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Unitary group tensor operator algebras for many-electron systems: II. One- and two-body matrix elements

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Relying on our earlier results in the unitary group Racah–Wigner algebra, specifically designed to facilitate quantum chemical calculations of molecular electronic structure, the tensor operator formalism required for an efficient evaluation of one- and two-body matrix elements of molecular electronic Hamiltonians within the spin-adapted Gel'fand–Tsetlin basis is developed. Introducing the second quantization-like creation and annihilation vector operators at the unitary group [U(n)] level, appropriate two-box symmetric and antisymmetric irreducible tensor operators as well as adjoint tensors are defined and their matrix elements evaluated in the electronic Gel'fand–Tsetlin basis as single products of segment values. Using these tensor operators, the matrix elements of one- and two-body components of a general electronic Hamiltonian are found. Explicit expressions for all relevant quantities pertaining to at most two-column irreducible representations that are required in molecular electronic structure calculations are given. Relationships with other approaches and possible future extensions of the formalism to partitioned bases or spin-dependent Hamiltonians are discussed.

1. Introduction

In the first communication of this series [1] [#1], referred to in the following as Part I, we have formulated the basic principles of unitary group Racah–Wigner calculus in a form that is particularly suitable for applications of the unitary group approach (UGA) [2–5] to many-electron systems (for review see refs. [6–14]). In

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[#1] In the following, this paper is referred to as Part I. We wish to point out a couple of misprints that crept into table 2 of Part I. For the I_t (I_s) factors (the last column for single occupancy), the factor $(b + e + t + 2)$ appearing in the numerator of the type C isoscalar factor should read $(b - e + t + 2)$ and, further, the factor $(e + 1)$in the denominator for the type D should equal $(e + 2)$.

this case, when only one- and two-column irreducible representations (irreps) come into play, multiplicity problems may be avoided, so that a relatively simple and versatile formalism results affording an efficient spin-adaptation of various quantum chemical methods that are used in investigations of molecular electronic structure (see, for example, refs. [15–29]).

In contrast to general approaches to U(n) Racah–Wigner calculus [30–33], whose objective is an exhaustive treatment of the problem that invariably leads to a rather formidable formalism, the present approach is entirely based on the well-known duality between unitary group U(n) and symmetric group S_N representation theory and affords a relatively simple machinery enabling the development of efficient algorithms for electronic structure calculations. Indeed, the main objective of this series of papers is to provide yet another viewpoint on the existing UGA methodologies and to maximally exploit the interrelationship between the U(n), S_N (see, e.g., refs. [34–36]) and SU(2) (see refs. [36–38]) approaches, obtaining a sufficiently general yet simple formalism that combines the convenient features of all the above listed approaches while enabling an extension to partitioned bases [1,39,40] or spin-dependent Hamiltonians [41].

In Part I of this series we have thus introduced the vector coupling of Clebsch–Gordan (CG) coefficients for both the U(n) and S_N groups and the related isoscalar factors or reduced Wigner coefficients. We employed the U(n)–S_N reciprocity of tensor product representations to interrelate the U(n) and S_N isoscalar factors. In addition to standard (GT for U(n) and genealogical for S_N) bases we also considered non-standard or partitioned bases that are essential for an eventual partitioning of larger molecular systems into their basic constituents. The derivation of explicit expressions for the isoscalar factors for the relevant two-column irreps was then based on the S_N representation theory, since in this way we were able to achieve an orbital number (n) independent formalism that enables an open-ended implementation for arbitrary basis sets defining the electronic model Hamiltonians exploited in quantum chemical computations. We have further examined U(n) Racah coefficients and derived explicit expressions for those that are pertinent to the UGA formalism.

In this part of our series we shall concentrate on the development of the U(n) irreducible tensor operator formalism and will exploit it to evaluate one- and two-body matrix elements within the standard UGA spin-adapted GT bases. We thus first summarize the necessary basic facts about the U(n) irreducible tensor operators in section 2 and introduce a convenient scaling of CG coefficients, isoscalar factors and reduced matrix elements that will enable us to considerably simplify the resulting formalism. We then introduce creation and annihilation-type vector operators at the U(n) level that will allow us to cast the entire formalism into a simpler form, thus facilitating a straightforward derivation of expressions for various matrix elements (MEs) that are required in practical implementations of UGA. These operators are reminiscent of those employed in both the second quantization formalism (at the U($2n$) spin-orbital level of the theory) and U(n) boson calculus

[30–33], but are unique and specific in that their definition is motivated by the S_N representation theory and due to the fact that they avoid the necessity to consider more than two-column irreps at any level of the theory (cf., e.g., very elegant and powerful Green–Gould [42–44] formalism based on invariant polynomial identities and related projection operators). The usefulness of these creation and annihilation-type vector operators is then demonstrated in section 4 where the standard segment level formulas are derived for U(n) generator MEs. At the same time, this derivation provides a new viewpoint on the group theoretical structure of various segment values.

In order to handle two-body operators in the same fashion, we explore in sections 5 and 6 two-body symmetric and antisymmetric tensors as well as adjoint tensors and develop the required formalism and explicit expressions for these quantities, which are then exploited in section 7 for the evaluation of two-body MEs. Although all the developments presented in this study may be generalized to arbitrary U(n) irreps, and many of the presented results are completely general in this regard, our emphasis is on UGA applications to molecular electronic structure and all final explicit expressions given in our tables are pertinent to this specific purpose. The last section 8 then summarizes the results and points out their specificity as well as the relationship with related approaches.

2. U(n) irreducible tensor operators

A general U(n) tensor operator T (see, e.g., refs. [30–33]), whose components transform according to some representation of U(n) under the action of U(n) operators, may be partitioned into the irreducible tensor operators by forming appropriate linear combinations. An irreducible U(n) tensor operator T_μ, associated with the μth irreducible representation (irrep) of U(n), is then a set of operators $T_\mu \equiv \{T_\mu(m)\}$ that may be labelled by the Gel'fand tableaux m labelling the basis vectors $|{}^{\langle\mu\rangle}_{m}\rangle$ of the carrier space of this irrep [#2] $\langle\mu\rangle \equiv \mu$. For our purposes it is convenient to replace the Gel'fand tableau labelling with the corresponding Weyl tableau labels, $|{}^{\mu}_{m}\rangle \equiv |{}^{\mu}_{W}\rangle$, and later, when we consider electronic Gel'fand–Tsetlin (GT) states, by the ABC or Paldus [2–4,11] tableaux. Even though either tableau automatically implies the relevant irrep label μ, it is convenient to display this label explicitly in designating our states or tensor operator components. Thus, the *irreducible tensor operator* associated with the irrep μ is defined as a set of operators $T_\mu \equiv \{T_\mu(W)\}$, with W ranging over all Weyl tableaux corresponding to this irrep, that transform under the action of U(n) generators E_{ij} in the following way

$$[E_{ij}, T_\mu(W)] = \sum_V \left\langle \begin{matrix}\mu\\ V\end{matrix} \middle| E_{ij} \middle| \begin{matrix}\mu\\ W\end{matrix} \right\rangle T_\mu(V)\,, \tag{1}$$

[#2] For the sake of simplicity, the highest weights $\langle\mu\rangle$ labelling U(n) irreps are written without the angular brackets unless the confusion could arise.

with the sum extending over all Weyl tableaux V of the same irrep μ.

When we consider a general representation space $\mathcal{V}$ for U(n) or, equivalently, a U(n)-module $\mathcal{V}$, we can reduce it to its irreducible components $\mathcal{V}_\mu, \mathcal{V} = \oplus_\mu \mathcal{V}_\mu$. An arbitrary operator $\hat{O}$ acting in $\mathcal{V}$ then maps an arbitrary $\mathcal{V}_\lambda$ into $\mathcal{V}$, so that

$$\hat{O}\left|\begin{matrix}\lambda\\U\end{matrix}\right\rangle = \sum_\nu \sum_W \left\langle \begin{matrix}\nu\\W\end{matrix}\middle|\hat{O}\middle|\begin{matrix}\lambda\\U\end{matrix}\right\rangle \left|\begin{matrix}\nu\\W\end{matrix}\right\rangle . \tag{2}$$

This is also true of a general tensor operator. However, for an irreducible tensor operator $\boldsymbol{T}_\mu$, the image space is restricted to only those irreps that are contained in the inner direct product of λ and μ, so that

$$\boldsymbol{T}_\mu : \mathcal{V}_\lambda \to \bigoplus_{\nu \in \mu \otimes \lambda} \mathcal{V}_\nu . \tag{3}$$

Thus, for $\hat{O} = \boldsymbol{T}_\mu$, the sum over ν in eq. (2) is restricted to only those irreps that are contained in the inner direct product of μ and λ, as given by the Littlewood–Richardson rules.

We can further decompose the irreducible tensor operator $\boldsymbol{T}_\mu$ into components, referred to as *unit tensor* (or *Wigner*) *operators*, that transform a given carrier space $\mathcal{V}_\lambda$ into another carrier space $\mathcal{V}_\gamma$ (see, e.g., eqs. (3.26) and (3.38) of ref. [31]). As was shown by Baird and Biedenharn [30], these unit tensor operators may then be labelled by a pair of Gel'fand tableaux belonging to the same irrep. In terms of Weyl tableaux we thus designate these operators as $T_\mu\binom{\Gamma}{V}$, Γ and V being Weyl tableaux associated with the irrep μ. The upper tableaux Γ determines a unique shift of the irrep labels, designated by $\Delta(\Gamma)$, so that

$$T_\mu\begin{pmatrix}\Gamma\\V\end{pmatrix} : \mathcal{V}_\lambda \to \mathcal{V}_{\lambda+\Delta(\Gamma)} . \tag{4}$$

Thus, eq. (2) for $\hat{O} = T_\mu\binom{\Gamma}{V}$ can now be written as

$$T_\mu\begin{pmatrix}\Gamma\\V\end{pmatrix}\left|\begin{matrix}\lambda\\U\end{matrix}\right\rangle = \sum_W \left\langle \begin{matrix}\lambda+\Delta(\Gamma)\\W\end{matrix}\middle|T_\mu(V)\middle|\begin{matrix}\lambda\\U\end{matrix}\right\rangle \left|\begin{matrix}\lambda+\Delta(\Gamma)\\W\end{matrix}\right\rangle , \tag{5}$$

where the sum extends only over the Weyl tableaux of the irrep $\gamma \equiv \lambda + \Delta(\Gamma)$. The shift $\Delta(\Gamma)$ is given by the weight of Γ (see, e.g., eqs. (3.24) and (3.25) of ref. [31]) and may also be characterized in terms of box addition and removal to the Young pattern associated with a given irrep. The latter description is more convenient when we label the basis vector (or states) and tensor operator components by Weyl tableaux, and is particularly efficient when only a few shift components are different from zero, as will be the case in our applications.

We must also mention that, generally, a given irrep ν may appear more than once in the direct product $\mu \otimes \lambda$, eq. (3). In such cases there exist several Gel'fand (or Weyl) tableaux having the same weight, so that $\Delta(\Gamma) = \Delta(\Gamma')$ while $\Gamma \neq \Gamma'$, and we need an additional label, say α, to distinguish the resulting irreps ν. Clearly, the operator tableaux Γ or W themselves may serve as such a multiplicity index.

One of the key problems of U(n) tensor calculus is the evaluation of matrix elements (MEs) of tensor operators. Relying on the Wigner–Eckart (WE) theorem, we can write MEs appearing in eq. (5) as a sum of products of reduced matrix elements (RMEs) and U(n) Clebsch–Gordan (CG) or Wigner coefficients,

$$\left\langle \begin{matrix} \nu \\ W \end{matrix} \middle| T_\mu(V) \middle| \begin{matrix} \lambda \\ U \end{matrix} \right\rangle = \sum_\alpha \langle \nu \| T_\mu \| \lambda \rangle_\alpha \left\langle \begin{matrix} \alpha\nu \\ W \end{matrix} \middle| \begin{matrix} \lambda & \mu \\ U & V \end{matrix} \right\rangle, \tag{6}$$

where α is the multiplicity index. In the multiplicity free case, we thus have a standard SU(2)-type WE theorem

$$\left\langle \begin{matrix} \nu \\ W \end{matrix} \middle| T_\mu(V) \middle| \begin{matrix} \lambda \\ U \end{matrix} \right\rangle = \langle \nu \| T_\mu \| \lambda \rangle \left\langle \begin{matrix} \nu \\ W \end{matrix} \middle| \begin{matrix} \lambda & \mu \\ U & V \end{matrix} \right\rangle. \tag{7}$$

When the basis of a chosen carrier space for a given U(n) irrep is adapted to an appropriate group chain, the corresponding CG coefficients can be factored into simple products of isoscalar factors (see Part I). Thus, employing the canonical GT basis, the U(n) CG coefficients may be expressed as a product of $U(m) \supset U(m-1)$ isoscalar factors with m ranging from 2 to n. This factorization may be regarded as the origin of ME segmentation in the unitary group approach [4,11,28,36–38]. However, when a multiplicity is present, either at the group or the subgroup level, the sum over the multiplicity label(s) must be carried out so that segmentation of MEs may involve more than one product. Nonetheless, we shall see that when dealing with many-electron systems, the multiplicity can be avoided, so that factorization may be achieved for MEs of any tensor operator, including spin-dependent ones. These results will be further exploited elsewhere.

In the following developments we shall find it convenient to employ properly scaled CG coefficients and isoscalar factors. We thus rewrite eq. (7) in terms of scaled quantities,

$$\left\langle \begin{matrix} \nu \\ W \end{matrix} \middle| T_\mu(V) \middle| \begin{matrix} \lambda \\ U \end{matrix} \right\rangle = \langle \nu \| T_\mu \| \lambda \rangle^{(s)} \left\langle \begin{matrix} \nu \\ W \end{matrix} \middle| \begin{matrix} \lambda & \mu \\ U & V \end{matrix} \right\rangle^{(s)}, \tag{8}$$

as indicated by the superscript (s). For an arbitrary scaling factor $c(\lambda, \mu; \nu)$ we thus define

$$\langle \nu \| T_\mu \| \lambda \rangle^{(s)} = \langle \nu \| T_\mu \| \lambda \rangle / c(\lambda, \mu; \nu), \tag{9a}$$

$$\left\langle \begin{matrix} \nu \\ W \end{matrix} \middle| \begin{matrix} \lambda & \mu \\ U & V \end{matrix} \right\rangle^{(s)} = c(\lambda, \mu; \nu) \left\langle \begin{matrix} \nu \\ W \end{matrix} \middle| \begin{matrix} \lambda & \mu \\ U & V \end{matrix} \right\rangle. \tag{9b}$$

With proper choice of phases, all quantities involved are real and the scaling factor $c(\lambda, \mu; \nu)$ is determined by the metric of scaled CG coefficients, namely

$$\sum_{U,V}\left[\left\langle \begin{matrix}\nu\\W\end{matrix}\middle|\begin{matrix}\lambda & \mu\\U & V\end{matrix}\right\rangle^{(s)}\right]^2 = [c(\lambda,\mu;\nu)]^2 . \tag{10}$$

The scaling of CG coefficients then implies a similar scaling for isoscalar factors. Recalling the definition of U(n) isoscalar factors, eq. (I.56)[#3], we can define the scaled isoscalar factors by

$$\left(\begin{matrix}\nu\\\nu'\end{matrix}\middle|\begin{matrix}\lambda & \mu\\\lambda' & \mu'\end{matrix}\right)^{(s)} = c(\lambda,\mu;\nu)\cdot c(\lambda',\mu';\nu')^{-1}\left(\begin{matrix}\nu\\\nu'\end{matrix}\middle|\begin{matrix}\lambda & \mu\\\lambda' & \mu'\end{matrix}\right). \tag{11}$$

With this choice, the relationship between CG coefficients and isoscalar factors is preserved, so that the scaled CG coefficients are given by the product of scaled isoscalar factors. An appropriate choice of scaling factors then greatly simplifies the explicit form of scaled isoscalar factors, making the ME evaluation more efficient. In fact, choosing the RMEs as scaling factors,

$$c(\lambda,\mu;\nu) = \langle\nu\|T_\mu\|\lambda\rangle , \tag{12}$$

the scaled RMEs equal to unity,

$$\langle\nu\|T_\mu\|\lambda\rangle^{(s)} = 1 , \tag{13}$$

so that the tensor operator MEs, eq. (8), are given by the properly scaled CG coefficients,

$$\left\langle \begin{matrix}\nu\\W\end{matrix}\middle|T_\mu(V)\middle|\begin{matrix}\lambda\\U\end{matrix}\right\rangle = \left\langle \begin{matrix}\nu\\W\end{matrix}\middle|\begin{matrix}\lambda & \mu\\U & V\end{matrix}\right\rangle^{(s)} . \tag{14}$$

This choice of scaling will be found very useful in the following sections.

3. Creation and annihilation vector operators

In order to facilitate the handling of various types of tensor operators, it is useful to introduce a suitable set of fundamental tensors in terms of which we can express all other tensors. Clearly, the components of such fundamental tensors, serving as our building blocks, should transform as a basis of the simplest nontrivial irrep $\langle 1\dot{0}\rangle \equiv (0,1)$, characterized by a single box Young tableau. (Recall [1] that $\langle 1\dot{0}\rangle \equiv \langle 1 0 \ldots 0\rangle$, while (a,b) designates the two-column U(n) irrep $\langle 2^a 1^b 0^{n-a-b}\rangle$.) In other words, these fundamental tensor operators represent a vector operator. We designate their components by $C_i^{\sigma\dagger}$ and define them as follows:

(1) The operators $C_i^{\sigma\dagger}$, $(1 \leqslant i \leqslant n)$ transform as a fundamental vector representation,

[#3] We refer to equation (x) or table x of Part I as eq. (I.x) or table I.x, respectively.

$$\left[E_{jk}, C_i^{\sigma\dagger}\right] = \delta_{ik} C_j^{\sigma\dagger} . \tag{15}$$

(2) The action of $C_i^{\sigma\dagger}$ on an arbitrary irrep carrier space is defined by its action on its canonical basis vectors, namely

$$C_i^{\sigma\dagger}\left|\begin{matrix}\lambda \\ U\end{matrix}\right\rangle = \sum_W \left\langle \begin{matrix}\lambda+\sigma \\ W\end{matrix}\right| C_i^{\sigma\dagger} \left|\begin{matrix}\lambda \\ U\end{matrix}\right\rangle \left|\begin{matrix}\lambda+\sigma \\ W\end{matrix}\right\rangle , \tag{16}$$

with MEs given by the WE theorem

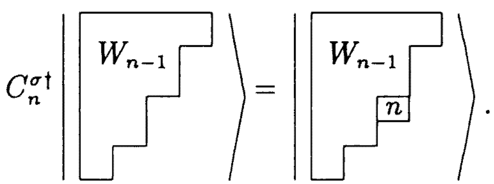
$$\left\langle \begin{matrix}\lambda+\sigma \\ W\end{matrix}\right| C_i^{\sigma\dagger} \left|\begin{matrix}\lambda \\ U\end{matrix}\right\rangle = \langle\lambda+\sigma\|C^\dagger\|\lambda\rangle \left\langle \begin{matrix}\lambda+\sigma \\ W\end{matrix}\right| \begin{matrix}\lambda & (0,1) \\ U & i\end{matrix} \Big\rangle , \tag{17}$$

where the first factor on the rhs is the RME of the $C^\dagger$ operator (see below) and the second factor is the U(n) CG coefficient for the coupling of canonical basis vectors of an arbitrary irrep λ and the one box vector irrep (0, 1) #4.

