end{array} \middle| \begin{array}{c} \lambda_1' \\ W_1' \end{array} \right\rangle^{(s)}$$
$$= \delta_{\sigma\tau}\delta_{\lambda_2'\lambda_2}\delta_{W_2'W_2} \left\langle \begin{array}{c} \lambda \\ \lambda_1'\lambda_2 \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1\lambda_2 \end{array} \right\rangle \left\langle \begin{array}{c} \lambda_1' \\ W_1' \end{array} \middle| \tilde{C}_\alpha^{\rho\dagger} \middle| \begin{array}{c} \lambda_1 \\ W_1 \end{array} \right\rangle, \quad (33)$$

where the shift ρ is given by $\lambda_1 + \rho = \lambda_1'$ and where we used the fact that the CG coefficients for vector operators of U(n_1) are equal to the U(n_1) MEs of $\tilde{C}_\alpha^{\rho\dagger}$ (cf., eq. (II.25)). Similarly, we have that

$$\left\langle \lambda \begin{array}{cc} \lambda_1' & \lambda_2' \\ W_1' & W_2' \end{array} \middle| C_i^{\sigma\dagger} \middle| \lambda - \tau \begin{array}{cc} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{array} \right\rangle$$
$$= \delta_{\sigma\tau}\delta_{\lambda_1'\lambda_1}\delta_{W_1'W_1} \left\langle \begin{array}{c} \lambda \\ \lambda_1\lambda_2' \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1\lambda_2 \end{array} \right\rangle \left\langle \begin{array}{c} \lambda_2 \\ W_2 \end{array} \begin{array}{c} (0,1) \\ i \end{array} \middle| \begin{array}{c} \lambda_2' \\ W_2' \end{array} \right\rangle^{(s)}$$
$$= \delta_{\sigma\tau}\delta_{\lambda_1'\lambda_1}\delta_{W_1'W_1} \left\langle \begin{array}{c} \lambda \\ \lambda_1\lambda_2' \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1\lambda_2 \end{array} \right\rangle \left\langle \begin{array}{c} \lambda_2' \\ W_2' \end{array} \middle| \tilde{C}_i^{\eta\dagger} \middle| \begin{array}{c} \lambda_2 \\ W_2 \end{array} \right\rangle, \quad (34)$$

where $\lambda_2 + \eta = \lambda_2'$. Again, we replaced the U(n_2) CG coefficient by the U(n_2) ME of $\tilde{C}_i^{\eta\dagger}$. We emphasize that the U(n) and U(n_i) vector operators are distinguished by a tilde. The first factor on the right-hand side of eq. (33) or (34) is the RME of a $C^\dagger$-type operator in a partitioned basis that depends on the U(n), U(n_1) and U(n_2) irreps. These RMEs remain to be determined. The MEs of annihilation operators are obtained by hermitian conjugation of eqs. (33) and (34).

In view of eqs. (31), (33) and (34) we can express MEs of $E_{\alpha i}$ in terms of MEs of $C_\alpha^{\tau\dagger}$ and C_i^{τ} operators. Comparing the result with eq. (8), we get the relationship between the RMEs of E operators in eq. (8) and the RMEs of $C^\dagger$ operators in eqs. (33)–(34):

$$\left\langle \begin{array}{c} \lambda \\ \lambda_1'\lambda_2' \end{array} \middle\| E \middle\| \begin{array}{c} \lambda \\ \lambda_1\lambda_2 \end{array} \right\rangle = \sum_\tau \left\langle \begin{array}{c} \lambda \\ \lambda_1'\lambda_2' \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1\lambda_2' \end{array} \right\rangle \left\langle \begin{array}{c} \lambda \\ \lambda_1\lambda_2 \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1\lambda_2' \end{array} \right\rangle$$
$$= \sum_\tau \left\langle \begin{array}{c} \lambda \\ \lambda_1'\lambda_2' \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1'\lambda_2 \end{array} \right\rangle \left\langle \begin{array}{c} \lambda \\ \lambda_1\lambda_2 \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1'\lambda_2 \end{array} \right\rangle, \quad (35)$$

where the second equation is a consequence of the symmetry properties of generator RMEs, eq. (30).

The evaluation of the RMEs of $C^\dagger$ operators is thus straightforward. We see from eqs. (33) and (34) that there are two kinds of $C^\dagger$ RMEs. In the first case, required for the evaluation of MEs of $U(n_2)$ vector operators, eq. (34), the $U(n_1)$ irreps are identical while the $U(n_2)$ irreps are different. In the second case, eq. (33), the $U(n_1)$ irreps are different while the $U(n_2)$ irreps are identical. Thus, the RMEs of the first kind may be obtained by considering the MEs of $C_n^{\tau\dagger}, n = n_1 + n_2$. If we choose for W_2' a tableau that is obtained by adding one box labeled with orbital index n to the diagram W_2 in which n is unoccupied (i.e., n is now singly occupied in W_2'), eq. (34) becomes

$$\langle C_n^{\tau\dagger}\rangle \equiv \left\langle \lambda \begin{array}{cc} \lambda_1 & \lambda_2' \\ W_1 & W_2' \end{array} \middle| C_n^{\tau\dagger} \middle| \lambda-\tau \begin{array}{cc} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{array} \right\rangle = \left\langle \begin{array}{c} \lambda \\ \lambda_1\lambda_2' \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1\lambda_2 \end{array} \right\rangle$$
$$\times \left(\begin{array}{cc} \lambda_2 & (0,1) \\ \lambda_2 & (0,0) \end{array} \middle| \begin{array}{c} \lambda_2' \\ \lambda_2 \end{array} \right)^{(s)} = \left\langle \begin{array}{c} \lambda \\ \lambda_1\lambda_2' \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1\lambda_2 \end{array} \right\rangle . \tag{36}$$

On the other hand, the ME of $C_n^{\tau\dagger}$ on the left-hand side of eq. (36) can be given the following form using the basis transformation, eq. (4):

$$\langle C_n^{\tau\dagger}\rangle = \sum_{W,W'} \left\langle \lambda \begin{array}{cc} \lambda_1 & \lambda_2' \\ W_1 & W_2' \end{array} \middle| \begin{array}{c} \lambda \\ W' \end{array} \right\rangle \left\langle \begin{array}{c} \lambda \\ W' \end{array} \middle| C_n^{\tau\dagger} \middle| \begin{array}{c} \lambda-\tau \\ W \end{array} \right\rangle$$
$$\times \left\langle \begin{array}{c} \lambda-\tau \\ W \end{array} \middle| \lambda-\tau \begin{array}{cc} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{array} \right\rangle , \tag{37}$$

where W and W' are such that they yield identical tableaux at the $U(n-1)$ level, i.e., $W_n \neq W_n'$ but $W_{n-1} = W_{n-1}'$. The ME of $C_n^{\tau\dagger}$ is simply an isoscalar factor. Expressing, further, the first coefficient on the right-hand side of eq. (37) as a product of an I_t factor and a $U(n-1)$ transformation coefficient, we get

$$\langle C_n^{\tau\dagger}\rangle = I_t \left(\begin{array}{cc} \lambda_1 & \lambda_2' \\ \lambda_1 & \lambda_2 \end{array} \middle| \begin{array}{c} \lambda \\ \lambda-\tau \end{array} \right) \left(\begin{array}{cc} \lambda-\tau & (0,1) \\ \lambda-\tau & (0,0) \end{array} \middle| \begin{array}{c} \lambda \\ \lambda-\tau \end{array} \right)^{(s)}$$
$$\times \sum_{\tilde{W}} \left| \left\langle \begin{array}{c} \lambda-\tau \\ \tilde{W} \end{array} \middle| \lambda-\tau \begin{array}{cc} \lambda_1 & \lambda_2 \\ \tilde{W}_1 & \tilde{W}_2 \end{array} \right\rangle \right|^2 , \tag{38}$$

where the scaled isoscalar factor equals 1, the transformation coefficients are normalized (cf., eq. (I.68)) and tilde indicates the $U(n-1)$ level tableaux. This implies that the RMEs of the first kind are simply I_t factors, i.e.

$$\left\langle \begin{array}{c} \lambda \\ \lambda_1\lambda_2' \end{array} \middle\| C^\dagger \middle\| \begin{array}{c} \lambda-\tau \\ \lambda_1\lambda_2 \end{array} \right\rangle = I_t \left(\begin{array}{cc} \lambda_1 & \lambda_2' \\ \lambda_1 & \lambda_2 \end{array} \middle| \begin{array}{c} \lambda \\ \lambda-\tau \end{array} \right) . \tag{39}$$

There are four RMEs of this kind that immediately follow from table I.2. Their explicit values are given in table 2.