(3) Finally, the action of the operator $C_n^{\sigma\dagger}$ on GT states of the irrep $\lambda \equiv \lambda_n$ in which the orbital n is unoccupied, is defined as

$$C_n^{\sigma\dagger}\left|\begin{matrix}\lambda_n \\ \lambda_{n-1} \\ W_{n-1}\end{matrix}\right\rangle = \left|\begin{matrix}\lambda_n+\sigma \\ \lambda_{n-1} \\ W_{n-1}\end{matrix}\right\rangle , \tag{18}$$

where $\lambda_n = \lambda_{n-1}$ are the irreps of U(n) and U($n-1$), respectively. Graphically, the Weyl tableau characterizing the resulting state of irrep $\lambda_n + \sigma$ is obtained by adding a box labelled with the orbital index n to the σth column of the Weyl tableau W_{n-1}, representing the initial state of the irrep λ_n, i.e.



(19)

Note that at this stage the action of the operators $C_i^{\sigma\dagger}$ is defined for a general U(n) irrep with an arbitrary number of columns.

It is obvious from the first condition above, defining $C^{\sigma\dagger}$ as a U(n) vector operator, that the superscript σ designates the operator pattern (or the shift component). We shall see shortly that the last condition (3) determines the required RMEs $\langle\lambda+\sigma\|C^\dagger\|\lambda\rangle$. Before we actually determine these RMEs, it is worth remarking that the above introduced operators $C^\dagger$ are similar to τ operators (referred to as fundamental Wigner operators) defined by Biedenharn, Louck and others [31–33,45]: they both represent unit vector operators, but differ in their RMEs, since τ

#4 Clearly, the index i in the vector irrep basis $|{}^{(0,1)}_{i}\rangle$, $i = 1, \dots, n$, represents the label in the single box Weyl tableau $\boxed{i}$.

operators are defined in such a way that their MEs are simply the corresponding CG coefficients, i.e. their RMEs are equal to unity. Another difference concerns the shift label. In the standard approach, the shift is defined through a row label rather than a column label used here. The latter has the advantage of yielding an n-independent formalism. It should also be noticed that for a given irrep all the operators $C_i^{\sigma\dagger}$ are not necessarily defined, since we require that a lexical state results. Thus, for example, the operator $C_i^{2\dagger}$ is not defined for any two-column irrep (a, b) when $b = 0$.

To complete the definition of the action of the $C_i^{\sigma\dagger}$ operator on any irrep carrier space, eqs. (16) and (17), we have to determine the RMEs $\langle \lambda + \sigma \| C^\dagger \| \lambda \rangle$. This can be done by exploiting eq. (18) or (19), since the RMEs depend only on the irrep labels involved. Thus, choosing a state in which the nth orbital is unoccupied, so that eq. (18) holds, we find that

$$\left\langle \begin{matrix} \lambda_n + \sigma \\ \lambda_{n-1} \\ W_{n-1} \end{matrix} \middle| C_n^{\sigma\dagger} \middle| \begin{matrix} \lambda_n \\ \lambda_{n-1} \\ W_{n-1} \end{matrix} \right\rangle = 1 = \langle \lambda_n + \sigma \| C^\dagger \| \lambda_n \rangle \left\langle \begin{matrix} \lambda_n + \sigma \\ W_{n-1} \end{matrix} \middle| \begin{matrix} \lambda_n & (0,1) \\ W_{n-1} & n \end{matrix} \right\rangle , \tag{20}$$

where $\lambda = \lambda_n = \lambda_{n-1}$. Consequently,

$$\langle \lambda + \sigma \| C^\dagger \| \lambda \rangle = \left(\begin{matrix} \lambda + \sigma \\ \lambda \end{matrix} \middle| \begin{matrix} \lambda & (0,1) \\ \lambda & 0 \end{matrix} \right)^{-1} = \left(\frac{N_{\lambda+\sigma} f_\lambda}{f_{\lambda+\sigma}} \right)^{1/2} , \tag{21}$$

where we have employed the results of Part I for the U(n) isoscalar factors, in particular eqs. (I.145) or (I.154). Clearly, $0 \equiv (0,0)$, N_μ designates the number of boxes (i.e. the particle number) associated with the irrep μ and f_μ designates the dimension of μ considered as an irrep of S_{N_μ}, i.e. $f_\mu = \dim([\mu])$, $[\mu]$ representing a symmetric group irrep (see Part I).

In the case of two column irreps $\langle 2^a\, 1^b\, \dot{0} \rangle \equiv (a, b)$, there are only two fundamental vector operators $C_i^{1\dagger}$ and $C_i^{2\dagger}$, whose action on a given irrep (a, b) module takes the form

$$C_i^{1\dagger} : (a, b) \rightarrow (a, b+1), \quad C_i^{2\dagger} : (a, b) \rightarrow (a+1, b-1) . \tag{22}$$

The corresponding shifts $\Delta(\sigma) \equiv \sigma$ for $\sigma = 1$ and $\sigma = 2$, that yield the resulting irrep $(a, b) + \sigma$, are thus given by (0, 1) and $(1, -1)$, respectively. For the relevant RMEs [#5], we find from eq. (21) (or using table I.2, types A and C) that

$$\langle (a, b+1) \| C^\dagger \| (a, b) \rangle = [(b+1)(a+b+2)/(b+2)]^{1/2} ,$$

$$\langle (a+1, b-1) \| C^\dagger \| (a, b) \rangle = [(a+1)(b+1)/b]^{1/2} . \tag{23}$$

The U(n) CG coefficients that appear in eq. (17) may be conveniently factored into a product of U(n) isoscalar factors [see Part I, eqs. (I.145) or (I.154)], i.e.

[#5] We drop the superscript σ from C since it is implied by the bra and ket irreps.

$$\left\langle \begin{array}{c|cc} \lambda & \mu & (0,1) \\ W & U & i \end{array} \right\rangle = \left(\prod_{k=1}^{i-1} \delta_{\lambda_k \mu_k} \right) \left(\begin{array}{c|cc} \lambda_i & \mu_i & (0,1) \\ \lambda_{i-1} & \mu_{i-1} & (0,0) \end{array} \right) \times \prod_{k=i+1}^{n} \left(\begin{array}{c|cc} \lambda_k & \mu_k & (0,1) \\ \lambda_{k-1} & \mu_{k-1} & (0,1) \end{array} \right), \tag{24}$$

where $\lambda_n = \lambda, \mu_n = \mu$. Thus, the bra and ket irreps for the subgroups $U(m), m = 1, 2, \ldots, i-1$ must be identical, since below the ith level of the canonical subgroup chain the operator $C_i^{\sigma\dagger}$ acts as the identity operator. We again emphasize that eqs. (17) and (24) are completely general, so that the MEs of $C_i^{\sigma\dagger}$ can be computed for any U(n) irreps as long as the relevant isoscalar factors are known. An explicit form of these isoscalar factors for two-column irreps was given in table 2 of Part I. These general expressions considerably simplify in the case that one of the coupled irreps is the single box fundamental vector representation, as required for isoscalar factors appearing in eq. (24). The relevant expressions for these factors are given in table 1. Choosing, further, the RMEs of $C^\dagger$, eq. (23), as the scaling factors $c(\lambda, \sigma; \lambda + \sigma), \lambda = (a, b)$, eq. (12), i.e.

$$c[(a,b),(0,1);(a,b)+\sigma] = \langle (a,b)+\sigma \| C^\dagger \| (a,b) \rangle, \tag{12'}$$

where $(a,b)+\sigma = (a,b+1)$ for $\sigma = 1$, and $(a,b)+\sigma = (a+1,b-1)$ for $\sigma = 2$ (for explicit values see eq. (23)), we obtain even simpler expressions for the scaled isoscalar factors, eq. (11), that are also listed in table 1. In fact, it is remarkable that these scaled factors are a-independent, so that only the corresponding SU(2) irreps

Table 1
Unscaled and scaled isoscalar factor $\left(\begin{array}{cc|c} \lambda' & (0,1) & (a,b) \\ \lambda & \mu & \nu \end{array} \right)$, required for MEs of vector operators[a]

μ	λ'	λ	ν	Unscaled	Scaled
(0, 1)	$(a,b-1)$	$(a,b-2)$	$(a,b-1)$	$-[(a+b)(b^2-1)/(a+b+1)]^{1/2}/b$	-1
		$(a-1,b)$	$(a,b-1)$	$-[a/(a+b+1)]^{1/2}/b$	$-1/(b+1)$
		$(a-1,b)$	$(a-1,b+1)$	1	$[b(b+2)]^{1/2}/(b+1)$
		$(a-1,b-1)$	$(a-1,b)$	$-[(a+b)/(a+b+1)]^{1/2}$	-1
	$(a-1,b+1)$	$(a-2,b+2)$	$(a-1,b+1)$	$-[(a-1)(b+1)(b+3)/a]^{1/2}/(b+2)$	-1
		$(a-1,b)$	$(a-1,b+1)$	$[(a+b+1)/a]^{1/2}/(b+2)$	$1/(b+1)$
		$(a-1,b)$	$(a,b-1)$	1	$[b(b+2)]^{1/2}/(b+1)$
		$(a-2,b+1)$	$(a-1,b)$	$-[(a-1)/a]^{1/2}$	-1
(0, 0)	$(a,b-1)$	$(a,b-1)$	$(a,b-1)$	$[(b+1)/b(a+b+1)]^{1/2}$	1
		$(a-1,b)$	$(a-1,b)$	$(a+b+1)^{-1/2}$	$[b/(b+1)]^{1/2}$
	$(a-1,b+1)$	$(a-1,b+1)$	$(a-1,b+1)$	$[(b+1)/a(b+2)]^{1/2}$	1
		$(a-1,b)$	$(a-1,b)$	$a^{-1/2}$	$[(b+2)/(b+1)]^{1/2}$

[a] Recall that the trivial isoscalar factors, i.e., in our case when $\lambda' = \lambda, \mu = (0,1)$ and $\nu = (a,b)$, both scaled and unscaled, equal 1.

play the role. The required matrix elements of $C_i^{\sigma\dagger}$ operators are then given by the product of these scaled isoscalar factors as implied by eq. (14), that now reads

$$\left\langle \begin{matrix} \lambda+\sigma \\ W \end{matrix} \middle| C_i^{\sigma\dagger} \middle| \begin{matrix} \lambda \\ U \end{matrix} \right\rangle = \left\langle \begin{matrix} \lambda & (0,1) \\ U & i \end{matrix} \middle| \begin{matrix} \lambda+\sigma \\ W \end{matrix} \right\rangle^{(s)} = \left\langle \begin{matrix} \lambda+\sigma \\ W \end{matrix} \middle| \begin{matrix} \lambda & (0,1) \\ U & i \end{matrix} \right\rangle^{(s)}, \tag{25}$$

assuming we use a real representation for U(n) CG coefficients. Thus, relying on eq. (24), we get when $i = n$,

$$\left\langle \begin{matrix} \lambda'_n \\ W'_n \end{matrix} \middle| C_n^{\sigma\dagger} \middle| \begin{matrix} \lambda_n \\ W_n \end{matrix} \right\rangle = \left(\begin{matrix} \lambda_n & (0,1) \\ \lambda_{n-1} & (0,0) \end{matrix} \middle| \begin{matrix} \lambda'_n \\ \lambda_{n-1} \end{matrix} \right)^{(s)}, \tag{25'}$$

while for $i < n$ we can write

$$\left\langle \begin{matrix} \lambda'_n \\ W'_n \end{matrix} \middle| C_i^{\sigma\dagger} \middle| \begin{matrix} \lambda_n \\ W_n \end{matrix} \right\rangle = \left(\begin{matrix} \lambda_n & (0,1) \\ \lambda_{n-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda'_n \\ \lambda'_{n-1} \end{matrix} \right)^{(s)} \left\langle \begin{matrix} \lambda'_{n-1} \\ W'_{n-1} \end{matrix} \middle| C_i^{\tau\dagger} \middle| \begin{matrix} \lambda_{n-1} \\ W_{n-1} \end{matrix} \right\rangle, \tag{25''}$$

where $\lambda'_n = \lambda_n + \sigma$ and $\lambda'_{n-1} = \lambda_{n-1} + \tau$.

We note, finally, that the corresponding Hermitian conjugate operators C_i^{σ}, representing annihilation-like operators, transform as the contragredient fundamental vector representation, namely

$$[E_{kj}, C_i^{\sigma}] = -\delta_{ik} C_j^{\sigma}\,. \tag{26}$$

Their action is given by the conjugate of eq. (16) and their MEs satisfy the relationship

$$\left\langle \begin{matrix} \lambda+\sigma \\ W \end{matrix} \middle| C_i^{\sigma\dagger} \middle| \begin{matrix} \lambda \\ U \end{matrix} \right\rangle = \left\langle \begin{matrix} \lambda \\ U \end{matrix} \middle| C_i^{\sigma} \middle| \begin{matrix} \lambda+\sigma \\ W \end{matrix} \right\rangle. \tag{27}$$

4. Generator matrix elements

There are several avenues open to us when deriving explicit expressions for the U(n) generator MEs. The most natural one is, of course, to regard the generators as adjoint tensor operators, associated with the irrep $\langle 1\dot{0} -1\rangle$, since E_{ij} "annihilates" a box labelled with j and "creates" one labelled with i. Such an approach, however, requires further development of the tensor operator formalism that will only be carried out in the following sections. Nonetheless, the same goal may be achieved using the simpler vector operator formalism that we have just outlined. The evaluation of U(n) generator MEs represents, in fact, a nice illustration of this formalism.

Since the MEs of raising and lowering generators are simply related, we only consider the former ones ($E_{ij}, i<j$). To represent the generators E_{ij} as vector operators, we observe that their MEs must vanish unless the bra and ket state (Gel'fand or Paldus) labels are identical above the jth level, so that these MEs are the same in all U(m) subgroups with $m = n, n-1, \ldots, j$. Thus, the U(n) MEs of $E_{ij}, i<j$ may be reduced to the corresponding U(j) MEs namely,

$$\left\langle \begin{matrix} \lambda \\ W' \end{matrix} \middle| E_{ij} \middle| \begin{matrix} \lambda \\ W \end{matrix} \right\rangle \equiv \left\langle \begin{matrix} \lambda_n \\ W'_n \end{matrix} \middle| E_{ij} \middle| \begin{matrix} \lambda_n \\ W_n \end{matrix} \right\rangle = \left(\prod_{k=j}^{n} \delta_{\lambda'_k \lambda_k}\right) \left\langle \begin{matrix} \lambda_j \\ W'_j \end{matrix} \middle| E_{ij} \middle| \begin{matrix} \lambda_j \\ W_j \end{matrix} \right\rangle . \tag{28}$$

It is now easy to realize that E_{ij} $(i<j)$ represents a U($j-1$) vector operator, since obviously (cf. eq. (15))

$$[E_{kl}, E_{ij}] = \delta_{il} E_{kj}, \quad 1 \leqslant k, l \leqslant j-1 . \tag{29}$$

We may thus write the required U(j) MEs, eq. (28), as a product of a certain factor that can only depend on the U(j) and U($j-1$) irrep labels and an ME of a fundamental vector operator $C_i^{\sigma\dagger}$, namely

$$\left\langle \begin{matrix} \lambda_j \\ W'_j \end{matrix} \middle| E_{ij} \middle| \begin{matrix} \lambda_j \\ W_j \end{matrix} \right\rangle = \left\langle \begin{matrix} \lambda_j \\ \lambda'_{j-1} \end{matrix} \middle| E \middle| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda'_{j-1} \\ W'_{j-1} \end{matrix} \middle| C_i^{\sigma\dagger} \middle| \begin{matrix} \lambda_{j-1} \\ W_{j-1} \end{matrix} \right\rangle , \tag{30}$$

where $\lambda'_{j-1} = \lambda_{j-1} + \sigma$. Expressing the last factor in eq. (30) as a product of the scaled RME and the CG coefficient, eq. (17), we can write

$$\left\langle \begin{matrix} \lambda_j \\ W'_j \end{matrix} \middle| E_{ij} \middle| \begin{matrix} \lambda_j \\ W_j \end{matrix} \right\rangle = \left\langle \begin{matrix} \lambda_j \\ \lambda'_{j-1} \end{matrix} \middle\| E \middle\| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right\rangle^{(s)} \left\langle \begin{matrix} \lambda_{j-1} & (0,1) \\ W_{j-1} & i \end{matrix} \middle| \begin{matrix} \lambda'_{j-1} \\ W'_{j-1} \end{matrix} \right\rangle^{(s)} , \tag{31}$$

where the first factor on the right-hand side, representing a (scaled) RME of E (a generator), is the same as the corresponding factor in eq. (30),

$$\begin{aligned} \left\langle \begin{matrix} \lambda_j \\ \lambda'_{j-1} \end{matrix} \middle\| E \middle\| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right\rangle^{(s)} &\equiv \left\langle \begin{matrix} \lambda_j \\ \lambda'_{j-1} \end{matrix} \middle| E \middle| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right\rangle \left\langle \lambda'_{j-1} \middle\| C^\dagger \middle\| \lambda_j \right\rangle^{(s)} \\ &= \left\langle \begin{matrix} \lambda_j \\ \lambda'_{j-1} \end{matrix} \middle| E \middle| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right\rangle , \end{aligned} \tag{32}$$

assuming that we choose the scaling according to eqs. (12) and (13). The second factor is then a scaled U($j-1$) CG coefficient (see also eq. (25)), whose general form is given by eq. (24) (where now all the quantities are appropriately scaled; we also note that in view of the chosen phase convention, all these quantities are real).

The unknown generator RMEs, eq. (32), may be easily determined from the elementary generator MEs given by Paldus formulae [2,3]. For example, when both $n_1 \equiv n-1$ and n are singly occupied in the bra and the ket, respectively, we have

$$\left\langle \begin{array}{c}(a,b)\\ \blacksquare\,\boxed{n_1}\end{array} \middle| E_{n-1,n} \middle| \begin{array}{c}(a,b)\\ \blacksquare\,\boxed{n}\end{array} \right\rangle = 1 = \left\langle \begin{array}{c}(a,b)\\(a,b)\end{array} \middle\| E \middle\| \begin{array}{c}(a,b)\\(a-1,b+1)\end{array} \right\rangle^{(s)}$$

$$\times \left(\begin{array}{cc}(a-1,b+1) & (0,1)\\ (a-1,b+1) & (0,0)\end{array} \middle| \begin{array}{c}(a,b)\\(a-1,b+1)\end{array} \right)^{(s)}, \quad n_1 = n-1 \tag{33}$$

and similarly for the other possibility that n and n_1 occur in the first column of the Weyl tableau, when $\lambda_{j-1} = (a, b-1)$. Since the scaled isoscalar factor on the right-hand side is equal to 1 in each case (see table 1), we find that the RMEs are also equal to 1. The remaining types may similarly be obtained by considering, say, the case with n doubly occupied in the ket and n and $n_1 \equiv n-1$ singly occupied in the bra. The relevant values of these RMEs are collected in table 2.

In summary, we can thus express the generator MEs (28) as a single product of segment values, namely

$$\left\langle \begin{array}{c}\lambda\\W'\end{array} \middle| E_{ij} \middle| \begin{array}{c}\lambda\\W\end{array} \right\rangle = \left(\prod_{k=j}^{n} \delta_{\lambda'_k \lambda_k} \right) \left\langle \begin{array}{c}\lambda_j\\ \lambda'_{j-1}\end{array} \middle\| E \middle\| \begin{array}{c}\lambda_j\\ \lambda_{j-1}\end{array} \right\rangle^{(s)}$$

$$\times \left\{ \prod_{k=i+1}^{j-1} \left(\begin{array}{cc}\lambda_k & (0,1)\\ \lambda_{k-1} & (0,1)\end{array} \middle| \begin{array}{c}\lambda'_k\\ \lambda'_{k-1}\end{array} \right)^{(s)} \right\}$$

$$\times \left(\begin{array}{cc}\lambda_i & (0,1)\\ \lambda_{i-1} & (0,0)\end{array} \middle| \begin{array}{c}\lambda'_i\\ \lambda'_{i-1}\end{array} \right)^{(s)} \prod_{k=1}^{i-1} \delta_{\lambda'_k \lambda_k} . \tag{34}$$

Comparing this result with that of UGA (or GUGA) we immediately see that the generator RMEs (32) represent the top segment values, the isoscalar factors within the braces the middle segment values, and the rightmost isoscalar factor the bottom segment value. We must emphasize, however, that this result is completely general and applies to any irrep whatsoever. Of course, in order to exploit it we must be able to determine the required isoscalar factors and RMEs. For two-column irreps are required segment values are contained in tables 1 and 2.

So far, we have treated the generators E_{ij} as U($j-1$) vector operators. We now

Table 2
Nonvanishing raising generator RMEs $\left\langle \begin{array}{c}(a,b)\\ \lambda\end{array} \middle| E \middle| \begin{array}{c}(a,b)\\ \nu\end{array} \right\rangle = \left\langle \begin{array}{c}(a,b)\\ \lambda\end{array} \middle\| E \middle\| \begin{array}{c}(a,b)\\ \nu\end{array} \right\rangle^{(s)}$, (cf., eq. (32)).

λ	ν	E
(a,b)	$(a,b-1)$	1
(a,b)	$(a-1,b+1)$	1
$(a,b-1)$	$(a-1,b)$	$[b/(b+1)]^{1/2}$
$(a-1,b+1)$	$(a-1,b)$	$[(b+2)/(b+1)]^{1/2}$

wish to proceed one step further and express the generators in terms of our U(n) creation and annihilation vector operators $C_i^{\sigma\dagger}$ and C_i^{σ}. Since E_{ij} represents an U(n) adjoint tensor operator (see section 6), as do the operators $C_i^{\sigma\dagger} C_j^{\tau}$ ($\sigma, \tau = 1, 2$), we can generally write

$$E_{ij} = \sum_{\sigma,\tau} \rho_{\sigma\tau} C_i^{\sigma\dagger} C_j^{\tau} . \tag{35}$$

In fact, the transformation matrix $\boldsymbol{\rho}$ must be diagonal, since E_{ij} leaves invariant any U(n) irrep module, so that

$$\rho_{\sigma\tau} = \rho_\tau \delta_{\sigma\tau} . \tag{35'}$$

In the special case of two-column irreps, only two values ρ_τ ($\tau = 1, 2$) are required (C_j^3 produces a vanishing result when acting on any two-column irrep module). In fact, $\boldsymbol{\rho}$ can be shown to be the 2×2 identity matrix in this case. The easiest way to see this is to consider the MEs of weight generator E_{nn} between states in which n is singly occupied. While the left-hand side of eq. (35) will always yield 1 in this case, the right-hand side equals ρ_k times the corresponding ME of $C_n^{k\dagger} C_n^{k}$, assuming that n occurs in the kth column of the Weyl tableau. Since the latter ME also equals 1, we have that $\rho_\tau = 1$, ($\tau = 1, 2$). Thus, we find that

$$E_{ij} = \sum_{\tau} \rho_\tau C_i^{\tau\dagger} C_j^{\tau} = \sum_{\tau} C_i^{\tau\dagger} C_j^{\tau} . \tag{36}$$

Using this result we can now express the generator MEs (28) in terms of MEs of $C^\dagger C$-type operators. Thus, for the E_{ij} in the U(j) basis, eq. (30), we find that

$$\begin{aligned} \left\langle \begin{matrix} \lambda_j \\ W_j' \end{matrix} \middle| E_{ij} \middle| \begin{matrix} \lambda_j \\ W_j \end{matrix} \right\rangle &= \sum_{\tau, W_j''} \left\langle \begin{matrix} \lambda_j \\ W_j' \end{matrix} \middle| C_i^{\tau\dagger} \middle| \begin{matrix} \lambda_j - \tau \\ W_j'' \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_j - \tau \\ W_j'' \end{matrix} \middle| C_j^{\tau} \middle| \begin{matrix} \lambda_j \\ W_j \end{matrix} \right\rangle \\ &= \sum_{\tau, W_j''} \left\langle \begin{matrix} \lambda_j - \tau & (0,1) \\ W_j'' & i \end{matrix} \middle| \begin{matrix} \lambda_j \\ W_j' \end{matrix} \right\rangle^{(s)} \left\langle \begin{matrix} \lambda_j - \tau & (0,1) \\ W_j'' & j \end{matrix} \middle| \begin{matrix} \lambda_j \\ W_j \end{matrix} \right\rangle^{(s)} , \end{aligned} \tag{37}$$

where in the last step we employed eq. (25), its conjugate, eq. (27), and the reality of CGs. Expressing, finally, the U(j) CG coefficients as a product of the U(j) $\supset$ U($j-1$) isoscalar factor and the U($j-1$) CG coefficient, we obtain

$$\begin{aligned} \left\langle \begin{matrix} \lambda_j \\ W_j' \end{matrix} \middle| E_{ij} \middle| \begin{matrix} \lambda_j \\ W_j \end{matrix} \right\rangle = & \left\{ \sum_{\tau} \left(\begin{matrix} \lambda_j - \tau & (0,1) \\ \lambda_{j-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda_j \\ \lambda_{j-1}' \end{matrix} \right)^{(s)} \left(\begin{matrix} \lambda_j - \tau & (0,1) \\ \lambda_{j-1} & (0,0) \end{matrix} \middle| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right)^{(s)} \right\} \\ & \times \left\langle \begin{matrix} \lambda_{j-1} & (0,1) \\ W_{j-1} & i \end{matrix} \middle| \begin{matrix} \lambda_{j-1}' \\ W_{j-1}' \end{matrix} \right\rangle^{(s)} , \end{aligned} \tag{38}$$

since the second CG coefficient on the right-hand side of the last eq. (37) simply equals an isoscalar factor in view of the fact that we must have $W_{j-1}'' = W_{j-1}$ (and thus, also $\lambda''_{j-1} = \lambda_{j-1}$). Comparing now this result with the preceding one, eq. (34), we see that the expression in curly brackets in eq. (38) represents in fact a general RME, so that

$$\left\langle \begin{matrix} \lambda_j \\ \lambda'_{j-1} \end{matrix} \middle\| E \middle\| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right\rangle = \sum_{\tau} \left(\begin{matrix} \lambda_j - \tau & (0,1) \\ \lambda_{j-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda_j \\ \lambda'_{j-1} \end{matrix} \right)^{(s)} \times \left(\begin{matrix} \lambda_j - \tau & (0,1) \\ \lambda_{j-1} & (0,0) \end{matrix} \middle| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right)^{(s)} . \tag{39}$$

Using the isoscalar factors listed in table 1 it is worthwhile to check that the RMEs given in table 2, that were obtained above with the help of Paldus formulas for elementary generators, do indeed satisfy the relationship (39) and may thus be obtained solely within the isoscalar factor formalism expounded in this series.

In concluding this section, we must emphasize that all the above derivations were made for the case of raising generators $E_{ij}, i<j$. In an exactly analogous way we can handle the corresponding lowering generators, using the fact that $E^{\dagger}_{ij} = E_{ji}$. Thus, for example, the generator RMEs that are required in this case are simply obtained from those given in table 2 by a transposition, since now

$$\left\langle \begin{matrix} \lambda_j \\ \lambda'_{j-1} \end{matrix} \middle\| E^{\mathrm{L}} \middle\| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right\rangle = \sum_{\tau} \left(\begin{matrix} \lambda_j - \tau & (0,1) \\ \lambda'_{j-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right)^{(s)} \times \left(\begin{matrix} \lambda_j - \tau & (0,1) \\ \lambda'_{j-1} & (0,0) \end{matrix} \middle| \begin{matrix} \lambda_j \\ \lambda'_{j-1} \end{matrix} \right)^{(s)} , \tag{39$'$}$$

so that

$$\left\langle \begin{matrix} \lambda \\ \lambda' \end{matrix} \middle\| E^{\mathrm{L}} \middle\| \begin{matrix} \lambda \\ \nu \end{matrix} \right\rangle = \left\langle \begin{matrix} \lambda \\ \nu \end{matrix} \middle\| E^{\mathrm{R}} \middle\| \begin{matrix} \lambda \\ \lambda' \end{matrix} \right\rangle \equiv \left\langle \begin{matrix} \lambda \\ \nu \end{matrix} \middle\| E \middle\| \begin{matrix} \lambda \\ \lambda' \end{matrix} \right\rangle , \tag{39$''$}$$

where the superscript designates the lowering (L) or raising (R) generator cases. We shall always employ raising generator RMEs in the following and thus drop the superscript to simplify the notation.

5. Symmetric and antisymmetric tensors

We have seen in the preceding section (eq. (36)) that the U(n) generators may be represented by a linear combination of products of creation and annihilation vector operators $C^{\dagger}$ and C. Consequently, generator products or two-body operators may be similarly represented using products of two $C^{\dagger}$ and two C operators.

The latter are basically of two types, namely $(C^\dagger C)(C^\dagger C)$ and $(C^\dagger C^\dagger)(CC)$. While the former type corresponds directly to the generator products $E_{ij}E_{kl}$, the latter type involves generators from the O(2n) extension of U(n) (cf. ref. [39]) and corresponds more directly to a standard second quantized form of two-body operators (see section 7). We refer to operators of the type $(C^\dagger C^\dagger)$ as *pairing operators* (CC being their conjugates). We shall now examine the MEs of these pairing operators, while those of the $(C^\dagger C)$-type, representing U(n) adjoint tensors, will be examined in the next section. Relying on these results we shall then be able to effectively handle MEs of two-body operators (see section 7).

The evaluation of pairing operator MEs leads us to the problem of handling the products of two irreducible tensors. Thus, for example, we can write

$$\left\langle \begin{matrix}\lambda\\ W\end{matrix}\middle| C_i^{\tau\dagger}C_j^{\sigma\dagger}\middle|\begin{matrix}\lambda_1\\ W_1\end{matrix}\right\rangle = \sum_U \left\langle \begin{matrix}\lambda\\ W\end{matrix}\middle| C_i^{\tau\dagger}\middle|\begin{matrix}\lambda_1+\sigma\\ U\end{matrix}\right\rangle\left\langle \begin{matrix}\lambda_1+\sigma\\ U\end{matrix}\middle| C_j^{\sigma\dagger}\middle|\begin{matrix}\lambda_1\\ W_1\end{matrix}\right\rangle$$

$$= \langle\lambda\|C^\dagger\|\lambda_1+\sigma\rangle\langle\lambda_1+\sigma\|C^\dagger\|\lambda_1\rangle$$

$$\times\sum_U \left\langle \begin{matrix}\lambda_1+\sigma & (0,1)\\ U & i\end{matrix}\middle|\begin{matrix}\lambda\\ W\end{matrix}\right\rangle\left\langle \begin{matrix}\lambda_1 & (0,1)\\ W_1 & j\end{matrix}\middle|\begin{matrix}\lambda_1+\sigma\\ U\end{matrix}\right\rangle, \quad (40)$$

where we have used the WE theorem, eq. (17), in the last step. Clearly, $\lambda = \lambda_1 + \sigma + \tau$. Although we could handle the quantities arising on the right-hand side of eq. (40) directly, it is much more convenient to exploit the recoupling procedure involving U(n) Racah coefficients. Indeed, considering the multiplicity free case and assuming that the CG coefficients are real, we easily transform the basic relationship (I.139), with the help of orthogonality properties of CG coefficients, into the form

$$\sum_{W_{12}} \left\langle \begin{matrix}\lambda_1 & \lambda_2\\ W_1 & W_2\end{matrix}\middle|\begin{matrix}\lambda_{12}\\ W_{12}\end{matrix}\right\rangle\left\langle \begin{matrix}\lambda_{12} & \lambda_3\\ W_{12} & W_3\end{matrix}\middle|\begin{matrix}\lambda\\ W\end{matrix}\right\rangle$$

$$= \sum_{\lambda_{23},W_{23}} U\{\lambda_1\lambda_2\lambda\lambda_3;\lambda_{12}\lambda_{23}\}\left\langle \begin{matrix}\lambda_2 & \lambda_3\\ W_2 & W_3\end{matrix}\middle|\begin{matrix}\lambda_{23}\\ W_{23}\end{matrix}\right\rangle\left\langle \begin{matrix}\lambda_1 & \lambda_{23}\\ W_1 & W_{23}\end{matrix}\middle|\begin{matrix}\lambda\\ W\end{matrix}\right\rangle. \quad (41)$$

Thus, assuming that the RMEs are equal to 1 and setting $\lambda_2 = \lambda_3 = (0,1)$, we can interpret the left-hand side of eq. (41) as the ME of a product of two tensor operators associated with irreps λ_2 and λ_3. With the help of recoupling, eq. (41), this ME reduces to the ME of a tensor associated with the irrep λ_{23} that arises from coupling of λ_2 and λ_3. In the case of pairing operators this leads to the coupling of two vector operators, each associated with the single box irrep (0, 1). This coupling produces tensors associated with the symmetic (1, 0) and antisymmetric (0, 2) two-box irreps. Exploiting, thus, the recoupling transformation (41) in eq. (40) we get

$$\left\langle \begin{matrix} \lambda \\ W \end{matrix} \middle| C_i^{\tau\dagger} C_j^{\sigma\dagger} \middle| \begin{matrix} \lambda_1 \\ W_1 \end{matrix} \right\rangle = \langle \lambda \| C^\dagger \| \lambda_1 + \sigma \rangle \langle \lambda_1 + \sigma \| C^\dagger \| \lambda_1 \rangle \times \sum_{\lambda_{23}, W_{23}} U\{\lambda_1(0,1)\lambda(0,1);(\lambda_1+\sigma)\lambda_{23}\} \times \left\langle \begin{matrix} (0,1) & (0,1) \\ j & i \end{matrix} \middle| \begin{matrix} \lambda_{23} \\ W_{23} \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_1 & \lambda_{23} \\ W_1 & W_{23} \end{matrix} \middle| \begin{matrix} \lambda \\ W \end{matrix} \right\rangle , \tag{42}$$

where again $\lambda = \lambda_1 + \sigma + \tau$, while λ_{23} runs over the irreps (1, 0) and (0, 2) and W_{23} is uniquely determined by labels i and j. To simplify notation, we designate either tableau, namely

$$\boxed{i}\boxed{j} \quad (i \leqslant j) \quad \text{or} \quad \begin{array}{|c|} \hline i \\ \hline j \\ \hline \end{array} \quad (i<j)$$

as $[ij]$ or $[ji]$, since irrep labels (1, 0) or (0, 2) immediately imply which one is involved. Clearly, the antisymmetric (0, 2) irrep cannot arise when $i = j$.

For the CG coefficients coupling two vector irreps we easily find (employing the same phase convention as in Part I) using table I.2 that

$$\left\langle \begin{matrix} (0,1) & (0,1) \\ i & j \end{matrix} \middle| \begin{matrix} (1,0) \\ [ij] \end{matrix} \right\rangle = [(1+\delta_{ij})/2]^{1/2}$$

and

$$\left\langle \begin{matrix} (0,1) & (0,1) \\ i & j \end{matrix} \middle| \begin{matrix} (0,2) \\ [ij] \end{matrix} \right\rangle = - \left\langle \begin{matrix} (0,1) & (0,1) \\ j & i \end{matrix} \middle| \begin{matrix} (0,2) \\ [ij] \end{matrix} \right\rangle = [(1-\delta_{ij})/2]^{1/2}, \quad (i \leqslant j) .$$

It is then easy to verify that

$$\left\langle \begin{matrix} (0,2) \\ [(n-1)n] \end{matrix} \middle| C_n^{1\dagger} C_{n-1}^{1\dagger} \middle| \begin{matrix} (0,0) \\ 0 \end{matrix} \right\rangle \equiv \left\langle \begin{array}{|c|} \hline n_1 \\ \hline n \\ \hline \end{array} \middle| C_n^{1\dagger} C_{n-1}^{1\dagger} \middle| 0 \right\rangle = 1 ,$$

where $n_1 \equiv n - 1$, which may also be regarded as a definition of the phase convention employed.

Now, within the spaces consisting of at most two-column irrep modules, the CG series involving symmetric and antisymmetric tensors are multiplicity free, namely

$$(a,b) \times (1,0) = (a+1,b) + \dots ,$$
$$(a,b) \times (0,2) = (a,b+2) + (1-\delta_{b,0})(a+1,b) + (a+2,b-2) + \dots ,$$

where the dots indicate more than two-column irreps. Thus, the symmetric tensor has only one shift component while the antisymmetric one has three (assuming $b \neq 0$). This is consistent with the fact that we have four $C^\dagger C^\dagger$ operators, namely $C_i^{1\dagger} C_j^{1\dagger}$ and $C_i^{2\dagger} C_j^{2\dagger}$ that are antisymmetric and shift (a,b) into $(a,b+2)$ and

$(a+2, b-2)$, respectively, and $C_i^{1\dagger} C_j^{2\dagger}$ and $C_i^{2\dagger} C_j^{1\dagger}$, both shifting (a, b) to $(a+1, b)$ and yielding one symmetric and one antisymmetric tensor.

The last CG coefficient on the right-hand side of eq. (42) that involves a symmetric or antisymmetric two-box irrep λ_{23} may be evaluated as a product of U(n) isoscalar factors whose explicit form may be found in table I.2. However, we can again simplify eq. (42) by using the RMEs as appropriate scaling factors. We thus observe that

$$c[(a-1,b),(1,0);(a,b)] = \langle (a,b) \| C^\dagger \| \nu \rangle \langle \nu \| C^\dagger \| (a-1,b) \rangle$$
$$= [a(a+b+1)]^{1/2}, \tag{43}$$

independently of the intermediate irrep ν, for which we have either $\nu = (a-1, b+1)$, or $\nu = (a, b-1)$. In a similar way we find that

$$c[(a,b-2),(0,2);(a,b)] = \langle (a,b) \| C^\dagger \| (a,b-1) \rangle \langle (a,b-1) \| C^\dagger \| (a,b-2) \rangle$$
$$= [(b-1)(a+b)(a+b+1)/(b+1)]^{1/2}, \tag{44a}$$

$$c[(a-1,b),(0,2);(a,b)] = c[(a-1,b),(1,0);(a,b)]$$
$$= [a(a+b+1)]^{1/2}, \tag{44b}$$

$$c[(a-2,b+2),(0,2);(a,b)] = \langle (a,b) \| C^\dagger \| (a-1,b+1) \rangle$$
$$\times \langle (a-1,b+1) \| C^\dagger \| (a-2,b+2) \rangle$$
$$= [(b+3)(a-1)a/(b+1)]^{1/2}. \tag{44c}$$

Employing these scaling factors, eq. (9b), we can rewrite eq. (42) in the form

$$\left\langle \begin{matrix} (d,e) \\ W' \end{matrix} \middle| C_i^{\tau\dagger} C_j^{\sigma\dagger} \middle| \begin{matrix} (a,b) \\ W \end{matrix} \right\rangle = \left\langle \begin{matrix} (a,b) \\ W \end{matrix} \middle| C_j^{\sigma} C_i^{\tau} \middle| \begin{matrix} (d,e) \\ W' \end{matrix} \right\rangle$$
$$= \sum_{\nu=(1,0),(0,2)} U\{(0,1)\,(0,1)\,(d,e)\,(a,b);\nu\,\mu\}$$
$$\times \left\langle \begin{matrix} (0,1) & (0,1) \\ j & i \end{matrix} \middle| \begin{matrix} \nu \\ [ij] \end{matrix} \right\rangle \left\langle \begin{matrix} (a,b) & \nu \\ W & [ij] \end{matrix} \middle| \begin{matrix} (d,e) \\ W' \end{matrix} \right\rangle^{(s)}, \tag{45}$$

where we have exploited the symmetry property of Racah coefficients, eq. (I.137) and where

$$(d,e) = (a,b) + \sigma + \tau, \quad \mu = (a,b) + \sigma = (d,e) - \tau. \tag{46}$$

The explicit form of (scaled) isoscalar factors that are required for the evaluation of the last (scaled) CG coefficient appearing in eq. (42) or (45) may be obtained from table I.2 and are listed in tables 3 and 4. Similarly, the required Racah coefficients are easily found in table I.3 (note that $(0,1) \equiv \langle 1 \rangle$ designates a one-box vector irrep). We thus arrive to the following explicit expressions for the MEs (45):

Table 3
Unscaled and scaled isoscalar factors $\left(\begin{matrix} (a-1,b) & (1,0) \\ \lambda & \mu \end{matrix}\middle| \begin{matrix} (a,b) \\ \nu \end{matrix}\right)$, required for MEs of symmetric tensors.