The derivation of the RMEs of the second kind is more laborious when we consider MEs of special operators, say $C_{n_1}^{\tau\dagger}$, since there are many levels between n_1 and n. However, a simple derivation may be carried out using eq. (35). Since the RMEs of E operators (table 1) and the RMEs of $C^\dagger$ operators of the first kind (eq. (39) and table 2) are known, we can solve eq. (35) to get the RMEs of $C^\dagger$ operators of the second kind. The four RMEs of this kind thus evaluated are given in table 2. These results show (table 2) that the $C^\dagger$ RMEs of the first and second kinds satisfy the following symmetry property:

$$\left\langle \begin{matrix} \lambda \\ \lambda_1'\lambda_2 \end{matrix} \middle\| C^\dagger \middle\| \begin{matrix} \lambda-\tau \\ \lambda_1\lambda_2 \end{matrix} \right\rangle = (-1)^{\lambda+[\lambda-\tau]+\lambda_1+\lambda_1'} \left\langle \begin{matrix} \lambda \\ \lambda_2\lambda_1' \end{matrix} \middle\| C^\dagger \middle\| \begin{matrix} \lambda-\tau \\ \lambda_2\lambda_1 \end{matrix} \right\rangle . \tag{40}$$

Finally, to gain a better insight into the nature of the above defined RMEs of $C^\dagger$ operators we exploit the well-known fact that follows from the Wigner–Eckart theorem, namely that a ME of an irreducible tensor operator that is adapted to the group chain $\mathrm{U}(n) \supset \mathrm{U}(n_1) \times \mathrm{U}(n_2)$ may be expressed as a product of a $\mathrm{U}(n)$

Table 2
The RMEs of $\mathrm{U}(n)$ $C^\dagger$ operators in a partitioned basis (3).

λ	λ_1	λ_2	$\left\langle \begin{matrix} (a,b) \\ (a_1,b_1)(a_2,b_2) \end{matrix} \middle\| C^\dagger \middle\| \begin{matrix} \lambda \\ \lambda_1\lambda_2 \end{matrix} \right\rangle$
$(a,b-1)$	(a_1,b_1)	(a_2,b_2-1)	$\frac{1}{2}\left[\frac{(b_2-b_1+b)(b_1+b_2+b+2)}{b_2(b+1)}\right]^{1/2}$
		(a_2-1,b_2+1)	$\frac{(-1)^{a_1+a_2+a+b_2}}{2}\left[\frac{(b_1+b_2-b+2)(b_1-b_2+b)}{(b_2+2)(b+1)}\right]^{1/2}$
$(a-1,b+1)$		(a_2,b_2-1)	$\frac{(-1)^{a_1+a_2+a+b_2}}{2}\left[\frac{(b_1+b_2-b)(b_1-b_2+b+2)}{b_2(b+1)}\right]^{1/2}$
		(a_2-1,b_2+1)	$\frac{1}{2}\left[\frac{(b_2-b_1+b+2)(b_1+b_2+b+4)}{(b_2+2)(b+1)}\right]^{1/2}$
$(a,b-1)$	(a_1,b_1-1)	(a_2,b_2)	$\frac{(-1)^{a_1+a+b_2}}{2}\left[\frac{(b_1-b_2+b)(b_1+b_2+b+2)}{b_1(b+1)}\right]^{1/2}$
	(a_1-1,b_1+1)		$\frac{(-1)^{a_2+b_2}}{2}\left[\frac{(b_1+b_2-b+2)(b_2-b_1+b)}{(b_1+2)(b+1)}\right]^{1/2}$
$(a-1,b+1)$	(a_1,b_1-1)		$\frac{(-1)^{a_2}}{2}\left[\frac{(b_1+b_2-b)(b_2-b_1+b+2)}{b_1(b+1)}\right]^{1/2}$
	(a_1-1,b_1+1)		$\frac{(-1)^{a_1+a}}{2}\left[\frac{(b_1-b_2+b+2)(b_1+b_2+b+4)}{(b_1+2)(b+1)}\right]^{1/2}$

RME, depending only on the U(n) irreps, and a general CG coefficient for the partitioned basis that is adapted to the $U(n) \supset U(n_1) \times U(n_2)$ chain. The CG (coupling) coefficient for the partitioned basis is then expressible as a product of an isoscalar factor for the group chain $U(n) \supset U(n_1) \times U(n_2)$ and of CG coefficients for the standard GT bases of $U(n_1)$ and $U(n_2)$, namely

$$\left\langle \begin{matrix} \mu & \nu \\ \mu_1\mu_2 & \nu_1\nu_2 \\ U_1U_2 & V_1V_2 \end{matrix} \middle| \begin{matrix} \lambda \\ \lambda_1\lambda_2 \\ W_1W_2 \end{matrix} \right\rangle = \left(\begin{matrix} \mu & \nu \\ \mu_1\mu_2 & \nu_1\nu_2 \end{matrix} \middle| \begin{matrix} \lambda \\ \lambda_1\lambda_2 \end{matrix} \right) \left\langle \begin{matrix} \mu_1 & \nu_1 \\ U_1 & V_1 \end{matrix} \middle| \begin{matrix} \lambda_1 \\ W_1 \end{matrix} \right\rangle \left\langle \begin{matrix} \mu_2 & \nu_2 \\ U_2 & V_2 \end{matrix} \middle| \begin{matrix} \lambda_2 \\ W_2 \end{matrix} \right\rangle,$$

where we now write $\left|\lambda \begin{smallmatrix} \mu & \nu \\ U & V \end{smallmatrix}\right\rangle$ as $\left|\begin{smallmatrix} \lambda \\ \mu\nu \\ UV \end{smallmatrix}\right\rangle$ (cf. also notation used in ref. [27]). Applying this result to MEs of, say, $C_i^{\tau\dagger}$ and noting that we deal with a vector operator of irrep (0, 1) of U(n_2) and a scalar (rank zero tensor) of irrep (0, 0) of U(n_1), we get

$$\begin{aligned} &\left\langle \lambda \begin{matrix} \lambda_1' & \lambda_2' \\ W_1' & W_2' \end{matrix} \middle| C_i^{\sigma\dagger} \middle| \lambda - \tau \begin{matrix} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{matrix} \right\rangle \\ &= \delta_{\sigma\tau}\delta_{\lambda_1'\lambda_1}\delta_{W_1'W_1}\langle\lambda\|C^\dagger\|\lambda-\tau\rangle \left(\begin{matrix} \lambda \\ \lambda_1\lambda_2' \end{matrix} \middle| \begin{matrix} \lambda-\tau & (0,1) \\ \lambda_1\lambda_2 & (0,0)(0,1) \end{matrix} \right) \\ &\quad \times \left\langle \begin{matrix} \lambda_2 & (0,1) \\ W_2 & i \end{matrix} \middle| \begin{matrix} \lambda_2' \\ W_2' \end{matrix} \right\rangle, \end{aligned} \tag{41}$$

where the first factor on the right-hand side of eq. (41) is an RME of $C^\dagger$ that depends only on the U(n) irreps (cf. eq. (II.23)) and the second factor is an isoscalar factor for $U(n) \supset U(n_1) \times U(n_2)$. Comparing now eq. (41), and an analogous equation for $C_\alpha^{\sigma\dagger}$, with eqs. (34) and (33), respectively, and using eq. (II.17), we immediately find for the $U(n) \supset U(n_1) \times U(n_2)$ isoscalar factors that

$$\begin{aligned} &\left(\begin{matrix} \lambda-\tau & (0,1) \\ \lambda_1\lambda_2 & (0,1)(0,0) \end{matrix} \middle| \begin{matrix} \lambda \\ \lambda_1'\lambda_2 \end{matrix} \right) \\ &= \langle\lambda\|C^\dagger\|\lambda-\tau\rangle^{-1}\langle\lambda_1'\|C^\dagger\|\lambda_1\rangle \left\langle \begin{matrix} \lambda \\ \lambda_1'\lambda_2 \end{matrix} \middle\| C^\dagger \middle\| \begin{matrix} \lambda-\tau \\ \lambda_1\lambda_2 \end{matrix} \right\rangle, \end{aligned} \tag{42}$$

$$\begin{aligned} &\left(\begin{matrix} \lambda-\tau & (0,1) \\ \lambda_1\lambda_2 & (0,0)(0,1) \end{matrix} \middle| \begin{matrix} \lambda \\ \lambda_1\lambda_2' \end{matrix} \right) \\ &= \langle\lambda\|C^\dagger\|\lambda-\tau\rangle^{-1}\langle\lambda_2'\|C^\dagger\|\lambda_2\rangle \left\langle \begin{matrix} \lambda \\ \lambda_1\lambda_2' \end{matrix} \middle\| C^\dagger \middle\| \begin{matrix} \lambda-\tau \\ \lambda_1\lambda_2 \end{matrix} \right\rangle. \end{aligned} \tag{43}$$

Alternatively, we can derive the second relationship, eq. (43), by specializing eq. (41) for the case $i = n$, in which case the ME of $C_n^{\sigma\dagger}$ on the left-hand side is given by the reduced element of $C^\dagger$, eq. (36). Evaluating subsequently the U(n_2) CG coefficient on the right-hand side of eq. (41) with the help of eqs. (II.9b, 12′, 25 and 25′) and table II.1, we find that it is equal to the inverse of the U(n_2) RME, i.e. to $\langle\lambda_2'\|C^\dagger\|\lambda_2\rangle^{-1}$, thus again obtaining eq. (43).