μ	λ	ν	Unscaled	Scaled
(1, 0)	$(a-2,b)$	$(a-1,b)$	$[(a-1)(a+b)/a(a+b+1)]^{1/2}$	1
	$(a-1,b-1)$	$(a,b-1)$	$-[(a+b)/(a+b+1)]^{1/2}$	-1
	$(a-2,b+1)$	$(a-1,b+1)$	$-[(a-1)/a]^{1/2}$	-1
(0, 1)	$(a-1,b-1)$	$(a-1,b)$	$-[b(a+b)/a(b+1)(a+b+1)]^{1/2}$	-1
	$(a-2,b+1)$	$(a-1,b)$	$-[(a-1)(b+2)/a(b+1)(a+b+1)]^{1/2}$	-1
	$(a-1,b)$	$(a,b-1)$	$(a+b+1)^{-1/2}$	$[b/(b+1)]^{1/2}$
	$(a-1,b)$	$(a-1,b+1)$	$a^{-1/2}$	$[(b+2)/(b+1)]^{1/2}$
(0, 0)	$(a-1,b)$	$(a-1,b)$	$[2/a(a+b+1)]^{1/2}$	$\sqrt{2}$

(i) For $\sigma = \tau$, only the antisymmetric term survives, since we cannot couple $(1,\ 0)$ and $(a, b-2)$ or $(a-2, b+2)$ to (a,b). Hence

$$\left\langle \begin{matrix} (d,e) \\ W' \end{matrix} \middle| C_i^{\sigma\dagger} C_j^{\sigma\dagger} \middle| \begin{matrix} (a,b) \\ W \end{matrix} \right\rangle = -\frac{a_{ij}}{\sqrt{2}} \left\langle \begin{matrix} (a,b) \\ W \end{matrix} \quad \begin{matrix} (0,2) \\ [ij] \end{matrix} \middle| \begin{matrix} (d,e) \\ W' \end{matrix} \right\rangle^{(s)}, \tag{47}$$

where

$$a_{ij} = \begin{cases} 1 & \text{if } i<j\,, \\ 0 & \text{if } i=j\,, \\ -1 & \text{if } i>j\,, \end{cases} \tag{48}$$

and

$$(d,e) = \begin{cases} (a, b+2) & \text{if } \sigma = 1\,, \\ (a+2, b-2) & \text{if } \sigma = 2\,. \end{cases} \tag{49}$$

Note that $a_{ji} = -a_{ij}$, while $[ij] \equiv [ji]$ by definition.

(ii) When $\sigma \neq \tau$, so that $\tau = \bar{\sigma}$ where $\bar{\sigma} = 3 - \sigma$, $(\sigma = 1,2)$, both symmetric and antisymmetric terms may contribute and we get

$$\begin{aligned} &\left\langle \begin{matrix} (a+1,b) \\ W' \end{matrix} \middle| C_i^{\bar{\sigma}\dagger} C_j^{\sigma\dagger} \middle| \begin{matrix} (a,b) \\ W \end{matrix} \right\rangle \\ &= (1+\delta_{ij})^{1/2} \rho_b^{(0)}(\sigma) \left\langle \begin{matrix} (a,b) \\ W \end{matrix} \quad \begin{matrix} (1,0) \\ [ij] \end{matrix} \middle| \begin{matrix} (a+1,b) \\ W' \end{matrix} \right\rangle^{(s)} \\ &+ a_{ij}(1-\delta_{b,0}) \rho_b^{(1)}(\sigma) \left\langle \begin{matrix} (a,b) \\ W \end{matrix} \quad \begin{matrix} (0,2) \\ [ij] \end{matrix} \middle| \begin{matrix} (a+1,b) \\ W' \end{matrix} \right\rangle^{(s)}, \end{aligned} \tag{50}$$

where

Table 4
Unscaled and scaled isoscalar factors $\begin{pmatrix} \lambda' & (0,2) & (a,b) \\ \lambda & \mu & \nu \end{pmatrix}$, required for MEs of antisymmetric tensors.

μ	λ'	λ	ν	Unscaled	Scaled
(0, 2)	$(a-2,b+2)$	$(a-2,b+1)$	$(a,b-1)$	1	$\left[\frac{b(b+3)}{(b+1)(b+2)}\right]^{1/2}$
		$(a-2,b+1)$	$(a-1,b+1)$	$\left[\frac{2(a+b+1)}{a(b+2)(b+3)}\right]^{1/2}$	$\left[\frac{2}{(b+1)(b+2)}\right]^{1/2}$
		$(a-3,b+3)$	$(a-1,b+1)$	$\left[\frac{(a-2)(b+1)(b+4)}{a(b+2)(b+3)}\right]^{1/2}$	1
		$(a-3,b+2)$	$(a-1,b)$	$[(a-2)/a]^{1/2}$	1
	$(a-1,b)$	$(a-1,b-1)$	$(a,b-1)$	$-\left[\frac{(a+b)(b-1)(b+2)}{(a+b+1)b(b+1)}\right]^{1/2}$	$-\left[\frac{(b-1)(b+2)}{b(b+1)}\right]^{1/2}$
		$(a-1,b-1)$	$(a-1,b+1)$	$\left[\frac{2(a+b)}{a(b+1)(b+2)}\right]^{1/2}$	$\left[\frac{2}{b(b+1)}\right]^{1/2}$
		$(a-2,b+1)$	$(a,b-1)$	$\left[\frac{2(a-1)}{(a+b+1)b(b+1)}\right]^{1/2}$	$\left[\frac{2}{(b+1)(b+2)}\right]^{1/2}$
		$(a-2,b+1)$	$(a-1,b+1)$	$-\left[\frac{(a-1)b(b+3)}{a(b+1)(b+2)}\right]^{1/2}$	$-\left[\frac{b(b+3)}{(b+1)(b+2)}\right]^{1/2}$
		$(a-2,b)$	$(a-1,b)$	$\left[\frac{(a-1)(a+b)}{a(a+b+1)}\right]^{1/2}$	1
	$(a,b-2)$	$(a,b-3)$	$(a,b-1)$	$\left[\frac{(a+b-1)(b-2)(b+1)}{(a+b+1)(b-1)b}\right]^{1/2}$	1
		$(a-1,b-1)$	$(a,b-1)$	$\left[\frac{2a}{(a+b+1)(b-1)b}\right]^{1/2}$	$\left[\frac{2}{b(b+1)}\right]^{1/2}$
		$(a-1,b-1)$	$(a-1,b+1)$	1	$\left[\frac{(b-1)(b+2)}{b(b+1)}\right]^{1/2}$
		$(a-1,b-2)$	$(a-1,b)$	$\left[\frac{a+b-1}{a+b+1}\right]^{1/2}$	1
(0, 1)	$(a-2,b+2)$	$(a-2,b+2)$	$(a-1,b+1)$	$\left[\frac{2(b+1)}{a(b+2)}\right]^{1/2}$	$\sqrt{2}$
		$(a-2,b+1)$	$(a-1,b)$	$(2/a)^{1/2}$	$\left[\frac{2(b+3)}{b+2}\right]^{1/2}$
	$(a-1,b)$	$(a-1,b)$	$(a,b-1)$	$\left[\frac{b+2}{(a+b+1)b}\right]^{1/2}$	$\left[\frac{b+2}{b+1}\right]^{1/2}$
		$(a-1,b)$	$(a-1,b+1)$	$-\left[\frac{b}{a(b+2)}\right]^{1/2}$	$-\left[\frac{b}{b+1}\right]^{1/2}$
		$(a-1,b-1)$	$(a-1,b)$	$\left[\frac{(a+b)(b+2)}{a(a+b+1)(b+1)}\right]^{1/2}$	$\left[\frac{b+2}{b}\right]^{1/2}$
		$(a-2,b+1)$	$(a-1,b)$	$-\left[\frac{(a-1)b}{a(a+b+1)(b+1)}\right]^{1/2}$	$-\left[\frac{b}{b+2}\right]^{1/2}$
	$(a,b-2)$	$(a,b-2)$	$(a,b-1)$	$\left[\frac{2(b+1)}{(a+b+1)b}\right]^{1/2}$	$\sqrt{2}$
		$(a-1,b-1)$	$(a-1,b)$	$\left[\frac{2}{a+b+1}\right]^{1/2}$	$\left[\frac{2(b-1)}{b}\right]^{1/2}$

$$\rho_b^{(\kappa)}(\sigma) = (-1)^{\kappa(\sigma-1)} \frac{1}{2} \left(\frac{b+1-(-1)^{\kappa+\sigma}}{b+1} \right)^{1/2} . \tag{51}$$

As already noted, the CG coefficients involving the symmetric and antisymmetric tensors are equal to single products of isoscalar factors whose explicit form is given in tables 3 and 4. For example, assuming that $i<j$, we have that

$$\begin{aligned} \left\langle \begin{matrix} \lambda_n & (1,0) \\ W_n & [ij] \end{matrix} \middle| \begin{matrix} \lambda_n' \\ W_n' \end{matrix} \right\rangle^{(s)} &= \left\{ \prod_{k=j+1}^{n} \left(\begin{matrix} \lambda_k & (1,0) \\ \lambda_{k-1} & (1,0) \end{matrix} \middle| \begin{matrix} \lambda_k' \\ \lambda_{k-1}' \end{matrix} \right)^{(s)} \right\} \\ &\times \left(\begin{matrix} \lambda_j & (1,0) \\ \lambda_{j-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda_j' \\ \lambda_{j-1}' \end{matrix} \right)^{(s)} \\ &\times \left\{ \prod_{k=i+1}^{j-1} \left(\begin{matrix} \lambda_k & (0,1) \\ \lambda_{k-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda_k' \\ \lambda_{k-1}' \end{matrix} \right)^{(s)} \right\} \\ &\times \left(\begin{matrix} \lambda_i & (0,1) \\ \lambda_{i-1} & (0,0) \end{matrix} \middle| \begin{matrix} \lambda_i' \\ \lambda_{i-1}' \end{matrix} \right)^{(s)} \prod_{k=1}^{i-1} \delta_{\lambda_k' \lambda_k} , \end{aligned} \tag{52}$$

and, similarly, for the antisymmetric tensor (0, 2).

As an illustration of eq. (50), we consider MEs of $C_n^{1\dagger} C_n^{2\dagger}$ and $C_n^{2\dagger} C_n^{1\dagger}$ operators. In this case only the symmetric term contributes and we find that

$$\left\langle \begin{array}{c} (a,b) \\ \boxed{W} \\ \quad\boxed{n} \\ \boxed{n} \end{array} \middle| C_n^{1\dagger} C_n^{2\dagger} \middle| \begin{array}{c} (a-1,b) \\ \boxed{W} \end{array} \right\rangle = \left(\frac{b}{b+1} \right)^{1/2} , \tag{53a}$$

$$\left\langle \begin{array}{c} (a,b) \\ \boxed{W} \\ \quad\boxed{n} \\ \boxed{n} \end{array} \middle| C_n^{2\dagger} C_n^{1\dagger} \middle| \begin{array}{c} (a-1,b) \\ \boxed{W} \end{array} \right\rangle = \left(\frac{b+2}{b+1} \right)^{1/2} . \tag{53b}$$

Note that we can obtain the same result by directly using the MEs of $C^\dagger$ operators. Clearly, $C_n^{1\dagger} C_n^{2\dagger}$ and $C_n^{2\dagger} C_n^{1\dagger}$ represent distinct operators so that, generally, $C_i^{1\dagger}$ and $C_j^{2\dagger}$ do not commute or anticommute.

6. Adjoint tensors

A tensor operator A_{ij} that satisfies the relationship

$$[E_{kl}, A_{ij}] = \delta_{il} A_{kj} - \delta_{kj} A_{il}, \quad (k,l = 1,2,\ldots,n) \tag{54}$$

is called an adjoint tensor operator belonging to the irrep $\langle 1 \dot{0} \bar{1} \rangle \equiv \langle 1 0 \ldots 0 \ -1 \rangle$.

Clearly, the generators E_{ij} are adjoint tensors, as are the four operators $C_i^{\sigma\dagger}C_j^{\tau}$, $(\sigma,\tau=1,2)$. The action of an adjoint tensor operator A_{ij} on a two-column U(n) irreducible module (a,b) produces modules associated with irreps given by the CG series

$$(a,b)\times\langle 1\,\dot{0}\,\bar{1}\rangle=(a-1,b+2)+(2-\delta_{b,0})(a,b)+(a+1,b-2)+\ldots\,, \quad (55)$$

the dots indicating more than two-column irreps. Thus, the four adjoint tensors $C_i^{\sigma\dagger}C_j^{\tau}$ $(\sigma,\tau=1,2)$ are associated with three distinct shifts, the zero-shift of (a,b) into itself having multiplicity 2 (assuming that $b\neq 0$). Indeed, the operator $C_i^{1\dagger}C_j^2$ shifts (a,b) into $(a-1,b+2)$, $C_i^{2\dagger}C_j^1$ shifts (a,b) into $(a+1,b-2)$, while both $C_i^{1\dagger}C_j^1$ and $C_i^{2\dagger}C_j^2$ shift (a,b) into itself. This multiplicity complicates the evaluation of adjoint tensor MEs, since a direct application of the WE theorem to the corresponding CG coefficients will not produce a single product of isoscalar factors. Instead, a sum over two multiplicity indices will be required, in general, at every level of the group chain.

A linear combination of two zero-shift adjoint tensors, $C_i^{1\dagger}C_j^1$ and $C_i^{2\dagger}C_j^2$, is again a zero-shift adjoint tensor. We have already established that a simple sum of these tensors gives the corresponding generator, eq. (36), namely

$$E_{ij}=C_i^{1\dagger}C_j^1+C_i^{2\dagger}C_j^2\,. \quad (56)$$

It is thus natural to ask which other linear combination of these zero-shift adjoint tensors will be the most useful in further development. Motivated by our earlier results, we shall look for a definition that would free us of any multiplicity problem and would lead to as simple a segmentation of the resulting MEs as possible. In general, we shall thus introduce three independent adjoint tensors producing distinct shifts as follows

$$N_{ij}^{(+)}=\eta^{(+)}(b)C_i^{1\dagger}C_j^2\,, \quad (57a)$$

$$N_{ij}^{(0)}=(1-\delta_{b,0})[\eta_1^{(0)}(b)C_i^{1\dagger}C_j^1+\eta_2^{(0)}(b)C_i^{2\dagger}C_j^2]\,, \quad (57b)$$

$$N_{ij}^{(-)}=\eta^{(-)}(b)C_i^{2\dagger}C_j^1\,, \quad (57c)$$

where η's represent suitable irrep module dependent scalar operators. Thus, these operators are invariant on any irrep module (a,b) and, as we shall see later, the scalars defining these operators depend only on the spin $b=2S$ of a given irrep, as the notation implies. Consequently, on a given irrep module (a,b), there is no need to distinguish these operators and the scalars that uniquely determine them. We may, of course, regard the three adjoint tensors $N_{ij}^{(\kappa)}$ $(\kappa=+,0,-)$ as forming a set N_{ij}, shifting (a,b) into $(a-1,b+2)$, (a,b) and $(a+1,b-2)$, respectively, in addition to the generator E_{ij} that also shifts (a,b) into (a,b). It should be noticed, however, that for $b=0$ there is only one zero-shift tensor, namely the generator E_{ij}, so that $N_{ij}^{(0)}$ does not exist in this case (note that eq. (57b) yields a trivial zero operator in this case).

Following the above outlined goal, we next attempt to find the irrep dependent scalar operators (or scalars) η that enable a segmentation of the resulting MEs of adjoint tensor $N_{ij}^{(\kappa)}$. We shall thus try to choose the irrep invariant operators η in such a way that the $N_{ij}^{(\kappa)}$ MEs satisfy the following two conditions:

(i) When $m \equiv r = \max\{i,j\}$, the $N_{ij}^{(\kappa)}$ MEs in the U(r) basis factorize as

$$\left\langle \begin{matrix} \lambda_r' \\ W_r' \end{matrix} \middle| N_{ij}^{(\kappa)} \middle| \begin{matrix} \lambda_r \\ W_r \end{matrix} \right\rangle = \left\langle \begin{matrix} \lambda_r' \\ \lambda_{r-1}' \end{matrix} \middle| N \middle| \begin{matrix} \lambda_r \\ \lambda_{r-1} \end{matrix} \right\rangle_p \left\langle \begin{matrix} \lambda_{r-1}' \\ W_{r-1}' \end{matrix} \middle| P \middle| \begin{matrix} \lambda_{r-1} \\ W_{r-1} \end{matrix} \right\rangle, \tag{58}$$

where $P = C_i^{\sigma\dagger}$, $p = C^\dagger$ when $r = j > i$, $P = C_j^\tau$, $p = C$ when $r = i > j$ and $P = 1, p = 0$ when $r = i = j$. The shift labels σ or τ are given by the irrep labels λ_{r-1} and λ_{r-1}', while λ_r and λ_r' uniquely determine the label κ. For example, $\lambda_r = (a,b)$ and $\lambda_r' = (a-1, b+2)$ imply immediately that $\kappa = +$. We shall refer to $r = \max\{i,j\}$ as a *turning point*, since below this level the vector operators $C_i^{\sigma\dagger}$ and C_j^τ, or the identity, come into play and determine the second factor in (58). We shall also call the first factor in (58) an *N–p connecting factor* for U(r) $\supset$ U($r-1$), since it provides a connection between the operators N and $P = C^\dagger$, C and 1. The MEs of P for the $C^\dagger$ and C type operators in the U($r-1$) basis are given by scaled CG factors, eq. (25), as shown in section 3.

(ii) When $m > i,j$, i.e. for levels above the turning point r, the $N_{ij}^{(\kappa)}$ MEs in U(m) basis factorize as

$$\left\langle \begin{matrix} \lambda_m' \\ W_m' \end{matrix} \middle| N_{ij}^{(\kappa)} \middle| \begin{matrix} \lambda_m \\ W_m \end{matrix} \right\rangle = \left\langle \begin{matrix} \lambda_m' \\ \lambda_{m-1}' \end{matrix} \middle| N \middle| \begin{matrix} \lambda_m \\ \lambda_{m-1} \end{matrix} \right\rangle \left\langle \begin{matrix} \lambda_{m-1}' \\ W_{m-1}' \end{matrix} \middle| N_{ij}^{(\kappa')} \middle| \begin{matrix} \lambda_{m-1} \\ W_{m-1} \end{matrix} \right\rangle. \tag{59}$$

The first factor on the right-hand side, that depends on the U(m) and U($m-1$) irreps, will be referred to as the *N-factor*, while the second factor represents an $N_{ij}^{(\kappa')}$ matrix element in the U($m-1$) basis. The labels κ and κ' are uniquely determined by the irrep labels λ_m, λ_m' and λ_{m-1}, λ_{m-1}', respectively. If there is no operator in the set N_{ij} that can shift λ_{m-1} into λ_{m-1}', the corresponding N-factor is defined as zero.

The first condition, eq. (58), may easily be shown to hold, since the action of operators P is multiplicity free, and represents in fact another form of the WE theorem. The second condition, eq. (59), on the other hand, represents a new requirement and cannot be proved using the WE theorem, since there are two zero-shift adjoint tensors when $\lambda_{m-1} = \lambda_{m-1}'$. Indeed, according to the WE theorem, the right-hand side of eq. (59) should involve a sum over MEs of both $N_{ij}^{(0)}$ and E_{ij}, so that the validity of the second condition, eq. (59), may only be fulfilled if we can define $N_{ij}^{(0)}$ in such a way that the E_{ij} and $N_{ij}^{(\kappa)}$ MEs are independently determined. Unfortunately, there is no general theorem that would ascertain the existence of such a factorization. We have thus proceeded in such a way that we first derived the form of the scalar factors η using special cases in which the above conjecture is fulfilled. Of course, the N_{ij} operators are not uniquely determined by conditions (58) and (59), since any constant multiple of N_{ij}'s or, equivalently, of irrep dependent scalar factors η, will also satisfy these conditions, although with different N and N–p factors. We may thus exploit this freedom to obtain N and N–p factors that are as simple as possible and satisfy the desirable symmetry properties. In this search for optimal η factors it is important to realize that while the non-zero shift tensors $N_{ij}^{(+)}$ and $N_{ij}^{(-)}$ are essentially unique (except for the adjustable factors $\eta^{(+)}(b)$ and $\eta^{(-)}(b)$, respectively, that may be chosen in an optimal way just mentioned), this is not the case for the zero-shift tensor $N_{ij}^{(0)}$ that is essentially determined by the ratio of $\eta_2^{(0)}(b)$ and $\eta_1^{(0)}(b)$. The overall scaling factor may then again be chosen in such a way that symmetric and simple N and N–p factors result.

Following this procedure, we arrived to the following optimal form for the irrep dependent scalar factors η:

$$\begin{aligned}\eta^{(+)}(b-1) &= \sqrt{\frac{b+2}{b+1}} = \eta^{(-)}(b+1),\\ \eta_1^{(0)}(b) &= \sqrt{\frac{b+2}{2b}} = -\left[2\eta_2^{(0)}(b)\right]^{-1}.\end{aligned} \tag{60}$$

Defining, thus, the $N_{ij}^{(\kappa)}$ operators acting on an (a,b) irrep module as follows

$$N_{ij}^{(+)} = \sqrt{\frac{b+3}{b+2}}\, C_i^{1\dagger} C_j^2\,, \tag{61a}$$

$$N_{ij}^{(0)} = (1-\delta_{b,0})\left(\sqrt{\frac{b+2}{2b}}\, C_i^{1\dagger} C_j^1 - \sqrt{\frac{b}{2(b+2)}}\, C_i^{2\dagger} C_j^2\right), \tag{61b}$$

$$N_{ij}^{(-)} = \sqrt{\frac{b+1}{b}}\, C_i^{2\dagger} C_j^1\,, \tag{61c}$$

we were able to show that eqs. (58) and (59) are satisfied in all possible cases, thus proving our conjecture for the case of two-column irreps. At the same time, we derived explicit expressions for the N and N–p connecting factors.

To illustrate this procedure, let us first consider the MEs of an operator $\tilde{N}_{ij}^{(+)} = C_i^{1\dagger} C_j^2$ in the U(m) basis with $m > i,j$. Taking $\lambda_m = (a,b)$, so that $\lambda'_m = (a-1, b+2)$, and using the resolution of the identity, we can write

$$\Theta \equiv \left\langle \begin{matrix}(a-1,b+2)\\ W'_m\end{matrix} \middle| \tilde{N}_{ij}^{(+)} \middle| \begin{matrix}(a,b)\\ W_m\end{matrix} \right\rangle = \sum_{U_m} \left\langle \begin{matrix}(a-1,b+2)\\ W'_m\end{matrix} \middle| C_i^{1\dagger} \middle| \begin{matrix}(a-1,b+1)\\ U_m\end{matrix} \right\rangle \times \left\langle \begin{matrix}(a-1,b+1)\\ U_m\end{matrix} \middle| C_j^2 \middle| \begin{matrix}(a,b)\\ W_m\end{matrix} \right\rangle. \tag{62}$$

The sum over U_m is obviously equivalent to the sum over μ_{m-1} and U_{m-1}, μ_{m-1} being the U($m-1$) irrep label for the intermediate configuration $|U_m\rangle$. Since $i,j<m$, the occupancy of the mth orbital must be the same in the bra and in the ket,

i.e. in W'_m and W_m. Assuming that this orbital is singly occupied and m appears in the second column of both W'_m and W_m (other cases may be treated in a similar way), we have that $\lambda'_{m-1} = (a-2, b+3)$ and $\lambda_{m-1} = (a-1, b+1)$. Then the only possible value for μ_{m-1} is $(a-2, b+2)$, so that relying on eq. (25) and factorization of CG coefficients in terms of isoscalar factors (see Part I and eq. (24)), we get

$$\begin{aligned}\Theta &= \left(\begin{matrix}(a-1,b+1) & (0,1) \\ (a-2,b+2) & (0,1)\end{matrix}\middle|\begin{matrix}(a-1,b+2) \\ (a-2,b+3)\end{matrix}\right)^{(s)} \\ &\times \left(\begin{matrix}(a-1,b+1) & (0,1) \\ (a-2,b+2) & (0,1)\end{matrix}\middle|\begin{matrix}(a,b) \\ (a-1,b+1)\end{matrix}\right)^{(s)} \\ &\times \sum_{U_{m-1}} \left\langle \begin{matrix}(a-2,b+3) \\ W'_{m-1}\end{matrix}\middle| C_i^{1\dagger} \middle| \begin{matrix}(a-2,b+2) \\ U_{m-1}\end{matrix}\right\rangle \\ &\times \left\langle \begin{matrix}(a-2,b+2) \\ U_{m-1}\end{matrix}\middle| C_j^{2} \middle| \begin{matrix}(a-1,b+1) \\ W_{m-1}\end{matrix}\right\rangle \\ &= \frac{\sqrt{(b+2)(b+4)}}{b+3}(-1)\left\langle \begin{matrix}(a-2,b+3) \\ W'_{m-1}\end{matrix}\middle| C_i^{1\dagger} C_j^{2} \middle| \begin{matrix}(a-1,b+1) \\ W_{m-1}\end{matrix}\right\rangle, \end{aligned} \tag{63}$$

where we used the explicit form of scaled isoscalar factors (see table 1) in the last step and deleted the sum over intermediate states at the $\mathrm{U}(m-1)$ level. The resulting factor $-[(b+2)(b+4)]^{1/2}/(b+3)$ thus represents the N-factor for the choice $\eta^{(+)}(b) = 1$. Using the properly scaled definition (61a) we thus get

$$\begin{aligned}&\left\langle \begin{matrix}(a-1,b+2) \\ (a-2,b+3)\end{matrix}\middle| N \middle| \begin{matrix}(a,b) \\ (a-1,b+1)\end{matrix}\right\rangle \\ &= \sqrt{\frac{b+3}{b+2}}\left(-\frac{\sqrt{(b+2)(b+4)}}{b+3}\right)\sqrt{\frac{b+3}{b+4}} = -1, \end{aligned} \tag{64}$$

since the operator $C_i^{1\dagger} C_j^2$ on the right-hand side of eq. (63) must be replaced by $\sqrt{(b+4)/(b+3)}\,C_i^{1\dagger} C_j^2$ (it now acts on the irrep $(a-1, b+1)$). We also see that the chosen scaling simplifies the resulting N-factor. It is worth emphasizing that the choice given by eqs. (60) and (61) was made after we examined all relevant cases as well as MEs of spin-dependent operators that will be the subject of future communications.

To illustrate the choice for the ratio of $\eta_2^{(0)}(b)$ and $\eta_1^{(0)}(b)$, we now choose the same irrep at the $\mathrm{U}(m-1)$ level in the matrix element Θ, eq. (62), ie. $\lambda'_{m-1} = \lambda_{m-1} = (a-1, b+1)$, which implies that m is singly occupied in the first column of W'_m and the second column of W_m. With this choice, the irrep μ_{m-1} can take on two distinct values, namely $(a-1, b)$ and $(a-2, b+2)$. Expressing again the MEs of C operators as a product of the $\mathrm{U}(m) \supset \mathrm{U}(m-1)$ isoscalar factor and $\mathrm{U}(m-1)$ ME, we can write

$$\Theta \equiv \sqrt{\frac{b+3}{b+2}} \Bigg\{ \begin{pmatrix} (a-1,b+1) & (0,1) & (a-1,b+2) \\ (a-1,b) & (0,1) & (a-1,b+1) \end{pmatrix}^{(s)}$$
$$\times \begin{pmatrix} (a-1,b+1) & (0,1) & (a,b) \\ (a-1,b) & (0,1) & (a-1,b+1) \end{pmatrix}^{(s)}$$
$$\times \sum_{U_{m-1}} \left\langle \begin{matrix} (a-1,b+1) \\ W'_{m-1} \end{matrix} \middle| C_i^{1\dagger} \middle| \begin{matrix} (a-1,b) \\ U_{m-1} \end{matrix} \right\rangle \left\langle \begin{matrix} (a-1,b) \\ U_{m-1} \end{matrix} \middle| C_j^{1} \middle| \begin{matrix} (a-1,b+1) \\ W_{m-1} \end{matrix} \right\rangle$$
$$+ \begin{pmatrix} (a-1,b+1) & (0,1) & (a-1,b+2) \\ (a-2,b+2) & (0,1) & (a-1,b+1) \end{pmatrix}^{(s)}$$
$$\times \begin{pmatrix} (a-1,b+1) & (0,1) & (a,b) \\ (a-2,b+2) & (0,1) & (a-1,b+1) \end{pmatrix}^{(s)}$$
$$\times \sum_{V_{m-1}} \left\langle \begin{matrix} (a-1,b+1) \\ W'_{m-1} \end{matrix} \middle| C_i^{2\dagger} \middle| \begin{matrix} (a-2,b+2) \\ V_{m-1} \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} (a-2,b+2) \\ V_{m-1} \end{matrix} \middle| C_j^{2} \middle| \begin{matrix} (a-1,b+1) \\ W_{m-1} \end{matrix} \right\rangle \Bigg\} . \tag{65}$$

The sums over U_{m-1} and V_{m-1} result in MEs of $C_i^{1\dagger} C_j^1$ and $C_i^{2\dagger} C_j^2$ operators, so that using the explicit form of the isoscalar factors (table 1) we get

$$\Theta = \sqrt{\frac{b+3}{b+2}} (-1) \frac{1}{b+1}$$
$$\times \left\langle \begin{matrix} (a-1,b+1) \\ W'_{m-1} \end{matrix} \middle| C_i^{1\dagger} C_j^1 - \frac{b+1}{b+3} C_i^{2\dagger} C_j^2 \middle| \begin{matrix} (a-1,b+1) \\ W_{m-1} \end{matrix} \right\rangle . \tag{66}$$

Thus, in order that the second factorization, eq. (59), holds, it is necessary that we choose for the ratio of $\eta_2^{(0)}$ and $\eta_1^{(0)}$ the value

$$\eta_2^{(0)}(b)/\eta_1^{(0)}(b) = -b/(b+2) , \tag{67}$$

assuming that the operators act on the irrep module (a,b) (note that in eq. (66) the operators are acting on the $(a-1,b+1)$ irrep module). Thus, with the definition of $N_{ij}^{(0)}$, eq. (61b), we find for the relevant N-factor the value

$$\left\langle \begin{matrix} (a-1,b+2) \\ (a-1,b+1) \end{matrix} \middle| N \middle| \begin{matrix} (a,b) \\ (a-1,b+1) \end{matrix} \right\rangle = \sqrt{\frac{b+3}{b+2}} (-1) \frac{1}{b+1} \sqrt{\frac{2(b+1)}{b+3}}$$
$$= -\left[\frac{2}{(b+1)(b+2)} \right]^{1/2} . \tag{68}$$

This calculation may be easily repeated for other cases. Remarkably enough, we always get the same value, eq. (67), for the ratio of $\eta_2^{(0)}$ and $\eta_1^{(0)}$ when acting on the (a,b) irrep module. For example, considering the $N_{ij}^{(-)}$ ME with $\lambda'_m = (a+1, b-2)$, $\lambda_m = (a,\ b)$, $\lambda'_{m-1} = \lambda_{m-1} = (a,\ b-1)$, we get for this ratio the value

$-(b-1)/(b+1)$, since the operators are now acting on the $(a,b-1)$ module. We can thus verify that the operators $N_{ij}^{(\kappa)}$ defined by eqs. (61) do indeed satisfy condition (59) in all possible cases. At the same time we obtain explicit values for nonvanishing N-factors that are collected in table 5 and possess the following symmetry property

$$\left\langle \begin{matrix} \lambda' \\ \lambda \end{matrix} \middle| N \middle| \begin{matrix} \nu' \\ \nu \end{matrix} \right\rangle = \left\langle \begin{matrix} \nu' \\ \nu \end{matrix} \middle| N \middle| \begin{matrix} \lambda' \\ \lambda \end{matrix} \right\rangle . \tag{69}$$

In a similar way we can derive explicit expressions for the N–$C^\dagger$, N–C and N–0 connecting factors: we simply take $m = r = \max\{i,j\}$ and consider all possible occupancies of the rth level. These connecting factors are essentially given by the product of two scaled isoscalar factors for vector operators in which at least one of the two (0, 1) irreps reduces to the scalar (0, 0) irrep. We find that these factors satisfy the following symmetry properties

$$\left\langle \begin{matrix} \lambda' \\ \lambda \end{matrix} \middle| N \middle| \begin{matrix} \nu' \\ \nu \end{matrix} \right\rangle_0 = \left\langle \begin{matrix} \nu' \\ \nu \end{matrix} \middle| N \middle| \begin{matrix} \lambda' \\ \lambda \end{matrix} \right\rangle_0 = \delta_{\lambda\nu} \left\langle \begin{matrix} \lambda' \\ \lambda \end{matrix} \middle| N \middle| \begin{matrix} \nu' \\ \lambda \end{matrix} \right\rangle_0 , \tag{70a}$$

and

$$\left\langle \begin{matrix} \lambda' \\ \lambda \end{matrix} \middle| N \middle| \begin{matrix} \nu' \\ \nu \end{matrix} \right\rangle_C = \left\langle \begin{matrix} \nu' \\ \nu \end{matrix} \middle| N \middle| \begin{matrix} \lambda' \\ \lambda \end{matrix} \right\rangle_{C^\dagger} . \tag{70b}$$

Table 5
N factors $\left\langle \begin{matrix} \lambda' \\ \lambda \end{matrix} \middle| N \middle| \begin{matrix} (a,b) \\ \nu \end{matrix} \right\rangle$, required for MEs of N operators. The unnecessary $(1-\delta_{b,0})$ factors are omitted.

λ'	λ	ν	N
$(a-1,b+2)$	$(a-2,b+2)$	$(a-1,b)$	1
	$(a-1,b+1)$	$(a,b-1)$	$-[b(b+3)/(b+1)(b+2)]^{1/2}$
	$(a-1,b+1)$	$(a-1,b+1)$	$-[2/(b+1)(b+2)]^{1/2}$
	$(a-2,b+3)$	$(a-1,b+1)$	-1
(a,b)	$(a-1,b)$	$(a-1,b)$	$1-\delta_{b,0}$
	$(a,b-1)$	$(a,b-1)$	$[(b-1)(b+2)/b(b+1)]^{1/2}$
	$(a,b-1)$	$(a-1,b+1)$	$-[2/(b+1)(b+2)]^{1/2}$
	$(a-1,b+1)$	$(a,b-1)$	$-[2/(b+1)(b+2)]^{1/2}$
	$(a-1,b+1)$	$(a-1,b+1)$	$[b(b+3)/(b+1)(b+2)]^{1/2}$
$(a+1,b-2)$	$(a,b-2)$	$(a-1,b)$	1
	$(a+1,b-3)$	$(a,b-1)$	$-[(b-2)(b+1)/(b-1)b]^{1/2}$
	$(a,b-1)$	$(a,b-1)$	$-[2/(b-1)b]^{1/2}$
	$(a,b-1)$	$(a-1,b+1)$	-1

Table 6
N–0 connecting factors $\left\langle \begin{matrix} \lambda' \\ \lambda \end{matrix} \middle| N \middle| \begin{matrix} (a,b) \\ \lambda \end{matrix} \right\rangle_0$. (Unnecessary $(1-\delta_{b,0})$ factor is omitted.) The symbol $\{x/y\}$ is defined in eq. (71).

λ'	λ	N–0
$(a-1,b+2)$	$(a-1,b+1)$	$\{3/2\}$
(a,b)	$(a-1,b)$	0
	$(a,b-1)$	$\{2/0\}/\sqrt{2}$
	$(a-1,b+1)$	$-\{0/2\}/\sqrt{2}$
	(a,b)	0
$(a+1,b-2)$	$(a,b-1)$	$\{1/0\}$

Their explicit values are collected in tables 6 and 7. Here and in the following it is convenient to define the symbol (cf. ref. [37])

$$\{k/l\} \equiv \sqrt{\frac{b+k}{b+l}}, \tag{71}$$

which enables a more compact representation of the resulting connecting factors (corresponding to the segment values of refs. [4,37] or ref. [11]) and is used in tables 6, 7, 9, 10, 12 and 13.

In summary, applying successively our factorization rules, eqs. (58) and (59), the MEs of $N_{ij}^{(\kappa)}$, $(\kappa = +, 0, -)$ tensors, eqs. (61), may be expressed as a single product of level segment values. Proceeding from the top level downwards, these segment values are given, respectively, by the N-factors (from the top level n to the turning level r), an N–$(C^\dagger, C, 0)$ connecting factor at level r, and vector operator scaled isoscalar factors for levels below r. When $i = j$, no segment values are needed for levels below r. Thus, for example, when $i<j = r$, we have that

Table 7
N–$C^\dagger$ connecting factors $\left\langle \begin{matrix} \lambda' \\ \lambda \end{matrix} \middle| N \middle| \begin{matrix} (a,b) \\ \nu \end{matrix} \right\rangle_{C^\dagger}$. (Unnecessary $(1-\delta_{b,0})$ factor is omitted.) The symbol $\{x/y\}$ is defined in eq. (71).