Assuming the same phase convention as in Parts I and II, so that the $C^\dagger$ RMEs are real, we immediately realize that they are identical with those obtained in Part II for the standard GT basis, since they are basis independent. Thus, recalling eq. (II.23), we can write

$$\begin{aligned}\langle(a,b)\|C^\dagger\|(a,b-1)\rangle &= [b(a+b+1)/(b+1)]^{1/2}\,,\\ \langle(a,b)\|C^\dagger\|(a-1,b+1)\rangle &= [a(b+2)/(b+1)]^{1/2}\,.\end{aligned} \tag{44}$$

Thus, relying on table 2 and eq. (44), we can easily derive the explicit form of the isoscalar factors given by eqs. (42) and (43). We can also verify that these factors satisfy the following orthogonality properties:

$$\sum_{\mu_1\mu_2\nu_1\nu_2}\left(\begin{matrix}\mu & \nu \\ \mu_1\mu_2 & \nu_1\nu_2\end{matrix}\middle|\begin{matrix}\lambda \\ \lambda_1\lambda_2\end{matrix}\right)\left(\begin{matrix}\mu & \nu \\ \mu_1\mu_2 & \nu_1\nu_2\end{matrix}\middle|\begin{matrix}\lambda' \\ \lambda_1\lambda_2\end{matrix}\right) = \delta_{\lambda\lambda'}\,, \tag{45}$$

$$\sum_{\lambda}\left(\begin{matrix}\mu & \nu \\ \mu_1\mu_2 & \nu_1\nu_2\end{matrix}\middle|\begin{matrix}\lambda \\ \lambda_1\lambda_2\end{matrix}\right)\left(\begin{matrix}\mu & \nu \\ \mu_1'\mu_2' & \nu_1'\nu_2'\end{matrix}\middle|\begin{matrix}\lambda \\ \lambda_1\lambda_2\end{matrix}\right) = \delta_{\mu_1\mu_1'}\delta_{\mu_2\mu_2'}\delta_{\nu_1\nu_1'}\delta_{\nu_2\nu_2'}\,. \tag{46}$$

5. Matrix element of two-body operators

As explained in section 7 of Part II, it is both more appropriate and convenient to examine directly the MEs of two-body operators, eq. (32), rather than MEs of generator products. Not only do they represent the required quantities, but they are in fact easier to obtain than the MEs of generator products. Throughout this section we employ the following shorthand notation $\langle e_{rs;r's'}\rangle$ for the required MEs, i.e.

$$\begin{aligned}\langle e_{rs;r's'}\rangle &\equiv \left\langle \lambda\ \begin{matrix}\lambda_1' & \lambda_2' \\ W_1' & W_2'\end{matrix}\middle| e_{rs;r's'} \middle| \lambda\ \begin{matrix}\lambda_1 & \lambda_2 \\ W_1 & W_2\end{matrix}\right\rangle \\ &\equiv \left\langle (a,b)\ \begin{matrix}(a_1',b_1') & (a_2',b_2') \\ W_1' & W_2'\end{matrix}\middle| e_{rs;r's'} \middle| (a,b)\ \begin{matrix}(a_1,b_1) & (a_2,b_2) \\ W_1 & W_2\end{matrix}\right\rangle,\end{aligned} \tag{47}$$

where r, s, r', s' are either U(n_1) or U(n_2) labels. As already noted in section 2 (cf. eq. (5)), the MEs of $e_{\alpha\beta;\alpha'\beta'}$ and $e_{ik;jl}$ are simply equal to their MEs in U(n_1) and

$\mathrm{U}(n_2)$ bases, respectively. Similarly, the MEs of $e_{\alpha\beta;ij} = e_{ij;\alpha\beta} = E_{\alpha\beta}E_{ij}$ are given by the product of the corresponding $\mathrm{U}(n_1)$ and $\mathrm{U}(n_2)$ MEs, namely

$$\langle e_{\alpha\beta;ij}\rangle = \delta_{\lambda_1'\lambda_1}\delta_{\lambda_2'\lambda_2}\left\langle \begin{matrix}\lambda_1\\ W_1'\end{matrix}\middle| E_{\alpha\beta} \middle| \begin{matrix}\lambda_1\\ W_1\end{matrix}\right\rangle \left\langle \begin{matrix}\lambda_2\\ W_2'\end{matrix}\middle| E_{ij} \middle| \begin{matrix}\lambda_2\\ W_2\end{matrix}\right\rangle . \tag{48}$$

The nontrivial cases which have to be considered are thus:

$$(1)\quad e_{\alpha i;\beta\gamma} = e_{\beta\gamma;\alpha i} = E_{\alpha i}E_{\beta\gamma}\,, \tag{49}$$

$$(2)\quad e_{ik;j\alpha} = e_{j\alpha;ik} = E_{j\alpha}E_{ik}\,, \tag{50}$$

$$(3)\quad e_{\alpha i;\beta j} = e_{\beta j;\alpha i} = E_{\alpha i}E_{\beta j}\,, \tag{51}$$

$$(4)\quad e_{\alpha i;j\beta} = e_{j\beta;\alpha i} = E_{\alpha i}E_{j\beta} - \delta_{ij}E_{\alpha\beta}\,. \tag{52}$$

The first two cases are associated with a one-electron charge transfer between the subsystems, case (3) with a two-electron charge transfer and case (4) with an interchange of electrons between the subsystems. All the remaining cases may be obtained by hermitian conjugation.

In the first case, eq. (49), we can express MEs of $E_{\alpha i}E_{\beta\gamma}$ in terms of MEs of $E_{\alpha i}$, for which eq. (8) applies, and $\mathrm{U}(n_1)$ MEs of $E_{\beta\gamma}$, i.e.,

$$\begin{aligned}\langle e_{\alpha i;\beta\gamma}\rangle &= \sum_{V_1}\left\langle \lambda \;\begin{matrix}\lambda_1' & \lambda_2'\\ W_1' & W_2'\end{matrix}\middle| E_{\alpha i}\middle| \lambda\;\begin{matrix}\lambda_1 & \lambda_2\\ V_1 & W_2\end{matrix}\right\rangle \left\langle \begin{matrix}\lambda_1\\ V_1\end{matrix}\middle| E_{\beta\gamma}\middle| \begin{matrix}\lambda_1\\ W_1\end{matrix}\right\rangle \\ &= \left\langle \begin{matrix}\lambda\\ \lambda_1'\lambda_2'\end{matrix}\middle\| E\middle\| \begin{matrix}\lambda\\ \lambda_1\lambda_2\end{matrix}\right\rangle \sum_{V_1}\left\langle \begin{matrix}\lambda_1'\\ W_1'\end{matrix}\middle| \tilde{C}_\alpha^{\sigma\dagger}\middle| \begin{matrix}\lambda_1\\ V_1\end{matrix}\right\rangle \\ &\quad\times \left\langle \begin{matrix}\lambda_2' & (0,1)\\ W_2' & i\end{matrix}\middle| \begin{matrix}\lambda_2\\ W_2\end{matrix}\right\rangle^{(s)} \left\langle \begin{matrix}\lambda_1\\ V_1\end{matrix}\middle| E_{\beta\gamma}\middle| \begin{matrix}\lambda_1\\ W_1\end{matrix}\right\rangle \\ &= \left\langle \begin{matrix}\lambda\\ \lambda_1'\lambda_2'\end{matrix}\middle\| E\middle\| \begin{matrix}\lambda\\ \lambda_1\lambda_2\end{matrix}\right\rangle \left\langle \begin{matrix}\lambda_2' & (0,1)\\ W_2' & i\end{matrix}\middle| \begin{matrix}\lambda_2\\ W_2\end{matrix}\right\rangle^{(s)} \left\langle \begin{matrix}\lambda_1'\\ W_1'\end{matrix}\middle| \tilde{G}^\sigma_{\alpha;\beta\gamma}\middle| \begin{matrix}\lambda_1\\ W_1\end{matrix}\right\rangle ,\end{aligned} \tag{53}$$

where the shift σ is fixed by the condition $\lambda_1 + \sigma = \lambda_1'$. In the last eq. (53), the generator RME (the first term) and the scaled $\mathrm{U}(n_2)$ CG coefficient (the second term) are known. The last term represents a ME of $\tilde{G}^\sigma_{\alpha;\beta\gamma} \equiv \tilde{C}^{\sigma\dagger}_\alpha E_{\beta\gamma}$ in the $\mathrm{U}(n_1)$ basis (cf., eq. (II.83′)). Similarly, for the case (2), eq. (50), we get an analogous expression

$$\langle e_{ik;j\alpha}\rangle = \left\langle \begin{matrix}\lambda\\ \lambda_1'\lambda_2'\end{matrix}\middle\| E\middle\| \begin{matrix}\lambda\\ \lambda_1\lambda_2\end{matrix}\right\rangle \left\langle \begin{matrix}\lambda_1' & (0,1)\\ W_1' & \alpha\end{matrix}\middle| \begin{matrix}\lambda_1\\ W_1\end{matrix}\right\rangle^{(s)} \left\langle \begin{matrix}\lambda_2'\\ W_2'\end{matrix}\middle| \tilde{G}^\sigma_{j;ik}\middle| \begin{matrix}\lambda_2\\ W_2\end{matrix}\right\rangle , \tag{54}$$