λ'	λ	ν	N–$C^\dagger$
$(a-1,b+2)$	$(a-1,b+1)$	$(a-1,b)$	$-\{3/1\}$
	$(a-1,b+2)$	$(a-1,b+1)$	$\{3/2\}$
(a,b)	$(a,b-1)$	$(a-1,b)$	$-\{2/1\}/\sqrt{2}$
	$(a-1,b+1)$	$(a-1,b)$	$\{0/1\}/\sqrt{2}$
	(a,b)	$(a,b-1)$	$\{2/0\}/\sqrt{2}$
	(a,b)	$(a-1,b+1)$	$-\{0/2\}/\sqrt{2}$
$(a+1,b-2)$	$(a,b-1)$	$(a-1,b)$	-1
	$(a+1,b-2)$	$(a,b-1)$	$\{1/0\}$

$$\left\langle \begin{matrix} \lambda_n' \\ W_n' \end{matrix} \middle| N_{ij}^{(\kappa)} \middle| \begin{matrix} \lambda_n \\ W_n \end{matrix} \right\rangle = \left\{ \prod_{k=j+1}^{n} \left\langle \begin{matrix} \lambda_k' \\ \lambda_{k-1}' \end{matrix} \middle| N \middle| \begin{matrix} \lambda_k \\ \lambda_{k-1} \end{matrix} \right\rangle \right\} \left\langle \begin{matrix} \lambda_j' \\ \lambda_{j-1}' \end{matrix} \middle| N \middle| \begin{matrix} \lambda_j \\ \lambda_{j-1} \end{matrix} \right\rangle_{C^\dagger}$$
$$\times \left\{ \prod_{k=i+1}^{j-1} \left(\begin{matrix} \lambda_k & (0,1) \\ \lambda_{k-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda_k' \\ \lambda_{k-1}' \end{matrix} \right)^{(s)} \right\} \left(\begin{matrix} \lambda_i & (0,1) \\ \lambda_{i-1} & (0,0) \end{matrix} \middle| \begin{matrix} \lambda_i' \\ \lambda_{i-1}' \end{matrix} \right)^{(s)} \prod_{k=1}^{i-1} \delta_{\lambda_k' \lambda_k} . \quad (72)$$

To conclude this section, we express the $C_i^{\sigma\dagger} C_j^{\tau}$ tensors in terms of the E_{ij} and $N_{ij}^{(\kappa)}$ operators. Inverting eqs. (56) and (61) we get

$$C_i^{1\dagger} C_j^2 = \sqrt{\frac{b+2}{b+3}}\, N_{ij}^{(+)} , \quad (73a)$$

$$C_i^{2\dagger} C_j^1 = \sqrt{\frac{b}{b+1}}\, N_{ij}^{(-)} , \quad (73b)$$

$$C_i^{1\dagger} C_j^1 = \frac{b}{2(b+1)} E_{ij} + \frac{1}{b+1} \sqrt{\frac{b(b+2)}{2}}\, N_{ij}^{(0)} , \quad (73c)$$

$$C_i^{2\dagger} C_j^2 = \frac{b+2}{2(b+1)} E_{ij} - \frac{1}{b+1} \sqrt{\frac{b(b+2)}{2}}\, N_{ij}^{(0)} . \quad (73d)$$

Hence, the MEs of $C_i^{1\dagger} C_j^2$ and $C_i^{2\dagger} C_j^1$ operators are simply related with the MEs of $N_{ij}^{(+)}$ and $N_{ij}^{(-)}$ tensors, respectively, both given by a single product of segment values. The MEs of $C_i^{1\dagger} C_j^1$ and $C_i^{2\dagger} C_j^2$ operators, on the other hand, are given by the sum of two terms corresponding to the MEs of E_{ij} and $N_{ij}^{(0)}$ tensors, each of which is expressible as a single product of segment values.

7. Two-body operators

We now finally turn our attention to generator products that appear in the two-electron part of the electronic Hamiltonian. In fact, it is both more appropriate and simpler to directly consider the MEs of two-body operators $e_{ik;jl}$, whose second quantized form is

$$e_{ik;jl} = \sum_{m,m'=\alpha,\beta} X_{jm}^{\dagger} X_{im'}^{\dagger} X_{km'} X_{lm} , \quad (74)$$

with $X_{jm}^{\dagger}(X_{jm})$ designating the creation (annihilation) operator associated with the orthonormal spin orbital $|jm\rangle$. Expressing the two-body operators $e_{ik;jl}$ in terms of $U(n)$ generators, we get a product term as well as a linear correcting term, namely

$$e_{ik;jl} = E_{ik} E_{jl} - \delta_{jk} E_{il} , \quad (75)$$

as is well known [2,3]. Using the relationship between the $U(n)$ generators and our vector operators, eq. (56), we can write for the generator product

$$E_{ik}E_{jl} = \sum_{\sigma} E_{ik} C_j^{\sigma\dagger} C_l^{\sigma} = \sum_{\sigma} (C_j^{\sigma\dagger} E_{ik} + \delta_{jk} C_i^{\sigma\dagger}) C_l^{\sigma}$$
$$= \sum_{\sigma,\tau} C_j^{\sigma\dagger} C_i^{\tau\dagger} C_k^{\tau} C_l^{\sigma} + \delta_{jk} E_{il} , \tag{76}$$

where we have used property (15) in the second step. Thus, we have that

$$e_{ik;jl} \equiv E_{ik}E_{jl} - \delta_{jk}E_{il} = \sum_{\sigma,\tau} C_j^{\sigma\dagger} C_i^{\tau\dagger} C_k^{\tau} C_l^{\sigma} , \tag{77}$$

is complete analogy to the second quantized form, eq. (74). In fact, this correspondence may be extended to the general k-body case,

$$\sum_{\tau_1,\tau_2,\ldots,\tau_k} C_{i_1}^{\tau_1\dagger} C_{i_2}^{\tau_2\dagger} \ldots C_{i_k}^{\tau_k\dagger} C_{j_k}^{\tau_k} \ldots C_{j_2}^{\tau_2} C_{j_1}^{\tau_1}$$
$$= \sum_{m_1,m_2,\ldots,m_k} X_{i_1m_1}^{\dagger} X_{i_2m_2}^{\dagger} \ldots X_{i_km_k}^{\dagger} X_{j_km_k} \ldots X_{j_2m_2} X_{j_1m_1} , \tag{78}$$

where the right-hand side sum extends over all spins and the left-hand side one over operator patterns. This correspondence, eq. (78), may be easily proved since the second quantization operators $X^\dagger$ and X have the same properties as the vector operators $C^\dagger$ and C under the action of U(n) generators, namely

$$\left[E_{ij}, X_{km}^{\dagger}\right] = \delta_{jk} X_{im}^{\dagger}, \quad \left[E_{ij}, X_{km}\right] = -\delta_{ik} X_{jm}, \quad E_{ij} = \sum_m X_{im}^{\dagger} X_{jm} . \tag{79}$$

Consequently, both sides of the correspondence relationship, eq. (78), are identical when expressed in terms of U(n) generators. This correspondence enables us to express k-body operators in terms of U(n) tensors. We must, however, emphasize that this correspondence relationship expresses only a formal similarity between the vector operators $C^\dagger$, C and second quantization operators $X^\dagger$, X since they are defined in different groups: while the vector operators $C^\dagger$ and C act on the orbital group U(n) modules, the second quantization operators $X^\dagger$ and X act on the modules of the spin orbital group U($2n$). The real meaning of this correspondence, eq. (78), is that we can either couple the fundamental U(n) tensors $C^\dagger$ and C within the U(n) framework to obtain higher rank U(n) tensors, for example the two-body operators in eq. (77), or we can express these U(n) operators as spin contractions of U($2n$) operators, as in eq. (74).

The first step in evaluating the two-body MEs is to classify the operators $e_{ik;jl}$, as was first done by Paldus and Boyle [37]. Without restricting the generality of our considerations, we can assume that l is the largest label, i.e. $l = \max\{i,j,k,l\}$, since

$$e_{ik;jl} = e_{jl;ik} = e_{lj,ki}^{\dagger} = e_{ki,lj}^{\dagger} . \tag{80}$$

We also assume that none of the generators involved in the product is a weight generator, i.e. that $i \neq k$ and $j \neq l$, since this case reduces to a single generator case.

The possible cases that arise are listed in table 8, where we also indicate the relationship with the classification given by Paldus and Boyle [37]. Moreover, the first case, when there is no overlap of generator regions $[i,k]$ and $[j,l]$, also reduces to a single generator case, since the ME in this case equals a simple product of ME's of the generators involved. Finally, we recall that the irrep labels in the bra and the ket associated with the subgroups $U(m)$ with $m \geqslant l = \max\{i,j,k,l\}$ and $m < p \equiv \min\{i,j,k,l\}$ must be identical lest the ME vanish, i.e.

$$\left\langle \begin{matrix} \lambda \\ W' \end{matrix} \middle| e_{ik;jl} \middle| \begin{matrix} \lambda \\ W \end{matrix} \right\rangle = \left(\prod_{m=l}^{n} \delta_{\lambda'_m \lambda_m} \right) \left\langle \begin{matrix} \lambda_l \\ W'_l \end{matrix} \middle| e_{ik;jl} \middle| \begin{matrix} \lambda_l \\ W_l \end{matrix} \right\rangle \left(\prod_{m=1}^{p-1} \delta_{\lambda'_m \lambda_m} \right) . \tag{81}$$

In the following developments we shall thus assume this requirement to be satisfied so that we can evaluate the required MEs in the $U(l)$ basis.

The tensor operator formalism that we briefly outlined at the outset of this paper offers numerous possibilities for the evaluation of the required MEs. The most obvious procedure is to decompose the operator, whose matrix elements we wish to evaluate, into its irreducible components and apply the WE theorem. In the case of two-body operators (77) we can expect the resulting irreducible tensors to contain two $C^\dagger$-type and two C-type operators. We shall examine this possibility more closely in our future communication [46] dealing with spin-dependent operators when more general two-body operators (non spin-preserving) must be considered. In this paper we shall follow a simpler route expressing MEs of two-body operators in terms of MEs of various tensor operators considered in the preceding sections. We thus first establish the relationship between the $e_{ik;jl}$ operators and vector, symmetric, antisymmetric and adjoint tensors.

We start by examining the possibilities at the highest level $l \equiv \max\{i,j,k,l\}$. Since we exclude trivial weight generators ($i \neq k, j \neq l$), at most two labels can be identical, so that we must distinguish three cases, namely (i) $e_{ik;jl}$ with $i,j,k<l$, (ii) $e_{il;jl}$ and (iii) $e_{lk;jl}$, which we now consider in turn:

(i) The first possibility, $e_{ik;jl}$ $(i,j,k<l)$, arises in cases 2, 4 and 6 of table 8 (recall that case 1 of table 8 reduces to a simple product of single generator MEs and

Table 8
Classification of two-body operators $e_{ik;jl}$ and its relationship with the classification of Paldus and Boyle (PB) [37].

Case	Condition	PB [37]
1	$i<k<j<l$, $\quad k<i<j<l$	$a1, b1$
2	$k<i=j<l$, $\quad i<j=k<l$	$a2, b2$
3	$i \leqslant j<k=l$	$a6, a7$
4	$i \leqslant j<k<l$, $\quad j<i<k<l$	$a3, a4, a5$
5	$j \leqslant k<i=l$	$b6, b7$
6	$j \leqslant k<i<l$, $\quad k<j<i<l$	$b3, b4, b5$

need not be considered here). Using the definition of $e_{ik;jl}$ in terms of U(n) [or U(l)] generators, eq. (75), we can write

$$\langle e_{ik;jl}\rangle \equiv \left\langle \begin{matrix}\lambda_l\\ W_l'\end{matrix}\middle| e_{ik;jl} \middle| \begin{matrix}\lambda_l\\ W_l\end{matrix}\right\rangle = \sum_{\mu_l,U_l} \left\langle \begin{matrix}\lambda_l\\ W_l'\end{matrix}\middle| E_{ik} \middle| \begin{matrix}\mu_l\\ U_l\end{matrix}\right\rangle \left\langle \begin{matrix}\mu_l\\ U_l\end{matrix}\middle| E_{jl} \middle| \begin{matrix}\lambda_l\\ W_l\end{matrix}\right\rangle$$

$$- \delta_{jk} \left\langle \begin{matrix}\lambda_l\\ W_l'\end{matrix}\middle| E_{il} \middle| \begin{matrix}\lambda_l\\ W_l\end{matrix}\right\rangle, \tag{82}$$

where $\mu_l = \lambda_l$ and, moreover, $\mu_{l-1} = \lambda'_{l-1}$ since $i,k<l$. Reducing matrix elements of E_{jl} and E_{il} generators using eq. (30) and subsequently exploiting commutation relation (15),we get

$$\langle e_{ik;jl}\rangle = \left\langle \begin{matrix}\lambda_l\\ \lambda'_{l-1}\end{matrix}\middle| E \middle| \begin{matrix}\lambda_l\\ \lambda_{l-1}\end{matrix}\right\rangle \left\langle \begin{matrix}\lambda'_{l-1}\\ W'_{l-1}\end{matrix}\middle| G^{\sigma}_{j;ik} \middle| \begin{matrix}\lambda_{l-1}\\ W_{l-1}\end{matrix}\right\rangle, \tag{83}$$

where we defined a new operator

$$G^{\sigma}_{j;ik} = C^{\sigma\dagger}_j E_{ik}\,, \tag{83'}$$

with σ given by the irreps at the U($l-1$) level,

$$\lambda_{l-1} + \sigma = \lambda'_{l-1}\,. \tag{83''}$$

We thus find that the required ME $\langle e_{ik;jl}\rangle$ is given by the product of a generator RME for U(l) $\supset$ U($l-1$) and a ME of a G-type operator in the U($l-1$) basis. We now proceed with our examination of basic types at the lth level and will return to the evaluation of the G-type MEs later on (see also our work on spin-dependent operators [46]). Thus, the ME of $e_{ik;jl}$, eq. (82), may be expressed in the form

$$\langle e_{ik;jl}\rangle = \left\langle \begin{matrix}\lambda_l\\ \lambda'_{l-1}\end{matrix}\middle| e \middle| \begin{matrix}\lambda_l\\ \lambda_{l-1}\end{matrix}\right\rangle_G \left\langle \begin{matrix}\lambda'_{l-1}\\ W'_{l-1}\end{matrix}\middle| G^{\sigma}_{j;ik} \middle| \begin{matrix}\lambda_{l-1}\\ W_{l-1}\end{matrix}\right\rangle, \tag{84}$$

where we introduced the so-called e–G connecting factor

$$\left\langle \begin{matrix}\lambda_l\\ \lambda'_{l-1}\end{matrix}\middle| e \middle| \begin{matrix}\lambda_l\\ \lambda_{l-1}\end{matrix}\right\rangle_G \equiv \left\langle \begin{matrix}\lambda_l\\ \lambda'_{l-1}\end{matrix}\middle| E \middle| \begin{matrix}\lambda_l\\ \lambda_{l-1}\end{matrix}\right\rangle = \left\langle \begin{matrix}\lambda_l\\ \lambda'_{l-1}\end{matrix}\middle\| E \middle\| \begin{matrix}\lambda_l\\ \lambda_{l-1}\end{matrix}\right\rangle^{(s)}, \tag{85}$$

i.e. as a product of an e–G connecting factor for U(l) $\supset$ U($l-1$) levels and a ME of a G-operator in the U($l-1$) basis.

(ii) The second possibility, $e_{il;jl}$ $(i,j<l)$ arises in case 3 of table 8 and produces a vanishing ME unless l is doubly occupied in the ket and unoccupied in the bra. Setting $\lambda_l = (a,b)$ we can write

$$\langle e_{il;jl}\rangle \equiv \left\langle \begin{matrix}(a,b)\\ W_l'\end{matrix}\middle| e_{il;jl} \middle| \begin{matrix}(a,b)\\ W_l\end{matrix}\right\rangle$$

$$= \left\langle \begin{matrix}(a,b)\\ W_l'\end{matrix}\middle| C^{1\dagger}_i C^{2\dagger}_j C^2_l C^1_l + C^{2\dagger}_i C^{1\dagger}_j C^1_l C^2_l \middle| \begin{matrix}(a,b)\\ W_l\end{matrix}\right\rangle, \tag{86}$$

since the shift labels of two C_l operators cannot be the same. Employing, thus, eqs. (53) and subsequently using eq. (50) we finally get

$$\begin{aligned}\langle e_{il;jl}\rangle &= \left\langle \begin{matrix}(a,b)\\ W'_{l-1}\end{matrix} \middle| \sqrt{\frac{b}{b+1}}C_i^{1\dagger}C_j^{2\dagger} + \sqrt{\frac{b+2}{b+1}}C_i^{2\dagger}C_j^{1\dagger} \middle| \begin{matrix}(a-1,b)\\ W_{l-1}\end{matrix}\right\rangle \\ &= (1+\delta_{ij})^{1/2}\left\langle \begin{matrix}(a-1,b) & (1,0)\\ W_{l-1} & [ij]\end{matrix} \middle| \begin{matrix}(a,b)\\ W'_{l-1}\end{matrix}\right\rangle^{(s)} \\ &\equiv \left\langle \begin{matrix}(a,b)\\ (a,b)\end{matrix} \middle| e \middle| \begin{matrix}(a,b)\\ (a-1,b)\end{matrix}\right\rangle_S \left\langle \begin{matrix}(a-1,b) & (1,0)\\ W_{l-1} & [ij]\end{matrix} \middle| \begin{matrix}(a,b)\\ W'_{l-1}\end{matrix}\right\rangle^{(s)}, \end{aligned} \tag{87}$$

where, for the sake of consistency, we introduced in the last step the e–S connecting factor (S stands for a symmetric tensor), given by $(1+\delta_{ij})^{1/2}$. Note that the contribution from the antisymmetric tensor cancels out, so that formally

$$\left\langle \begin{matrix}(a,b)\\ (a,b)\end{matrix} \middle| e \middle| \begin{matrix}(a,b)\\ (a-1,b)\end{matrix}\right\rangle_S = (1+\delta_{ij})^{1/2}, \quad \left\langle \begin{matrix}(a,b)\\ (a,b)\end{matrix} \middle| e \middle| \begin{matrix}(a,b)\\ (a-1,b)\end{matrix}\right\rangle_A = 0. \tag{88}$$

(iii) In the last case, $e_{lk;jl}$ $(j,k<l)$, corresponding to case 5 of table 8, we can write

$$e_{lk;jl} = \sum_\sigma C_j^{\sigma\dagger} E_{lk} C_l^\sigma, \tag{89}$$

so that

$$\begin{aligned}\langle e_{lk;jl}\rangle &\equiv \left\langle \begin{matrix}\lambda_l\\ W'_l\end{matrix} \middle| e_{lk;jl} \middle| \begin{matrix}\lambda_l\\ W_l\end{matrix}\right\rangle \\ &= \sum_{\sigma,\mu_l,U_l,V_l} \left\langle \begin{matrix}\lambda_l\\ W'_l\end{matrix} \middle| C_j^{\sigma\dagger} \middle| \begin{matrix}\mu_l\\ U_l\end{matrix}\right\rangle \left\langle \begin{matrix}\mu_l\\ U_l\end{matrix} \middle| E_{lk} \middle| \begin{matrix}\mu_l\\ V_l\end{matrix}\right\rangle \left\langle \begin{matrix}\mu_l\\ V_l\end{matrix} \middle| C_l^{\sigma} \middle| \begin{matrix}\lambda_l\\ W_l\end{matrix}\right\rangle \\ &= \sum_{\sigma,U_l} \left\langle \begin{matrix}\lambda_l\\ W'_l\end{matrix} \middle| C_j^{\sigma\dagger} \middle| \begin{matrix}\mu_l\\ U_l\end{matrix}\right\rangle \left\langle \begin{matrix}\mu_l\\ U_l\end{matrix} \middle| E_{lk} \middle| \begin{matrix}\mu_l\\ V_l\end{matrix}\right\rangle \left(\begin{matrix}\mu_l & (0,1)\\ \lambda_{l-1} & (0,0)\end{matrix} \middle| \begin{matrix}\lambda_l\\ \lambda_{l-1}\end{matrix}\right)^{(s)}, \end{aligned} \tag{90}$$

where $V_{l-1} = W_{l-1}$ and $\mu_l = \lambda_l - \sigma$. In the last step we employed eq. (25′) at the U(l) level. Employing, next, eqs. (30), (32) and (27) for the generator matrix elements and eq. (25″) with $n = l$ for the vector operator matrix elements, we find that the ME (90) reduces to

$$\begin{aligned}\langle e_{lk;jl}\rangle = &\sum_{\sigma,\tau} \left(\begin{matrix}\lambda_l-\sigma & (0,1)\\ \lambda'_{l-1}-\tau & (0,1)\end{matrix} \middle| \begin{matrix}\lambda_l\\ \lambda'_{l-1}\end{matrix}\right)^{(s)} \left\langle \begin{matrix}\lambda_l-\sigma\\ \lambda_{l-1}\end{matrix} \middle\| E \middle\| \begin{matrix}\lambda_l-\sigma\\ \lambda'_{l-1}-\tau\end{matrix}\right\rangle \\ &\times \left(\begin{matrix}\lambda_l-\sigma & (0,1)\\ \lambda_{l-1} & (0,0)\end{matrix} \middle| \begin{matrix}\lambda_l\\ \lambda_{l-1}\end{matrix}\right)^{(s)} \left\langle \begin{matrix}\lambda'_{l-1}\\ W'_{l-1}\end{matrix} \middle| C_j^{\tau\dagger} C_k^{\rho} \middle| \begin{matrix}\lambda_{l-1}\\ W_{l-1}\end{matrix}\right\rangle, \end{aligned} \tag{91}$$

where $\rho = \lambda_{l-1} - \lambda'_{l-1} + \tau$. We can then express the ME of $C_j^{\tau\dagger} C_k^\rho$ in terms of MEs of E_{jk} and $N_{jk}^{(\kappa)}$ tensors using eqs. (73a)–(73d), so that we can finally write

$$\langle e_{lk;jl}\rangle = \left\langle \begin{matrix}\lambda_l\\ \lambda'_{l-1}\end{matrix}\middle| e \middle| \begin{matrix}\lambda_l\\ \lambda_{l-1}\end{matrix}\right\rangle_E \left\langle \begin{matrix}\lambda'_{l-1}\\ W'_{l-1}\end{matrix}\middle| E_{jk} \middle| \begin{matrix}\lambda_{l-1}\\ W_{l-1}\end{matrix}\right\rangle + \left\langle \begin{matrix}\lambda_l\\ \lambda'_{l-1}\end{matrix}\middle| e \middle| \begin{matrix}\lambda_l\\ \lambda_{l-1}\end{matrix}\right\rangle_N \left\langle \begin{matrix}\lambda'_{l-1}\\ W'_{l-1}\end{matrix}\middle| N_{jk}^{(\kappa)} \middle| \begin{matrix}\lambda_{l-1}\\ W_{l-1}\end{matrix}\right\rangle, \tag{92}$$

where $\kappa = +, 0$ or $-$ is uniquely fixed by the irreps λ_{l-1} and λ'_{l-1} (in fact, for $\rho - \tau = \lambda_{l-1} - \lambda'_{l-1} = 1, \kappa = +$, for $\rho - \tau = -1, \kappa = -$ and for $\rho = \tau, \kappa = 0$; recall that for the shift labels σ, τ, ρ we use the convention that $\sigma = 1 \equiv (0,1)$ and $\sigma = 2 \equiv (1,-1)$). Thus, the *e–E* and *e–N* connecting factors depend on two isoscalar factors and an RME appearing in eq. (91) as well as on the coefficients relating the adjoint tensor components with E_{ij} and $N_{ij}^{(\kappa)}$ tensors, eq. (73a)–(73d). It must be remembered that the latter coefficients are irrep label dependent. We have collected all the relevant *e–E* and *e–N* factors in table 9.

To illustrate how the results listed in table 9 may be easily derived, we provide an example. Clearly, in this case, the lth orbital must have the same occupancy in the bra and in the ket. We set $\lambda_l = (a,b)$ and assume, for example, that the lth level is singly occupied in the first column of both W_l and W'_l, so that $\lambda_{l-1} = \lambda'_{l-1} = (a, b-1)$. Then the second isoscalar factor on the right-hand side of eq. (91) vanishes unless $\sigma = 1$, in which case $\lambda_l - \sigma = (a, b-1)$. Further, since $\lambda_{l-1} = \lambda'_{l-1}$, we have that $\rho = \tau$ and thus for $\rho = \tau = 1$ we find that $\lambda'_{l-1} - \tau = (a, b-2)$ while for $\rho = \tau = 2$ we have $\lambda'_{l-1} - \tau = (a-1, b)$. Finding the appropriate values for the resulting isoscalar factors from table 1 and of the corresponding RMEs from table 2, eq. (91) yields in this case

$$\left\langle \begin{matrix}(a,b)\\ (a,b-1)\\ W'_{l-1}\end{matrix}\middle| e_{lk;jl} \middle| \begin{matrix}(a,b)\\ (a,b-1)\\ W_{l-1}\end{matrix}\right\rangle = -\left\langle \begin{matrix}(a,b-1)\\ W'_{l-1}\end{matrix}\middle| C_j^{1\dagger}C_k^1 + \frac{1}{b+1} C_j^{2\dagger}C_k^2 \middle| \begin{matrix}(a,b-1)\\ W_{l-1}\end{matrix}\right\rangle . \tag{93}$$

Table 9
e–E and *e–N* connecting factors $\left\langle \begin{matrix}(a,b)\\ \lambda\end{matrix}\middle| e \middle| \begin{matrix}(a,b)\\ \nu\end{matrix}\right\rangle_{E,N}$, providing top segment value at level $i = l(>j,k)$ for the evaluation of $e_{ik;jl}$ MEs in terms of MEs of E_{jk} and $N_{jk}^{(\kappa)}$ operators. Notation of eq. (71) is employed.

λ	ν	*e–E*	*e–N*	κ
(a,b)	(a,b)	0	0	0
$(a,b-1)$	$(a,b-1)$	$-1/2$	$-\{-1/1\}/\sqrt{2}$	0
$(a-1,b+1)$	$(a-1,b+1)$	$-1/2$	$\{3/1\}/\sqrt{2}$	0
$(a,b-1)$	$(a-1,b+1)$	0	$\{0/1\}$	$-$
$(a-1,b+1)$	$(a,b-1)$	0	$\{0/1\}$	$+$
$(a-1,b)$	$(a-1,b)$	-1	0	0

Recalling (eqs. (73c), (73d)) that

$$C_j^{1\dagger} C_k^1 = \frac{b-1}{2b} E_{jk} + \frac{1}{b}\sqrt{\frac{(b-1)(b+1)}{2}}\, N_{jk}^{(0)}\,, \tag{94a}$$

and

$$C_j^{2\dagger} C_k^2 = \frac{b+1}{2b} E_{jk} - \frac{1}{b}\sqrt{\frac{(b-1)(b+1)}{2}}\, N_{jk}^{(0)}\,, \tag{94b}$$

when acting on the $(a, b-1)$ irrep module, we finally find that

$$\left\langle \begin{matrix} (a,b) \\ (a,b-1) \\ W'_{l-1} \end{matrix} \middle| e_{lk;jl} \middle| \begin{matrix} (a,b) \\ (a,b-1) \\ W_{l-1} \end{matrix} \right\rangle = -\frac{1}{2}\left\langle \begin{matrix} (a,b-1) \\ W'_{l-1} \end{matrix} \middle| E_{jk} \middle| \begin{matrix} (a,b-1) \\ W_l \end{matrix} \right\rangle$$
$$- \sqrt{\frac{b-1}{2(b+1)}}\left\langle \begin{matrix} (a,b-1) \\ W'_{l-1} \end{matrix} \middle| N_{jk}^{(0)} \middle| \begin{matrix} (a,b-1) \\ W_l \end{matrix} \right\rangle, \tag{95}$$

yielding immediately the e–E and e–N factors (as well as κ) listed in the second row of table 9. Other cases are treated in an analogous way. It is worth noting that the e–E and e–N connecting factors are symmetric

$$\left\langle \begin{matrix} \lambda \\ \mu \end{matrix} \middle| e \middle| \begin{matrix} \lambda \\ \nu \end{matrix} \right\rangle_X = \left\langle \begin{matrix} \lambda \\ \nu \end{matrix} \middle| e \middle| \begin{matrix} \lambda \\ \mu \end{matrix} \right\rangle_X, \quad X = E, N \tag{96}$$

as follows from table 9.

We now return to the evaluation of G-type MEs that are required in case (i) above, eq. (84). Introducing again the resolution of the identity,

$$\langle G_{j;ik}^{\sigma} \rangle \equiv \left\langle \begin{matrix} \lambda'_{l-1} \\ W'_{l-1} \end{matrix} \middle| G_{j;ik}^{\sigma} \middle| \begin{matrix} \lambda_{l-1} \\ W_{l-1} \end{matrix} \right\rangle$$
$$= \sum_{\mu_{l-1}, U_{l-1}} \left\langle \begin{matrix} \lambda'_{l-1} \\ W'_{l-1} \end{matrix} \middle| C_j^{\sigma\dagger} \middle| \begin{matrix} \mu_{l-1} \\ U_{l-1} \end{matrix} \right\rangle \left\langle \begin{matrix} \mu_{l-1} \\ U_{l-1} \end{matrix} \middle| E_{ik} \middle| \begin{matrix} \lambda_{l-1} \\ W_{l-1} \end{matrix} \right\rangle,$$

we see immediately that we must have that $\mu_m = \lambda_m$ for $m = l-1, l-2, \ldots, s$ where $s = \max\{i,k\}$. In fact, it is convenient to choose $r = \max\{i,j,k\} \geqslant s$ and to reduce the right-hand side MEs to the $U(r)$ basis. This is easily achieved realizing that the E_{ik} MEs are the same in both $U(l-1)$ and $U(r)$ (in fact $U(s)$) bases, while stepping down each level in the MEs of $C_j^{\sigma\dagger}$ introduces an appropriate isoscalar factor, eq. (25″), so that

$$\langle G_{j;ik}^{\sigma} \rangle = \prod_{m=r+1}^{l-1} \left(\begin{matrix} \lambda_m & (0,1) \\ \lambda_{m-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda'_m \\ \lambda'_{m-1} \end{matrix} \right)^{(s)} \left\langle \begin{matrix} \lambda'_r \\ W'_r \end{matrix} \middle| G_{j;ik}^{\sigma} \middle| \begin{matrix} \lambda_r \\ W_r \end{matrix} \right\rangle,$$
$$r = \max\{i,j,k\}\,. \tag{97}$$

After the rth level, only MEs of simpler tensors, that were considered earlier, can appear. Four cases may arise at this step that we now consider in turn (we again ignore the trivial case when there is no overlap of generator regions):

(a) When $k<i=j=r, r=\max\{i,j,k\}$, the G operator ME reduces to the ME of C_k^τ, since the ME of $C_i^{\sigma\dagger}$ in $\mathrm{U}(i)$ basis is given by a simple isoscalar factor, eq. (25′), while the ME of E_{ij} is given by the product of a RME of E and the ME of C_k^τ in the $\mathrm{U}(i-1)$ basis. We thus get

$$\begin{aligned}\left\langle\begin{matrix}\lambda'_i\\ W'_i\end{matrix}\right|G^{\sigma}_{i;ik}\left|\begin{matrix}\lambda_i\\ W_i\end{matrix}\right\rangle &= \sum_{U_i}\left\langle\begin{matrix}\lambda'_i\\ W'_i\end{matrix}\right|C_i^{\sigma\dagger}\left|\begin{matrix}\lambda_i\\ U_i\end{matrix}\right\rangle\left\langle\begin{matrix}\lambda_i\\ U_i\end{matrix}\right|E_{ik}\left|\begin{matrix}\lambda_i\\ W_i\end{matrix}\right\rangle\\ &= \left(\begin{matrix}\lambda_i & (0,1)\\ \lambda'_{i-1} & (0,0)\end{matrix}\left|\begin{matrix}\lambda'_i\\ \lambda'_{i-1}\end{matrix}\right.\right)^{(s)}\\ &\quad\times\left\langle\begin{matrix}\lambda_i\\ \lambda_{i-1}\end{matrix}\right\|E\left\|\begin{matrix}\lambda_i\\ \lambda'_{i-1}\end{matrix}\right\rangle\left\langle\begin{matrix}\lambda'_{i-1}\\ W'_{i-1}\end{matrix}\right|C_k^{\tau}\left|\begin{matrix}\lambda_{i-1}\\ W_{i-1}\end{matrix}\right\rangle\\ &\equiv\left\langle\begin{matrix}\lambda'_i\\ \lambda'_{i-1}\end{matrix}\right|G\left|\begin{matrix}\lambda_i\\ \lambda_{i-1}\end{matrix}\right\rangle_C\left\langle\begin{matrix}\lambda'_{i-1} & (0,1)\\ W'_{i-1} & k\end{matrix}\left|\begin{matrix}\lambda_{i-1}\\ W_{i-1}\end{matrix}\right.\right\rangle^{(s)},\end{aligned}\tag{98}$$

where $\lambda'_{i-1}+\tau=\lambda_{i-1}$ and where we defined the G–C connecting factor

$$\left\langle\begin{matrix}\lambda'_i\\ \lambda'_{i-1}\end{matrix}\right|G\left|\begin{matrix}\lambda_i\\ \lambda_{i-1}\end{matrix}\right\rangle_C = \left(\begin{matrix}\lambda_i & (0,1)\\ \lambda'_{i-1} & (0,0)\end{matrix}\left|\begin{matrix}\lambda'_i\\ \lambda'_{i-1}\end{matrix}\right.\right)^{(s)}\left\langle\begin{matrix}\lambda_i\\ \lambda_{i-1}\end{matrix}\right\|E\left\|\begin{matrix}\lambda_i\\ \lambda'_{i-1}\end{matrix}\right\rangle.\tag{99}$$

In fact, since the ith level must be doubly occupied in the bra and unoccupied in the ket, we must have that $\lambda'_i\equiv(a,b)$ and $\lambda'_{i-1}=(a-1,b)$, while $\lambda_i=\lambda_{i-1}$. The only possible values for the latter irrep labels $\nu\equiv\lambda_i=\lambda_{i-1}$ that yield a nonvanishing isoscalar factor on the right-hand side of eq. (99) are $\nu=(a,b-1)$ and $\nu=(a-1,b+1)$, as may easily be seen from table 1. Since in each case the relevant RME equals 1, the G–C connecting factors are in fact given by the isoscalar factor on the right-hand side of eq. (99). The possible values of this connecting factor are listed in table 10.

(b) In a similar way, when $i<j=k=r=\max\{i,j,k\}$, we find that

$$\begin{aligned}\left\langle\begin{matrix}\lambda'_k\\ W'_k\end{matrix}\right|G^{\sigma}_{k;ik}\left|\begin{matrix}\lambda_k\\ W_k\end{matrix}\right\rangle &= \left(\begin{matrix}\lambda_k & (0,1)\\ \lambda'_{k-1} & (0,0)\end{matrix}\left|\begin{matrix}\lambda'_k\\ \lambda'_{k-1}\end{matrix}\right.\right)^{(s)}\\ &\quad\times\left\langle\begin{matrix}\lambda_k\\ \lambda'_{k-1}\end{matrix}\right\|E\left\|\begin{matrix}\lambda_k\\ \lambda_{k-1}\end{matrix}\right\rangle\left\langle\begin{matrix}\lambda'_{k-1}\\ W'_{k-1}\end{matrix}\right|C_i^{\tau\dagger}\left|\begin{matrix}\lambda_{k-1}\\ W_{k-1}\end{matrix}\right\rangle\\ &\equiv\left\langle\begin{matrix}\lambda'_k\\ \lambda'_{k-1}\end{matrix}\right|G\left|\begin{matrix}\lambda_k\\ \lambda_{k-1}\end{matrix}\right\rangle_{C^\dagger}\left\langle\begin{matrix}\lambda_{k-1} & (0,1)\\ W_{k-1} & i\end{matrix}\left|\begin{matrix}\lambda'_{k-1}\\ W'_{k-1}\end{matrix}\right.\right\rangle^{(s)},\end{aligned}\tag{100}$$

where $\lambda_{k-1}+\tau=\lambda'_{k-1}$ and where we defined the G–$C^\dagger$ connecting factor

Table 10
G–C connecting factors $\left\langle \begin{matrix} (a,b) \\ \lambda \end{matrix} \middle| G \middle| \begin{matrix} \nu' \\ \nu \end{matrix} \right\rangle_C$, providing connection between the MEs of $G^{\sigma}_{i;ik} \equiv C^{\sigma\dagger}_i E_{ik}$ and C^{τ}_k operators at level $i = j\ (>k)$. Since i must be doubly occupied in the bra and unoccupied in the ket, we can only have that $\lambda = (a-1,b)$ and $\nu' = \nu$. Definition (71) is employed.

ν	G–C
$(a,b-1)$	$\{0/1\}$
$(a-1,b+1)$	$\{2/1\}$

$$\left\langle \begin{matrix} \lambda'_k \\ \lambda'_{k-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_k \\ \lambda_{k-1} \end{matrix} \right\rangle_{C^\dagger} = \left(\begin{matrix} \lambda_k & (0,1) \\ \lambda'_{k-1} & (0,0) \end{matrix} \middle| \begin{matrix} \lambda'_k \\ \lambda'_{k-1} \end{matrix} \right)^{(s)} \left\langle \begin{matrix} \lambda_k \\ \lambda'_{k-1} \end{matrix} \middle\| E \middle\| \begin{matrix} \lambda_k \\ \lambda_{k-1} \end{matrix} \right\rangle . \tag{101}$$

The relevant values of this factor are listed in table 11.

(c) The next possibility arises when $k = r = \max\{i,j,k\}$, i.e. when $i,j<k=r$. In this case we reduce the ME of $C^{\sigma\dagger}_j$ using eq. (25″) with $n = k$ to the ME of $C^{\rho\dagger}_j$ in the U$(k-1)$ basis times an appropriate isoscalar factor, while the generator matrix element is expressed as a product of a corresponding RME and ME of $C^{\tau\dagger}_i$ in the U$(i-1)$ basis using eq. (30). Eliminating then the sum over intermediate states we get

$$\left\langle \begin{matrix} \lambda'_k \\ W'_k \end{matrix} \middle| G^{\sigma}_{j;ik} \middle| \begin{matrix} \lambda_k \\ W_k \end{matrix} \right\rangle = \sum_{\tau} \left(\begin{matrix} \lambda_k & (0,1) \\ \lambda_{k-1}+\tau & (0,1) \end{matrix} \middle| \begin{matrix} \lambda'_k \\ \lambda'_{k-1} \end{matrix} \right)^{(s)} \left\langle \begin{matrix} \lambda_k \\ \lambda_{k-1}+\tau \end{matrix} \middle\| E \middle\| \begin{matrix} \lambda_k \\ \lambda_{k-1} \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} \lambda'_{k-1} \\ W'_{k-1} \end{matrix} \middle| C^{\rho\dagger}_j C^{\tau\dagger}_i \middle| \begin{matrix} \lambda_{k-1} \\ W_{k-1} \end{matrix} \right\rangle , \tag{102}$$

where $\rho = \lambda'_{k-1} - \lambda_{k-1} - \tau$. It is now straightforward to express the pairing opera-

Table 11
G–$C^\dagger$ connecting factors $\left\langle \begin{matrix} (a,b) \\ \lambda \end{matrix} \middle| G \middle| \begin{matrix} \nu' \\ \nu \end{matrix} \right\rangle_{C^\dagger}$, providing connection between the MEs of $G^{\sigma}_{k;ik} \equiv C^{\sigma\dagger}_k E_{ik}$ and $C^{\tau\dagger}_i$ operators at level $j = k\ (>i)$.