with the shift σ given by $\lambda_2 + \sigma = \lambda_2'$. The MEs of G operators, eq. (II.83), were examined in detail in Part II. We recall that these MEs may be evaluated as simple products of segment values. Defining $r_1 \equiv \max\{\alpha, \beta, \gamma\}, r_2 \equiv \max(\{\alpha, \beta, \gamma\}\backslash\{r_1\})$ and $r_3 \equiv \min\{\alpha, \beta, \gamma\}$, this segmentation formalism involves in general: (1) A simple product of segment values from the top level n_1 to level r_1 and from level r_2 to level r_3, where the segment values are given by scaled isoscalar factors of $C^\dagger$ vector operators. (2) In the region between the levels r_1 and r_2, two terms are generally required, each of which is a simple product of segment values. The character of these two terms depends on the nature of the two smaller labels, r_2 and r_3. If both r_2 and r_3 are of a creation type in $\tilde{G}^{\sigma}_{\alpha;\beta\gamma} \equiv \tilde{C}^{\sigma\dagger}_{\alpha} E_{\beta\gamma}$, i.e., α and β, these terms are given by the MEs of symmetric and antisymmetric tensors, and the corresponding segment values are the isoscalar factors associated with these tensors. On the other hand, if one of the lables r_2 and r_3 is of a creation type and another one of an annihilation type in $\tilde{G}^{\sigma}_{\alpha;\beta\gamma} \equiv \tilde{C}^{\sigma\dagger}_{\alpha} E_{\beta\gamma}$, e.g., α, γ or β, γ, then the adjoint tensors, namely the generators E and the operators N (cf. section 6 of Part II) come into play. Consequently, the required segment values in this region are then the E and N factors defined in Part II. (3) Finally, below the level r_3, all the irreps in the bra and the ket must be identical lest the ME vanishes. We refer to Part II for the details and for the explicit values of required segment values.

In the third case, eq. (51), involving two $\mathrm{U}(n_1)$ labels and two $\mathrm{U}(n_2)$ labels, the operators involved annihilates two boxes from W_2 and creates two boxes in W_1. Their MEs may thus be expressed in terms of the MEs of $E_{\alpha i}$ and $E_{\beta j}$, namely

$$\langle e_{\alpha i;\beta j}\rangle = \sum_{\nu_1\nu_2 V_1 V_2} \left\langle \lambda \begin{array}{cc} \lambda_1' & \lambda_2' \\ W_1' & W_2' \end{array} \right| E_{\alpha i} \left| \lambda \begin{array}{cc} \nu_1 & \nu_2 \\ V_1 & V_2 \end{array} \right\rangle \times \left\langle \lambda \begin{array}{cc} \nu_1 & \nu_2 \\ V_1 & V_2 \end{array} \right| E_{\beta j} \left| \lambda \begin{array}{cc} \lambda_1 & \lambda_2 \\ W_1 & W_2 \end{array} \right\rangle . \tag{55}$$

Applying eq. (8), we thus obtain a rather complex formula that contains two generator RMEs, two $\mathrm{U}(n_1)$ MEs involving $\tilde{C}^\dagger$ operators and two $\mathrm{U}(n_2)$ MEs of $\tilde{C}$-type operators. The sum over V_1 and V_2 leads then to an ME of a product of two $\tilde{C}^\dagger$ operators and another ME of a product of two $\tilde{C}$ operators. Moreover, the sum over the intermediate irrep labels can be replaced by the sum over shift components σ and ρ defined by $\nu_1 \equiv \lambda_1 + \sigma$ and $\nu_2 \equiv \lambda_2 - \rho$. We thus get

$$\langle e_{\alpha i;\beta j}\rangle = \sum_{\sigma\rho} \left\langle \begin{array}{c} \lambda \\ \lambda_1'\lambda_2' \end{array} \right\| E \left\| \begin{array}{c} \lambda \\ (\lambda_1+\sigma)(\lambda_2-\rho) \end{array} \right\rangle \left\langle \begin{array}{c} \lambda \\ (\lambda_1+\sigma)(\lambda_2-\rho) \end{array} \right\| E \left\| \begin{array}{c} \lambda \\ \lambda_1\lambda_2 \end{array} \right\rangle \times \left\langle \begin{array}{c} \lambda_1' \\ W_1' \end{array} \right| \tilde{C}^{\tau\dagger}_{\alpha} \tilde{C}^{\sigma\dagger}_{\beta} \left| \begin{array}{c} \lambda_1 \\ W_1 \end{array} \right\rangle \left\langle \begin{array}{c} \lambda_2' \\ W_2' \end{array} \right| \tilde{C}^{\eta}_{i} \tilde{C}^{\rho}_{j} \left| \begin{array}{c} \lambda_2 \\ W_2 \end{array} \right\rangle , \tag{56}$$

where the shift labels τ and η are fixed by the conditions $\lambda_1 + \sigma + \tau = \lambda_1'$ and $\lambda_2 - \rho - \eta = \lambda_2'$.

It thus remains to evaluate the MEs of $U(n_1)$ and $U(n_2)$ pairing operators. We showed in Part II that these MEs may be written in terms of MEs of symmetric and antisymmetric tensors. The required relationships (originally derived for $U(n)$ but, of course, applicable to $U(n_1)$ and $U(n_2)$) have the form (cf., eqs. (II.47–51))

$$\left\langle \begin{matrix} (a,b) \\ W' \end{matrix} \middle| C_r^{1\dagger} C_s^{1\dagger} \middle| \begin{matrix} (a,b-2) \\ W \end{matrix} \right\rangle = -\frac{a_{rs}}{\sqrt{2}} \left\langle \begin{matrix} (a,b-2) \\ W \end{matrix} \quad \begin{matrix} (0,2) \\ [rs] \end{matrix} \middle| \begin{matrix} (a,b) \\ W' \end{matrix} \right\rangle^{(s)}, \tag{57}$$

$$\left\langle \begin{matrix} (a,b) \\ W' \end{matrix} \middle| C_r^{2\dagger} C_s^{2\dagger} \middle| \begin{matrix} (a-2,b+2) \\ W \end{matrix} \right\rangle = -\frac{a_{rs}}{\sqrt{2}} \left\langle \begin{matrix} (a-2,b+2) \\ W \end{matrix} \quad \begin{matrix} (0,2) \\ [rs] \end{matrix} \middle| \begin{matrix} (a,b) \\ W' \end{matrix} \right\rangle^{(s)}, \tag{58}$$

$$\begin{aligned} \left\langle \begin{matrix} (a,b) \\ W' \end{matrix} \middle| C_r^{1\dagger} C_s^{2\dagger} \middle| \begin{matrix} (a-1,b) \\ W \end{matrix} \right\rangle =& (1+\delta_{rs})^{1/2} \frac{1}{2} \sqrt{\frac{b}{b+1}} \\ & \times \left\langle \begin{matrix} (a-1,b) \\ W \end{matrix} \quad \begin{matrix} (1,0) \\ [rs] \end{matrix} \middle| \begin{matrix} (a,b) \\ W' \end{matrix} \right\rangle^{(s)} \\ & - a_{rs} \tilde{\delta}_{b,0} \frac{1}{2} \sqrt{\frac{b+2}{b+1}} \left\langle \begin{matrix} (a-1,b) \\ W \end{matrix} \quad \begin{matrix} (0,2) \\ [rs] \end{matrix} \middle| \begin{matrix} (a,b) \\ W' \end{matrix} \right\rangle^{(s)}, \end{aligned} \tag{59}$$

$$\begin{aligned} \left\langle \begin{matrix} (a,b) \\ W' \end{matrix} \middle| C_r^{2\dagger} C_s^{1\dagger} \middle| \begin{matrix} (a-1,b) \\ W \end{matrix} \right\rangle =& (1+\delta_{rs})^{1/2} \frac{1}{2} \sqrt{\frac{b+2}{b+1}} \\ & \times \left\langle \begin{matrix} (a-1,b) \\ W \end{matrix} \quad \begin{matrix} (1,0) \\ [rs] \end{matrix} \middle| \begin{matrix} (a,b) \\ W' \end{matrix} \right\rangle^{(s)} \\ & + a_{rs} \tilde{\delta}_{b,0} \frac{1}{2} \sqrt{\frac{b}{b+1}} \left\langle \begin{matrix} (a-1,b) \\ W \end{matrix} \quad \begin{matrix} (0,2) \\ [rs] \end{matrix} \middle| \begin{matrix} (a,b) \\ W' \end{matrix} \right\rangle^{(s)}, \end{aligned} \tag{60}$$

where $\tilde{\delta}_{b,0} = 1 - \delta_{b,0}$ and

$$a_{rs} = \begin{cases} 1 & \text{if } r<s, \\ 0 & \text{if } r=s, \\ -1 & \text{if } r>s. \end{cases} \tag{61}$$

In view of these relationships, eq. (56) may be written in the following general form:

$$\langle e_{\alpha i;\beta j}\rangle = \sum_{P,Q=S,A} C_{PQ} \left\langle \begin{matrix} \lambda_1 & \lambda_P \\ W_1 & [\alpha\beta] \end{matrix} \middle| \begin{matrix} \lambda_1' \\ W_1' \end{matrix} \right\rangle^{(s)} \left\langle \begin{matrix} \lambda_2' & \lambda_Q \\ W_2' & [ij] \end{matrix} \middle| \begin{matrix} \lambda_2 \\ W_2 \end{matrix} \right\rangle^{(s)}, \tag{62}$$

where $\lambda_S \equiv (1,0)$, $\lambda_A \equiv (0,2)$, and $[\alpha\beta]$ and $[ij]$ designate the appropriate two-box Weyl tableaux (see section 5 of Part II for details). The coefficients C_{PQ} depend on all $U(n)$, $U(n_1)$ and $U(n_2)$ irrep labels and orbital labels ij and $\alpha\beta$.

It is straightforward though laborious to work out the explicit form of the coefficients C_{PQ} using the RMEs of table 1 and eqs. (57)–(60). There are nine possible choices for the irreps λ_1' and λ_2' that are listed in the first and second columns of table 3, respectively. Formally, the sum in eq. (56) contains four terms. However, some of them vanish except in the case when $b_1' = b_1$ and $b_2' = b_2$. In four cases (when $b_1' - b_1 = \pm 2$ and $b_2' - b_2 = \pm 2$), the sum in eq. (56) reduces to only one term, while in the remaining four cases, it contains two terms. Let us illustrate this on an example. When $\lambda_1' = (a_1, b_1 + 2)$ and $\lambda_2' = (a_2, b_2 - 2)$, all shifts σ, τ, ρ, η must equal 1 and eq. (56) becomes

$$\begin{aligned} \langle e_{\alpha i;\beta j}\rangle = & \left\langle \begin{matrix} (a,b) \\ (a_1,b_1+2)(a_2,b_2-2) \end{matrix} \middle\| E \middle\| \begin{matrix} (a,b) \\ (a_1,b_1+1)(a_2,b_2-1) \end{matrix} \right\rangle \\ & \times \left\langle \begin{matrix} (a_1,b_2+2) \\ W_1' \end{matrix} \middle| \tilde{C}_\alpha^{1\dagger}\tilde{C}_\beta^{1\dagger} \middle| \begin{matrix} (a_1,b_1) \\ W_1 \end{matrix} \right\rangle \\ & \times \left\langle \begin{matrix} (a,b) \\ (a_1,b_1+1)(a_2,b_2-1) \end{matrix} \middle\| E \middle\| \begin{matrix} (a,b) \\ (a_1,b_1)(a_2,b_2) \end{matrix} \right\rangle \\ & \times \left\langle \begin{matrix} (a_2,b_2-2) \\ W_2' \end{matrix} \middle| \tilde{C}_i^1\tilde{C}_j^1 \middle| \begin{matrix} (a_2,b_2) \\ W_2 \end{matrix} \right\rangle. \end{aligned} \tag{63}$$

In view of eq. (57), the MEs of $\tilde{C}_\alpha^{1\dagger}\tilde{C}_\beta^{1\dagger}$ and $\tilde{C}_i^1\tilde{C}_j^1$ involve only antisymmetric terms, so that $C_{SS} = C_{SA} = C_{AS} = 0$ and C_{AA} is given by the product of two generator RMEs and of two coefficients $(-a_{\alpha\beta}/\sqrt{2})$ and $(-a_{ij}/\sqrt{2})$ arising from eq. (57), so that

$$\begin{aligned} C_{AA} = & \, a_{\alpha\beta}a_{ij} \\ & \times \frac{1}{8}\left[\frac{(b_2-b_1+b-2)(b_2-b_1+b)(b_1-b_2+b+2)(b_1-b_2+b+4)}{(b_1+1)(b_1+2)(b_2-1)b_2}\right]^{1/2}. \end{aligned} \tag{64}$$

In fact, we can prove that from among the coefficients C_{SS}, C_{SA}, C_{AS} and C_{AA}, those corresponding to mixed symmetry, namely C_{SA} and C_{AS}, always vanish. This may be achieved by comparing MEs of $e_{\alpha i;\beta j}$ and $e_{\beta j;\alpha i}$, or by a direct calculation using eq. (56). Thus, we finally get

$$\langle e_{\alpha i;\beta j}\rangle = C_{SS}\left\langle \begin{matrix} (a_1,b_1) & (1,0) \\ W_1 & [\alpha\beta] \end{matrix} \middle| \begin{matrix} (a_1',b_1') \\ W_1' \end{matrix} \right\rangle^{(s)} \left\langle \begin{matrix} (a_2',b_2') & (1,0) \\ W_2' & [ij] \end{matrix} \middle| \begin{matrix} (a_2,b_2) \\ W_2 \end{matrix} \right\rangle^{(s)}$$
$$+ C_{AA}\left\langle \begin{matrix} (a_1,b_1) & (0,2) \\ W_1 & [\alpha\beta] \end{matrix} \middle| \begin{matrix} (a_1',b_1') \\ W_1' \end{matrix} \right\rangle^{(s)} \left\langle \begin{matrix} (a_2',b_2') & (0,2) \\ W_2' & [ij] \end{matrix} \middle| \begin{matrix} (a_2,b_2) \\ W_2 \end{matrix} \right\rangle^{(s)}, \tag{65}$$

with the coefficients C_{SS} and C_{AA} for all possible cases given in table 3. It is worth noting that the C_{SS} term survives only in one case, namely when $b_1 = b_1'$ and $b_2 = b_2'$. Finally, we recall that the CG coefficients of the symmetric and antisymmetric tensors are given by simple products of relevant isoscalar factors that were given in Part II (cf. eq. (II.52) and tables II.3 and 4).

Similarly as in the third case, eq. (51), the operator characterizing case (4), eq. (52), also contains two $U(n_1)$ and two $U(n_2)$ labels but, in contrast to case (3), preserves the particle number in both subsystems. In view of eq. (32),

$$e_{\alpha i;j\beta} = e_{j\beta;\alpha i} = \sum_{\sigma} C_\alpha^{\sigma\dagger} E_{j\beta} C_i^\sigma\,, \tag{66}$$

so that the MEs of $e_{\alpha i;j\beta}$ may be expressed in terms of those for $C_\alpha^{\sigma\dagger}$, $E_{j\beta}$ and C_i^σ. Exploiting eq. (8) for MEs of $E_{j\beta}$, and eqs. (33) and (34) for those of $C_\alpha^{\sigma\dagger}$ and C_i^σ, respectively, we can write

$$\langle e_{\alpha i;j\beta}\rangle = \sum_{\sigma\nu_1\nu_2V_1V_2} \left\langle \begin{matrix} \lambda \\ \lambda_1'\lambda_2' \end{matrix} \middle\| C^\dagger \middle\| \begin{matrix} \lambda-\sigma \\ \nu_1\lambda_2' \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_1' \\ W_1' \end{matrix} \middle| \tilde{C}_\alpha^{\rho\dagger} \middle| \begin{matrix} \nu_1 \\ V_1 \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda-\sigma \\ \nu_1\lambda_2' \end{matrix} \middle\| E \middle\| \begin{matrix} \lambda-\sigma \\ \lambda_1\nu_2 \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} \nu_1 \\ V_1 \end{matrix} \middle| \tilde{C}_\beta^\tau \middle| \begin{matrix} \lambda_1 \\ W_1 \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_2' \\ W_2' \end{matrix} \middle| \tilde{C}_j^{\xi\dagger} \middle| \begin{matrix} \nu_2 \\ V_2 \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} \lambda \\ \lambda_1\lambda_2 \end{matrix} \middle\| C^\dagger \middle\| \begin{matrix} \lambda-\sigma \\ \lambda_1\nu_2 \end{matrix} \right\rangle \left\langle \begin{matrix} \nu_2 \\ V_2 \end{matrix} \middle| \tilde{C}_i^\eta \middle| \begin{matrix} \lambda_2 \\ W_2 \end{matrix} \right\rangle, \tag{67}$$

where the shifts τ, η and the intermediate irreps ν_1, ν_2 satisfy the relationships $\nu_1 = \lambda_1 - \tau, \nu_2 = \lambda_2 - \eta$, and the shifts ρ and ξ are fixed by the conditions $\lambda_1 - \tau + \rho = \nu_1 + \rho = \lambda_1'$ and $\lambda_2 - \eta + \xi = \nu_2 + \xi = \lambda_2'$. Eliminating the sums over V_1 and V_2 then gives

$$\langle e_{\alpha i;j\beta}\rangle = \sum_{\sigma\tau\eta} \left\langle \begin{matrix} \lambda-\sigma \\ (\lambda_1-\tau)\lambda_2' \end{matrix} \middle\| E \middle\| \begin{matrix} \lambda-\sigma \\ \lambda_1(\lambda_2-\eta) \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda \\ \lambda_1'\lambda_2' \end{matrix} \middle\| C^\dagger \middle\| \begin{matrix} \lambda-\sigma \\ (\lambda_1-\tau)\lambda_2' \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} \lambda \\ \lambda_1\lambda_2 \end{matrix} \middle\| C^\dagger \middle\| \begin{matrix} \lambda-\sigma \\ \lambda_1(\lambda_2-\eta) \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_1' \\ W_1' \end{matrix} \middle| \tilde{C}_\alpha^{\rho\dagger}\tilde{C}_\beta^\tau \middle| \begin{matrix} \lambda_1 \\ W_1 \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_2' \\ W_2' \end{matrix} \middle| \tilde{C}_j^{\xi\dagger}\tilde{C}_i^\eta \middle| \begin{matrix} \lambda_2 \\ W_2 \end{matrix} \right\rangle. \tag{68}$$

Table 3
The coefficients C_{SS} and C_{AA} in eq. (65) that depend on all bra and ket irreps of $U(n_1)$, $U(n_2)$ and $U(n)$. The irrep of $U(n)$ is fixed as (a,b) and the ket irreps of $U(n_1)$ and $U(n_2)$ are fixed as (a_1,b_1) and (a_2,b_2), respectively. Thus C_{SS} and C_{AA} are given as functions of the bra irreps (a_1',b_1') and (a_2',b_2') of $U(n_1)$ and $U(n_2)$, respectively. To avoid repetition we define $C_{AA} \equiv \frac{1}{8} a_{\alpha\beta} a_{ij} \tilde{C}_{AA}$ and tabulate $\tilde{C}_{AA}$, using the shorthand notation given below [a].

(a_1',b_1')	(a_2',b_2')	C_{SS}	$\tilde{C}_{AA}$
(a_1+2,b_1-2)	(a_2,b_2-2)	0	$\frac{\{-2\}_1\{0\}_4}{[0,1;-1,0]}$
	(a_2-1,b_2)	0	$\tilde{\delta}_{b_2,0}\frac{\sqrt{2}(-1)^{a_1+a_2+a+b_2}(0,0,2,2)}{[0,1;0,2]}$
	(a_2-2,b_2+2)	0	$\frac{\{-2\}_2\{2\}_3}{[0,1;2,3]}$
(a_1+1,b_1)	(a_2,b_2-2)	0	$\tilde{\delta}_{b_1,0}\frac{\sqrt{2}(-1)^{a_1+a_2+a+1}(0,2,0,2)}{[0,2;-1,0]}$
	(a_2-1,b_2)	$(-1)^{b_2}N^{ij}_{\alpha\beta}$	$\tilde{\delta}_{b_1,0}\tilde{\delta}_{b_2,0}\frac{2(-1)^{b_2+1}(b_1^2+b_2^2-b^2+2b_1+2b_2-2b)}{[0,2;0,2]}$
	(a_2-2,b_2+2)	0	$\tilde{\delta}_{b_1,0}\frac{\sqrt{2}(-1)^{a_1+a_2+a}(2,0,2,4)}{[0,2;2,3]}$
(a_1,b_1+2)	(a_2,b_2-2)	0	$\frac{\{2\}_2\{-2\}_3}{[1,2;-1,0]}$
	(a_2-1,b_2)	0	$\tilde{\delta}_{b_2,0}\frac{\sqrt{2}(-1)^{a_1+a_2+a+b_2+1}(2,2,0,4)}{[1,2;0,2]}$
	(a_2-2,b_2+2)	0	$\frac{\{2\}_1\{4\}_4}{[1,2;2,3]}$

[a] The following shorthand notation is used:

$$N^{ij}_{\alpha\beta} = \tfrac{1}{2}[(1+\delta_{\alpha\beta})(1+\delta_{ij})]^{1/2},$$

$$\{m\}_1 = [(b_1+b_2-b+m)(b_1+b_2-b+m+2)]^{1/2},$$

$$\{m\}_2 = [(b_1-b_2+b+m)(b_1-b_2+m+2)]^{1/2},$$

$$\{m\}_3 = [(-b_1+b_2+b+m)(-b_1+b_2+b+m+2)]^{1/2},$$

$$\{m\}_4 = [(b_1+b_2+b+m)(b_1+b_2+b+m+2)]^{1/2},$$

$$(m_1,m_2,m_3,m_4) = [(b_1+b_2-b+m_1)(b_1-b_2+b+m_2)(-b_1+b_2+b+m_3)(b_1+b_2+b+m_4)]^{1/2},$$

$$[m_1,m_2;m_3,m_4] = [(b_1+m_1)(b_1+m_2)(b_2+m_3)(b_2+m_4)]^{1/2}.$$

Equivalently, writing $e_{\alpha i;j\beta}$ as $\sum_\sigma C_j^{\sigma\dagger} E_{\alpha i} C_\beta^\sigma$, we find that also

$$\langle e_{\alpha i;j\beta}\rangle = \sum_{\sigma\tau\eta} \left\langle \begin{matrix}\lambda-\sigma\\ \lambda_1'(\lambda_2'-\eta)\end{matrix} \middle\| E \middle\| \begin{matrix}\lambda-\sigma\\ (\lambda_1'-\tau)\lambda_2\end{matrix} \right\rangle \left\langle \begin{matrix}\lambda\\ \lambda_1'\lambda_2'\end{matrix} \middle\| C^\dagger \middle\| \begin{matrix}\lambda-\sigma\\ \lambda_1'(\lambda_2'-\eta)\end{matrix} \right\rangle$$

$$\times \left\langle \begin{matrix}\lambda\\ \lambda_1\lambda_2\end{matrix} \middle\| C^\dagger \middle\| \begin{matrix}\lambda-\sigma\\ (\lambda_1'-\tau)\lambda_2\end{matrix} \right\rangle \left\langle \begin{matrix}\lambda_1'\\ W_1'\end{matrix} \middle| \tilde{C}_\alpha^{\tau\dagger} \tilde{C}_\beta^\rho \middle| \begin{matrix}\lambda_1\\ W_1\end{matrix} \right\rangle \left\langle \begin{matrix}\lambda_2'\\ W_2'\end{matrix} \middle| \tilde{C}_j^{\eta\dagger} \tilde{C}_i^\xi \middle| \begin{matrix}\lambda_2\\ W_2\end{matrix} \right\rangle, \tag{68'}$$

where $\rho = \lambda_1 - \lambda_1' + \tau$ and $\xi = \lambda_2 - \lambda_2' + \eta$. Again, although there are 8 terms on the right-hand side of eq. (68) or (68′), in most cases at least half of them vanish. For example, when $\lambda_1' = (a_1 - 1, b_1 + 2)$ and $\lambda_2' = (a_2 - 1, b_2 + 2)$, we have that $\sigma = 2, \rho = 1$ and $\eta = 2, \xi = 1$, so that only two terms ($\tau = 1$ and 2) survive. Only when $\lambda_1' = (a_1, b_1) = \lambda_1$ and $\lambda_2' = (a_2, b_2) = \lambda_2$, all 8 terms must be considered.

Through eq. (68), the MEs of two-body operators are reduced to MEs of $U(n_1)$ and $U(n_2)$ adjoint tensors. We showed in Part II that any adjoint tensor can be constructed from a corresponding generator E and operators N, whose MEs are given by simple products of segment values. The relationship between the $C^\dagger C$ operators and E and N adjoint tensors on a given $U(n)$ irrep module (a, b) is given as (cf., eqs. (II.73a-d))

$$C_r^{1\dagger} C_s^1 = \frac{b}{2(b+1)} E_{rs} + \frac{1}{b+1}\sqrt{\frac{b(b+2)}{2}} N_{rs}^{(0)}, \tag{69}$$

$$C_r^{2\dagger} C_s^2 = \frac{b+2}{2(b+1)} E_{rs} - \frac{1}{b+1}\sqrt{\frac{b(b+2)}{2}} N_{rs}^{(0)}, \tag{70}$$

$$C_r^{1\dagger} C_s^2 = \sqrt{\frac{b+2}{b+3}} N_{rs}^{(+)}, \tag{71}$$

$$C_r^{2\dagger} C_s^1 = \sqrt{\frac{b}{b+1}} N_{rs}^{(-)}. \tag{72}$$

Using these relations, eqs. (69)–(72), and tables 1 and 2 for the RMEs appearing in eq. (68), we can express eq. (68) in the form

$$\langle e_{\alpha i;j\beta}\rangle = \sum_{P,Q=E,N^\kappa} C_{PQ} \left\langle \begin{matrix}\lambda_1'\\ W_1'\end{matrix} \middle| P_{\alpha\beta} \middle| \begin{matrix}\lambda_1\\ W_1\end{matrix} \right\rangle \left\langle \begin{matrix}\lambda_2'\\ W_2'\end{matrix} \middle| Q_{ji} \middle| \begin{matrix}\lambda_2\\ W_2\end{matrix} \right\rangle, \tag{73}$$

where the coefficients C_{PQ} depend on all the irreps involved. We find again that the mixed terms C_{EN} and C_{NE} always vanish. We can thus write

$$\langle e_{\alpha i;j\beta}\rangle = C_{EE}\left\langle \begin{matrix}(a'_1,b'_1)\\ W'_1\end{matrix}\middle| E_{\alpha\beta} \middle| \begin{matrix}(a_1,b_1)\\ W_1\end{matrix}\right\rangle \left\langle \begin{matrix}(a'_2,b'_2)\\ W'_2\end{matrix}\middle| E_{ji} \middle| \begin{matrix}(a_2,b_2)\\ W_2\end{matrix}\right\rangle + C_{N^\kappa N^{\kappa'}}\left\langle \begin{matrix}(a'_1,b'_1)\\ W'_1\end{matrix}\middle| N^\kappa_{\alpha\beta} \middle| \begin{matrix}(a_1,b_1)\\ W_1\end{matrix}\right\rangle \left\langle \begin{matrix}(a'_2,b'_2)\\ W'_2\end{matrix}\middle| N^{\kappa'}_{ji} \middle| \begin{matrix}(a_2,b_2)\\ W_2\end{matrix}\right\rangle, \quad (74)$$

where the actual shifts κ and κ' for $N[\kappa,\kappa'=(+),(0),(-)]$ are uniquely determined by the irreps λ'_1,λ_1 and λ'_2,λ_2, respectively, and may thus be omitted. The explicit form of the coefficients C_{EE} and C_{NN} for nine possible cases is given in table 4, together with the corresponding shifts κ and κ'. We note that again the C_{EE} term survives only for the fifth case when $\lambda'_1=\lambda_1$ and $\lambda'_2=\lambda_2$. As shown in Part II, the

Table 4
The coefficients C_{EE} and C_{NN} and shifts κ,κ' in eq. (74) that depend on all bra and ket irreps of $U(n_1)$, $U(n_2)$ and $U(n)$. The irrep of $U(n)$ is fixed as (a,b) and the ket irreps of $U(n_1)$ and $U(n_2)$ are fixed as (a_1,b_1) and (a_2,b_2), respectively. Thus C_{EE} and C_{NN} are given as functions of the bra irreps (a'_1,b'_1) and (a'_2,b'_2) of $U(n_1)$ and $U(n_2)$, respectively. The same shorthand notation as in table 3 is used.

(a'_1,b'_1)	(a'_2,b'_2)	C_{EE}	$4C_{NN}$ [a)]	κ	κ'
(a_1+1,b_1-2)	(a_2+1,b_2-2)	0	$\frac{(-1)^{b_2+1}\{-2\}_1\{0\}_4}{[0,1;0,1]}$	$(-)$	$(-)$
	(a_2,b_2)	0	$\frac{\sqrt{2}(-1)^{a_1+a_2+a+1}(0,0,2,2)}{[0,1;0,2]}$	$(-)$	(0)
	(a_2-1,b_2+2)	0	$\frac{(-1)^{b_2+1}\{-2\}_2\{2\}_3}{[0,1;2,3]}$	$(-)$	$(+)$
(a_1,b_1)	(a_2+1,b_2-2)	0	$\frac{\sqrt{2}(-1)^{a_1+a_2+a+b_2}(0,2,0,2)}{[0,2;0,1]}$	(0)	$(-)$
	(a_2,b_2)	$-\frac{1}{2}$	$\frac{2(b_1^2+b_2^2-b^2+2b_1+2b_2-2b)}{[0,2;0,2]}$	(0)	(0)
	(a_2-1,b_2+2)	0	$\frac{\sqrt{2}(-1)^{a_1+a_2+a+b_2+1}(2,0,2,4)}{[0,2;2,3]}$	(0)	$(+)$
(a_1-1,b_1+2)	(a_2+1,b_2-2)	0	$\frac{(-1)^{b_2+1}\{2\}_2\{-2\}_3}{[2,3;0,1]}$	$(+)$	$(-)$
	(a_2,b_2)	0	$\frac{\sqrt{2}(-1)^{a_1+a_2+a}(2,2,0,4)}{[2,3;0,2]}$	$(+)$	(0)
	(a_2-1,b_2+2)	0	$\frac{(-1)^{b_2+1}\{2\}_1\{4\}_4}{[2,3;2,3]}$	$(+)$	$(+)$

a) To avoid special cases we assume that $C_{NN}=0$ if the numerator vanishes.

MEs of E and N operators are given by simple products of corresponding segment values (cf., eq. (II.34) and tables II.1, 2 as well as eq. (II.72) and tables II.1, 5–7).

The similarity between the coefficients appearing in eqs. (62) and (73) is worth pointing out. In both cases, the mixed terms always vanish and the C_{SS} and C_{EE} coefficients survive only when the spins of U(n_1) and U(n_2) irreps are preserved (i.e., when $b_1' = b_1$ and $b_2' = b_2$). Moreover, both C_{AA} and C_{NN} coefficients (cf. tables 3 and 4) have the same numerators except for a phase factor and Kronecker delta symbols. This similitude arises due to an analogous shift behavior between the generators and symmetric tensors on the one hand and between the N operators and antisymmetric tensors on the other hand. Indeed, both generators and symmetric tensors possess only one shift component that preserves spin (or the b value), while both N operators and antisymmetric tensors have three shift components, inducing a spin shift of 1, 0 and -1 (or, correspondingly, a change in b by 2, 0 and -2, respectively).

6. Discussion and conclusions

In the preceding sections we applied the unitary group tensor operator algebra formalism, developed in Parts I and II of this series, to the U(n) $\supset$ U(n_1) $\times$ U(n_2) partitioned bases. Our results indicate that the evaluation of one- and two-body MEs in partitioned bases may be carried out in very much the same way as for the standard GT bases, relying on their factorization involving segment values. All the additional quantities that are required for partitioned bases are listed in tables 1–4. Similarly as for the standard bases, their values depend on the intermediate spin quantum numbers at a given level (b values), although the phase factor may now also depend on double occupancies (a values). For the generator (or one-body) MEs, eq. (8), we require generator RMEs that basically represent Racah coefficients (table 1) as well as CG coefficients associated with standard U(n_1) and U(n_2) GT bases that are given by simple products of scaled isoscalar factors for vector operators as shown in Part II. For two-body operator MEs, we have to distinguish four new types, eqs. (49)–(52), involving intershell (or intergroup) operators. In general, these are given by the sum involving two terms, each of which is a simple product of segment values (cf. eqs. (53), (54), (65) and (74) corresponding to types 1–4, eqs. (49)– (52), respectively). These two terms represent either symmetric and antisymmetric tensors, or adjoint tensors expressed in terms of a generator and N operators. For the first two cases, eqs. (53) and (54), we have to evaluate a simple product for one of the subgroups and the above-mentioned sum involving two terms for the other subgroup. In the remaining two cases, eqs. (65) and (74), each term is a product of U(n_1) and U(n_2) MEs. Except for the top level segment values which are listed in tables 1, 3 and 4, the segment values for all other levels are identical with those required for standard GT bases and tabulated in Part II.

All the developments presented in this paper are based on the U(n) tensor operator techniques that were developed in Parts I and II of this series. Our primary objective was to interrelate the MEs of U(n) generators in a partitioned basis with those for the standard U(n_1) and U(n_2) bases. We have seen that in fact we only need a few additional quantities in addition to those already established earlier for the canonical GT bases (cf. Part II). The development of the required formalism was made easy thanks to the introduction of the creation and annihilation-type vector operators at the orbital U(n) level in Part II. In fact, these operators represent basic building blocks in terms of which we can express all the desired operators, similarly as in the standard second quantization formalism. Of course, in view of more intricate symmetry properties of these orbital creation and annihilation operators (in contrast to creation and annihilation operators of the second quantization formalism that transform according to the totally antisymmetric, single-column irreps), an appropriate recoupling must be carried out when these operators are combined and when evaluating MEs in partitioned bases. Although the actual derivations, particularly for two-body operators, may be quite laborious, the final results are just as simple as for standard GT bases. In fact, only a few additional segment values, represented by generator and vector operator RMEs (tables 1 and 2) are required.

Similarly as in the case of standard GT bases, our tensor operator formalism closely parallels that based on Green–Gould representation theory [28,29] that was employed in ref. [27]. Our generator RMEs are essentially those used in ref. [27a] and, likewise, our vector operator RMEs parallel the reduced Wigner coefficients of ref. [27a]. Note, however, that while only one-body MEs were considered earlier [27], this work provides complete results for both one- and two-body operators. As we already announced in Part II, we shall provide a more detailed comparison of both approaches in one of the future installments of this series [34].

Let us finally point out that the results of this paper, where we restricted ourselves to a system partitioning involving two subsystems, may be generalized to composite bases involving more than two subgroups. Regardless of how complicated is the partitioned basis employed, we can always express the MEs of one- and two-body operators in terms of MEs of their building blocks, namely the $C^\dagger$ and C-type operators, which may be suitably recoupled within each subgroup. The final result will thus always be given in terms of rank one $(C^\dagger, C)$ and rank two (S, A, E, N) tensors, whose MEs were given in Part II. For operators whose orbital labels belong to two distinct subgroups, all necessary coupling coefficients were essentially derived in this paper. For operators containing orbital labels associated with three distinct subgroups, certain additional coefficients will have to be worked out. Since the most general two-body operator involves at most four orbital labels, the most complicated case will involve four distinct subgroups. However, we must keep in mind, that this is a purely formal analysis of the partitioning problem. Obviously, the main usefulness of system partitioning stems from the fact that numerous two-body terms, particularly those associated with a multi-electron charge transfer between weakly interacting subsystems, may be safely neglected.

It is thus important to consider the partitioning problem in an actual physical or chemical context, where it will lead to substantial simplifications resulting in reduced computational requirements. We will examine this aspect in the future when applying the formalism to actual systems.

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Appendix

In order to derive the Racah coefficients appearing in eqs. (17) and (23), we apply the results of Part I, in particular eq. (I.141), which expresses an important relationship between the Racah coefficients and $U(n) \supset U(n-1)$ isoscalar factors (referred to as I_u factors for short). Let us choose the irreps in eq. (I.141) as follows:

$$\begin{aligned} &\lambda_1 = (0, b_2 - 1), \quad \lambda_2 = (0,1), \quad \lambda_3 = (a_1, b_1), \\ &\lambda_{12} = (0, b_2), \quad \lambda_{23} = (a_1, b_1 + 1), \quad \lambda = (\tilde{a}, b), \\ &\mu_1 = (0, b_2 - 2), \quad \mu_{23} = (a_1, b_1 + 1), \quad \mu = (\tilde{a} - 1, b + 1). \end{aligned} \tag{A.1}$$

First, we notice that all multiplicity labels are unnecessary in this case. Second, the choice of $\mu_{23} = \lambda_{23}$ implies that $\mu_2 = \lambda_2$ and $\mu_3 = \lambda_3$, since when we do not remove any box from λ_{23}, we cannot remove any box from λ_2 and λ_3 either. Third, there is only one possibility for μ_{12}, namely $\mu_{12} = (0, b_2 - 1)$. Since the irrep $\lambda = (\tilde{a}, b)$ is obtained by adding b_2 boxes of $\lambda_{12} = (0, b_2)$ to $\lambda_3 = (a_1, b_1)$, we have that

$$\tilde{a} = a_1 + k, \quad b = b_1 + b_2 - 2k, \tag{A.2}$$

for some k. Substituting thus these values into eq. (I.141) we get

$$\begin{aligned} &U\{(0, b_2 - 1), (0,1), (\tilde{a}, b), (a_1, b_1); (0, b_2), (a_1, b_1 + 1)\} \\ &\quad \times I_u \left(\begin{array}{cc|c} (0, b_2 - 1) & (a_1, b_1 + 1) & (\tilde{a}, b) \\ (0, b_2 - 2) & (a_1, b_1 + 1) & (\tilde{a} - 1, b + 1) \end{array} \right) \\ &= U\{(0, b_2 - 2), (0,1), (\tilde{a} - 1, b + 1), (a_1, b_1); (0, b_2 - 1), (a_1, b_1 + 1)\} \\ &\quad \times I_u \left(\begin{array}{cc|c} (0, b_2 - 1) & (0,1) & (0, b_2) \\ (0, b_2 - 2) & (0,1) & (0, b_2 - 1) \end{array} \right) \end{aligned}$$

$$\times I_u\begin{pmatrix} (0,b_2) & (a_1,b_1) & (\tilde{a},b) \\ (0,b_2-1) & (a_1,b_1) & (\tilde{a}-1,b+1) \end{pmatrix}, \tag{A.3}$$

where the last isoscalar factor on the right-hand side of eq. (I.141), being equal to 1, was dropped. Using table I.2 for the above I_u factors and eq. (A.2), we obtain the following recursion formula for Racah coefficients:

$$U\{(0,b_2-1),(0,1),(a_1+k,b_1+b_2-2k),(a_1,b_1);(0,b_2),(a_1,b_1+1)\}$$
$$= -\left[\frac{(b_2-1)(b_1-k+1)}{b_2(b_1-k+2)}\right]^{1/2}$$
$$\times\ U\{(0,b_2-2),(0,1),(a_1+k-1,b_1+b_2-2k+1),(a_1,b_1);(0,b_2-1),(a_1,b_1+1)\}\,. \tag{A.4}$$

Using the orthogonality of Racah coefficients, we can prove that when $(\tilde{a},b)=(a_1,b_1+b_2)$, or $k=0$, the Racah coefficients in eq. (A.4) equal 1, i.e.

$$U\{(0,\tilde{b}_2-1),(0,1),(a_1,b_1+\tilde{b}_2),(a_1,b_1);(0,\tilde{b}_2),(a_1,b_1+1)\}=1\,, \tag{A.5}$$

for any $\tilde{b}_2\geqslant 1$. Indeed, eq. (I.133b) implies that

$$\sum_{\lambda_{12}} U\{(0,\tilde{b}_2-1),(0,1),(a_1,b_1+\tilde{b}_2),(a_1,b_1);\lambda_{12},(a_1,b_1+1)\}^2=1\,, \tag{A.6}$$

where λ_{12} results from the coupling of $(0,\tilde{b}_2-1)$ and (0, 1) and thus can only be equal to $(0,\tilde{b}_2)$ or $(1,\tilde{b}_2-2)$. However, coupling (a_1,b_1) with $(1,\tilde{b}_2-2)$ cannot yield $(a_1,b_1+\tilde{b}_2)$, so that only $\lambda_{12}=(0,b_2)$ is possible, implying eq. (A.5). We then iterate eq. (A.4) k-times until we reach U with $\lambda=(a_1,b_1+b_2-k)$, so that applying (A.5) for $\tilde{b}=b_2-k$ we get

$$U\{(0,b_2-1),(0,1),(a_1+k,b_1+b_2-2k),(a_1,b_1);(0,b_2),(a_1,b_1+1)\}$$
$$=(-1)^k\left[\frac{(b_2-k)(b_1-k+1)}{b_2(b_1+1)}\right]^{1/2}. \tag{A.7}$$

Since $a_1+k=a$ and $b_1+b_2-2k=b$, eq. (A.2), this relationship yields immediately eq. (17).

To derive the Racah coefficient arising in eq. (23), we choose the irreps in eq. (I.141) as follows:

$$\begin{aligned} &\lambda_1=(0,b_2-1)\,, \quad \lambda_2=(0,1)\,, && \lambda_3=(a_1,b_1)\,,\\ &\lambda_{12}=(0,b_2)\,, \quad \lambda_{23}=(a_1+1,b_1-1)\,, && \lambda=(\tilde{a},b)\\ &&& \quad =(a_1+b_2-k,b_1-b_2+2k)\,,\\ &\mu_1=(0,b_2-2)\,, \quad \mu_{23}=(a_1+1,b_1-1)\,, && \mu=(\tilde{a},b-1)\\ &&& \quad =(a_1+b_2-k,b_1-b_2+2k-1)\,, \end{aligned} \tag{A.8}$$

where $k=(b-b_1+b_2)/2$. This choice implies that $\mu_2=\lambda_2,\mu_3=\lambda_3$, and $\mu_{12}=(0,b_2-1)$. We thus get

$$U\{(0,b_2-1),(0,1),(\tilde{a},b),(a_1,b_1);(0,b_2),(a_1+1,b_1-1)\} \times I_u\begin{pmatrix} (0,b_2-1) & (a_1+1,b_1-1) & (\tilde{a},b) \\ (0,b_2-2) & (a_1+1,b_1-1) & (\tilde{a},b-1) \end{pmatrix}$$
$$= U\{(0,b_2-2),(0,1),(\tilde{a},b-1),(a_1,b_1);(0,b_2-1),(a_1+1,b_1-1)\}$$
$$\times I_u\begin{pmatrix} (0,b_2-1) & (0,1) & (0,b_2) \\ (0,b_2-2) & (0,1) & (0,b_2-1) \end{pmatrix} I_u\begin{pmatrix} (0,b_2) & (a_1,b_1) & (\tilde{a},b) \\ (0,b_2-1) & (a_1,b_1) & (\tilde{a},b-1) \end{pmatrix}, \tag{A.9}$$

where the irrep $(\tilde{a},b)$ is defined by eq. (A.8). Substituting the I_u factors from table I.2, we obtain another recursion formula

$$U\{(0,b_2-1),(0,1),(a',b'),(a_1,b_1);(0,b_2),(a_1+1,b_1-1)\}$$
$$= \left[\frac{(b_2-1)(b_1+k+1)}{b_2(b_1+k)}\right]^{1/2}$$
$$\times U\{(0,b_2-2),(0,1),(a',b'-1),(a_1,b_1);(0,b_2-1),(a_1+1,b_1-1)\}, \tag{A.10}$$

where $a' = a_1+b_2-k, b' = b_1-b_2+2k$. From eq. (I.133a) we find that

$$\sum_{\lambda_{23}} U\{(0,\tilde{b}_2-1),(0,1),(a_1+\tilde{b}_2,b_1-\tilde{b}_2),(a_1,b_1);(0,\tilde{b}_2),\lambda_{23}\}^2 = 1\,, \tag{A.11}$$

where λ_{23} can equal (a_1+1,b_1-1) or (a_1,b_1+1). However, only the first one yields $(a_1+\tilde{b}_2,b_1-\tilde{b}_2)$ when coupled with $(0,\tilde{b}_2-1)$. Thus (choosing positive phase factor)

$$U\{(0,\tilde{b}_2-1),(0,1),(a_1+\tilde{b}_2,b_1-\tilde{b}_2),(a_1,b_1);(0,\tilde{b}_2),(a_1+1,b_1-1)\} = 1\,, \tag{A.12}$$

for any $\tilde{b}_2 \geqslant 1$. Using this fact for $\tilde{b}_2 = b_2-k$ and iterating eq. (A.10) k-times, we obtain the desired relationship:

$$U\{(0,b_2-1),(0,1),(\tilde{a},b),(a_1,b_1);(0,b_2),(a_1+1,b_1-1)\}$$
$$= \left[\frac{(b_1+k+1)(b_2-k)}{(b_1+1)b_2}\right]^{1/2} = \frac{1}{2}\left[\frac{(b_1+b_2-b)(b_1+b_2+b+2)}{(b_1+1)b_2}\right]^{1/2}. \tag{A.13}$$

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