ν'	λ	ν	G–$C^\dagger$
$(a,b-1)$	$(a-1,b)$	$(a-1,b-1)$	1
	$(a,b-1)$	$(a,b-2)$	1
	$(a,b-1)$	$(a-1,b)$	1
	$(a-1,b+1)$	$(a,b+2)$	0
	$(a-1,b+1)$	$(a-1,b)$	0
$(a-1,b+1)$	$(a-1,b)$	$(a-2,b+1)$	1
	$(a,b-1)$	$(a-1,b)$	0
	$(a,b-1)$	$(a-2,b+2)$	0
	$(a-1,b+1)$	$(a-1,b)$	1
	$(a-1,b+1)$	$(a-2,b+2)$	1

tor $C_j^{\rho\dagger} C_i^{\tau\dagger}$ MEs in terms of those for symmetric and antisymmetric tensors by employing eqs. (47)–(51). Introducing again appropriate G–S and G–A connecting factors, we obtain

$$\left\langle \begin{matrix} \lambda'_k \\ W'_k \end{matrix} \middle| G^{\sigma}_{j;ik} \middle| \begin{matrix} \lambda_k \\ W_k \end{matrix} \right\rangle = \left\langle \begin{matrix} \lambda'_k \\ \lambda'_{k-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_k \\ \lambda_{k-1} \end{matrix} \right\rangle_S \left\langle \begin{matrix} \lambda_{k-1} & (1,0) \\ W_{k-1} & [ij] \end{matrix} \middle| \begin{matrix} \lambda'_{k-1} \\ W'_{k-1} \end{matrix} \right\rangle^{(s)} + \left\langle \begin{matrix} \lambda'_k \\ \lambda'_{k-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_k \\ \lambda_{k-1} \end{matrix} \right\rangle_A \left\langle \begin{matrix} \lambda_{k-1} & (0,2) \\ W_{k-1} & [ij] \end{matrix} \middle| \begin{matrix} \lambda'_{k-1} \\ W'_{k-1} \end{matrix} \right\rangle^{(s)} . \quad (103)$$

All possible G–S and G–A connecting factors are given in table 12. To illustrate their evaluation, we consider the following example.

Consider the case that level k is unoccupied in W'_k but is singly occupied in the second column of W_k. Thus, setting $\lambda'_k = (a,b)$, we have that $\lambda_k = (a, b-1)$ and $\lambda'_{k-1} = (a,b), \lambda_{k-1} = (a-1,b)$. Now, for $\tau = 1 \equiv (0,1)$, we have $\rho = (a,b) -(a-1,b) - \tau = (1,0) - \tau = (1,-1) \equiv 2$ and for $\tau = 2 \equiv (1,-1)$, $\rho = (1,0) -(1,-1) = (0,1) \equiv 1$. However, both the isoscalar factor and the RME on the right-hand side of eq. (102) vanish when $\tau = 1$, so that we get

$$\left\langle \begin{matrix} (a,b) \\ (a,b) \\ W'_{k-1} \end{matrix} \middle| G^{\sigma}_{j;ik} \middle| \begin{matrix} (a,b-1) \\ (a-1,b) \\ W_{k-1} \end{matrix} \right\rangle = \left\langle \begin{matrix} (a,b) \\ W'_{k-1} \end{matrix} \middle| C_j^{1\dagger} C_i^{2\dagger} \middle| \begin{matrix} (a-1,b) \\ W_{k-1} \end{matrix} \right\rangle . \quad (104)$$

Thus, applying eqs. (50) and (51) we find for the desired connecting factors the following values

$$\left\langle \begin{matrix} (a,b) \\ (a,b) \end{matrix} \middle| G \middle| \begin{matrix} (a,b-1) \\ (a-1,b) \end{matrix} \right\rangle_S = \tfrac{1}{2}(1+\delta_{ij})^{1/2} \sqrt{\frac{b}{b+1}}, \quad (105a)$$

Table 12

G–S and G–A connecting factors $\left\langle \begin{matrix} (a,b) \\ \lambda \end{matrix} \middle| G \middle| \begin{matrix} \nu' \\ \nu \end{matrix} \right\rangle_{S,A}$, providing connection between the MEs of $G^{\sigma}_{j;ik} \equiv C_j^{\sigma\dagger} E_{ik}$ and MEs of symmetric and antisymmetric tensors of $[ij]$ at level $k(>i,j)$. We define $s_{ij} = (1+\delta_{ij})^{1/2}/2$ and use notation of eq. (71). Unnecessary $(1-\delta_{b,0})$ factors are avoided.

ν'	λ	ν	G–S	G–A
$(a,b-1)$	(a,b)	$(a,b-2)$	0	$a_{ij}/\sqrt{2}$
	(a,b)	$(a-1,b)$	$s_{ij}\{0/1\}$	$a_{ij}\{2/1\}/2$
	$(a,b-1)$	$(a-1,b-1)$	$-s_{ij}$	$-a_{ij}\{-1/1\}/2$
	$(a-1,b+1)$	$(a-1,b-1)$	0	$a_{ij}\{2/1\}/\sqrt{2}$
$(a-1,b+1)$	(a,b)	$(a-2,b+2)$	0	$a_{ij}/\sqrt{2}$
	(a,b)	$(a-1,b)$	$s_{ij}\{2/1\}$	$-a_{ij}\{0/1\}/2$
	$(a-1,b+1)$	$(a-2,b+1)$	$-s_{ij}$	$a_{ij}\{3/1\}/2$
	$(a,b-1)$	$(a-2,b+1)$	0	$a_{ij}\{0/1\}/\sqrt{2}$

$$\left\langle \begin{matrix} (a,b) \\ (a,b) \end{matrix} \middle| G \middle| \begin{matrix} (a,b-1) \\ (a-1,b) \end{matrix} \right\rangle_A = \tfrac{1}{2} a_{ij} (1-\delta_{b,0}) \sqrt{\frac{b+2}{b+1}}, \tag{105b}$$

with a_{ij} defined by eq. (48). The remaining possibilities are treated in a similar manner and the results are collected in table 12.

(d) The last possibility occurs when $i = r = \max\{i,j,k\}$, i.e. when $j,k < i = r$, which leads to G–E and G–N connecting factors. Similarly as in the preceding case (c) we find that

$$\left\langle \begin{matrix} \lambda'_i \\ W'_i \end{matrix} \middle| G^{\sigma}_{j;ik} \middle| \begin{matrix} \lambda_i \\ W_i \end{matrix} \right\rangle = \sum_{\tau} \left(\begin{matrix} \lambda_i & (0,1) \\ \lambda'_{i-1} - \tau & (0,1) \end{matrix} \middle| \begin{matrix} \lambda'_i \\ \lambda'_{i-1} \end{matrix} \right)^{(s)} \left\langle \begin{matrix} \lambda_i \\ \lambda_{i-1} \end{matrix} \middle\| E \middle\| \begin{matrix} \lambda_i \\ \lambda'_{i-1} - \tau \end{matrix} \right\rangle \times \left\langle \begin{matrix} \lambda'_{i-1} \\ W'_{i-1} \end{matrix} \middle| C^{\tau\dagger}_j C^{\rho}_k \middle| \begin{matrix} \lambda_{i-1} \\ W_{i-1} \end{matrix} \right\rangle, \tag{106}$$

where $\rho = \lambda_{i-1} - \lambda'_{i-1} + \tau$. Expressing the MEs of $C^{\tau\dagger}_j C^{\rho}_k$ in terms of MEs of generators E_{jk} and adjoint tensors $N^{(\kappa)}_{jk}$, eqs. (73), and introducing the corresponding G–E and G–N connecting factors, we can write

$$\left\langle \begin{matrix} \lambda'_i \\ W'_i \end{matrix} \middle| G^{\sigma}_{j;ik} \middle| \begin{matrix} \lambda_i \\ W_i \end{matrix} \right\rangle = \left\langle \begin{matrix} \lambda'_i \\ \lambda'_{i-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_i \\ \lambda_{i-1} \end{matrix} \right\rangle_E \left\langle \begin{matrix} \lambda'_{i-1} \\ W'_{i-1} \end{matrix} \middle| E_{jk} \middle| \begin{matrix} \lambda_{i-1} \\ W_{i-1} \end{matrix} \right\rangle + \left\langle \begin{matrix} \lambda'_i \\ \lambda'_{i-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_i \\ \lambda_{i-1} \end{matrix} \right\rangle_N \left\langle \begin{matrix} \lambda'_{i-1} \\ W'_{i-1} \end{matrix} \middle| N^{(\kappa)}_{jk} \middle| \begin{matrix} \lambda_{i-1} \\ W_{i-1} \end{matrix} \right\rangle, \tag{107}$$

where κ is implied by the irrep labels λ'_{i-1} and λ_{i-1}. All possible connecting factors of the G–E and G–N types, together with the corresponding superscripts κ, are listed in table 13.

As an example of evaluating these connecting factors, consider the case charac-

Table 13
G–E and G–N connecting factors $\left\langle \begin{matrix} (a,b) \\ \lambda \end{matrix} \middle| G \middle| \begin{matrix} \nu' \\ \nu \end{matrix} \right\rangle_{E,N}$, providing connection between the MEs of $G^{\sigma}_{j;ik} \equiv C^{\sigma\dagger}_j E_{ik}$ and MEs of E_{jk} and $N^{(\kappa)}_{jk}$ at level i ($>j,k$). Definition (71) is employed.

ν'	λ	ν	G–E	G–N	κ
$(a,b-1)$	$(a,b-1)$	$(a,b-1)$	$-1/2$	$-\{-1/1\}/\sqrt{2}$	0
	$(a-1,b+1)$	$(a,b-1)$	0	$\{0/1\}$	+
	$(a-1,b)$	$(a,b-2)$	0	$-\{-1/1\}$	+
	$(a-1,b)$	$(a-1,b)$	$-\{0/1\}/2$	$-\{2/1\}/\sqrt{2}$	0
$(a-1,b+1)$	$(a,b-1)$	$(a-1,b+1)$	0	$\{0/1\}$	−
	$(a-1,b+1)$	$(a-1,b+1)$	$-1/2$	$\{3/1\}/\sqrt{2}$	0
	$(a-1,b)$	$(a-1,b)$	$-\{2/1\}/2$	$\{0/1\}/\sqrt{2}$	0
	$(a-1,b)$	$(a-2,b+2)$	0	-1	−

terized by the irreps $\lambda'_i = (a,b)$ and $\lambda_i = \lambda_{i-1} = \lambda'_{i-1} = (a, b-1)$. In this case $\rho = \tau$ and we obtain from eq. (106) that

$$\left\langle \begin{matrix} (a,b) \\ (a,b-1) \\ W'_{i-1} \end{matrix} \middle| G^{\sigma}_{j;ik} \middle| \begin{matrix} (a,b-1) \\ (a,b-1) \\ W_{i-1} \end{matrix} \right\rangle$$
$$= -\left\langle \begin{matrix} (a,b-1) \\ W'_{i-1} \end{matrix} \middle| C^{1\dagger}_j C^1_k + \frac{1}{b+1} C^{2\dagger}_j C^2_k \middle| \begin{matrix} (a,b-1) \\ W_{i-1} \end{matrix} \right\rangle$$
$$= -\frac{1}{2}\left\langle \begin{matrix} (a,b-1) \\ W'_{i-1} \end{matrix} \middle| E_{jk} \middle| \begin{matrix} (a,b-1) \\ W_{i-1} \end{matrix} \right\rangle$$
$$- \sqrt{\frac{b-1}{2(b+1)}} \left\langle \begin{matrix} (a,b-1) \\ W'_{i-1} \end{matrix} \middle| N^{(0)}_{jk} \middle| \begin{matrix} (a,b-1) \\ W_{i-1} \end{matrix} \right\rangle, \tag{108}$$

yielding the first row of table 13.

This completes the evaluation of required connecting factors or segment values in terms of which MEs of any two-body operator may be expressed, similarly as first derived by Paldus and Boyle [37] (cf. also ref. [36] for segmentation formulas based on the S_N formalism). The required MEs are thus expressed in the following "segmented" form

$$\langle e_{ik;jl} \rangle \equiv \left\langle \begin{matrix} \lambda_l \\ W'_l \end{matrix} \middle| e_{ik;jl} \middle| \begin{matrix} \lambda_l \\ W_l \end{matrix} \right\rangle$$
$$= \prod_{m_1 \in \Omega_1} W^P_{m_1} \left\{ \prod_{m_2 \in \Omega_2} W^X_{m_2} + \prod_{m_2 \in \Omega_2} W^Y_{m_2} \right\} \prod_{m_3 \in \Omega_3} W^Q_{m_3}, \tag{109}$$

where $W^Z_m (Z = P, X, Y, Q)$ designates an appropriate mth level segment value of type Z that depends solely on the bra and the ket irrep labels of $\mathrm{U}(m)$ and $\mathrm{U}(m-1)$ subgroups. Depending on the type, the segment values are given by various connecting and scaled isoscalar factors. The index set Ω_2 designates the overlap region of the corresponding generator ranges $[i,k] \cap [j,l]$, where the symmetric and antisymmetric tensor $(X = S, Y = A)$ or adjoint tensors $(X = E, Y = N)$ come into play. The sets Ω_1 and Ω_3 correspond then to single generator regions, where the factors pertinent to the evaluation of one-body MEs (section 4) apply. We now indicate the specific form of the generic expression (109) for all relevant cases listed in table 8.

(1) As already stated, the first case when $\Omega_2 = \emptyset$ reduces to the product of one-body MEs that were handled in section 4.

(2) In case 2, again only a single product of segment values emerges. Thus, when $k < i = j < l$, we get from eqs. (84), (97) and (98) that

$$\langle e_{ik;il}\rangle = \left\langle \begin{matrix} \lambda_l \\ \lambda'_{l-1} \end{matrix} \middle| e \middle| \begin{matrix} \lambda_l \\ \lambda_{l-1} \end{matrix} \right\rangle_G \prod_{m=i+1}^{l-1} \left(\begin{matrix} \lambda_m & (0,1) \\ \lambda_{m-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda'_m \\ \lambda'_{m-1} \end{matrix} \right)^{(s)}$$
$$\times \left\langle \begin{matrix} \lambda'_i \\ \lambda'_{i-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_i \\ \lambda_{i-1} \end{matrix} \right\rangle_C \left\langle \begin{matrix} \lambda'_{i-1} & (0,1) \\ W'_{i-1} & k \end{matrix} \middle| \begin{matrix} \lambda_{i-1} \\ W_{i-1} \end{matrix} \right\rangle^{(s)}, \tag{110}$$

or, when $i<j=k<l$ (using eq. (100) instead of eq. (98))

$$\langle e_{ik;kl}\rangle = \left\langle \begin{matrix} \lambda_l \\ \lambda'_{l-1} \end{matrix} \middle| e \middle| \begin{matrix} \lambda_l \\ \lambda_{l-1} \end{matrix} \right\rangle_G \prod_{m=k+1}^{l-1} \left(\begin{matrix} \lambda_m & (0,1) \\ \lambda_{m-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda'_m \\ \lambda'_{m-1} \end{matrix} \right)^{(s)}$$
$$\times \left\langle \begin{matrix} \lambda'_k \\ \lambda'_{k-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_k \\ \lambda_{k-1} \end{matrix} \right\rangle_{C^\dagger} \left\langle \begin{matrix} \lambda_{k-1} & (0,1) \\ W_{k-1} & i \end{matrix} \middle| \begin{matrix} \lambda'_{k-1} \\ W'_{k-1} \end{matrix} \right\rangle^{(s)}, \tag{111}$$

where the last CG factor represents a simple product of isoscalar factors (cf., e.g., eq. (24)).

(3) In case 3 of table 8, i.e. when $i \leqslant j < k = l$, the MEs $\langle e_{il,jl}\rangle$ are given by eq. (87). The required symmetric tensor CG coefficients are evaluated using eq. (52) as a simple product of relevant isoscalar factors (tables 1 and 3). Note that the irrep (1, 0) remains unchanged from the $(l-1)$st level to the level $r = \max\{i,j\}$, when it changes to a single box irrep (0, 1) if $i \neq j$ or to the trivial scalar irrep (0, 0) if $i = j$. In the former case, the vector operator isoscalar factors are involved following the rth level.

(4) In case 4 of table 8, when $i,j<k<l$, we encounter both symmetric and antisymmetric tensors in the overlap region (from the kth level to the level $\max\{i,j\}$). In view of eqs. (84), (97) and (109) we have

$$\langle e_{ik;jl}\rangle = \left\langle \begin{matrix} \lambda_l \\ \lambda'_{l-1} \end{matrix} \middle| e \middle| \begin{matrix} \lambda_l \\ \lambda_{l-1} \end{matrix} \right\rangle_G \prod_{m=k+1}^{l-1} \left(\begin{matrix} \lambda_m & (0,1) \\ \lambda_{m-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda'_m \\ \lambda'_{m-1} \end{matrix} \right)^{(s)}$$
$$\times \left\{ \left\langle \begin{matrix} \lambda'_k \\ \lambda'_{k-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_k \\ \lambda_{k-1} \end{matrix} \right\rangle_S \left\langle \begin{matrix} \lambda_{k-1} & (1,0) \\ W_{k-1} & [ij] \end{matrix} \middle| \begin{matrix} \lambda'_{k-1} \\ W'_{k-1} \end{matrix} \right\rangle^{(s)} \right.$$
$$\left. + \left\langle \begin{matrix} \lambda'_k \\ \lambda'_{k-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_k \\ \lambda_{k-1} \end{matrix} \right\rangle_A \left\langle \begin{matrix} \lambda_{k-1} & (0,2) \\ W_{k-1} & [ij] \end{matrix} \middle| \begin{matrix} \lambda'_{k-1} \\ W'_{k-1} \end{matrix} \right\rangle^{(s)} \right\}. \tag{112}$$

When $i<j$, both CG coefficients in curly bracket involve the same factor

$$\left\langle \begin{matrix} \lambda_{j-1} & (0,1) \\ W_{j-1} & i \end{matrix} \middle| \begin{matrix} \lambda'_{j-1} \\ W'_{j-1} \end{matrix} \right\rangle^{(s)}, \tag{113}$$

corresponding to the non-overlap portion of the E_{ik} generator range, that can be taken outside the curly bracket and represents in fact the W^Q part in eq. (109).

(5) In case 5 of table 8, i.e. when $j \leqslant k < i = l$, the MEs $\langle e_{lk;jl}\rangle$ are given by eq. (92) in terms of the MEs of E_{jk} and $N_{jk}^{(\kappa)}$ operators that were examined in detail in

sections 4 and 6. In this case, the W^P part in eq. (109) equals 1. Following the level $\max\{j,k\}$, the MEs of E_{jk} and $N_{jk}^{(\kappa)}$ may contain the following common factor

$$\left\langle \begin{matrix} \lambda_{k-1} & (0,1) \\ W_{k-1} & j \end{matrix} \middle| \begin{matrix} \lambda'_{k-1} \\ W'_{k-1} \end{matrix} \right\rangle^{(s)}, \quad (j<k) \tag{114}$$

representing the W^Q part in eq. (109). Likewise, when $k<j$ (which corresponds in fact to the case c6 of ref. [37]), this factor becomes

$$\left\langle \begin{matrix} \lambda'_{j-1} & (0,1) \\ W'_{j-1} & k \end{matrix} \middle| \begin{matrix} \lambda_{j-1} \\ W_{j-1} \end{matrix} \right\rangle^{(s)}. \tag{115}$$

(6) For the last case 6 of table 8, when $j,k<i<l$, the overlap region involves adjoint tensor operators E_{jk} and $N_{jk}^{(\kappa)}$ (from the ith level to the level $\max\{j,k\}$). In view of eqs. (84), (97) and (107) we get

$$\begin{aligned} \langle e_{ik;jl}\rangle = & \left\langle \begin{matrix} \lambda_l \\ \lambda'_{l-1} \end{matrix} \middle| e \middle| \begin{matrix} \lambda_l \\ \lambda_{l-1} \end{matrix} \right\rangle_G \prod_{m=i+1}^{l-1} \left(\begin{matrix} \lambda_m & (0,1) \\ \lambda_{m-1} & (0,1) \end{matrix} \middle| \begin{matrix} \lambda'_m \\ \lambda'_{m-1} \end{matrix} \right)^{(s)} \\ & \times \left\{ \left\langle \begin{matrix} \lambda'_i \\ \lambda'_{i-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_i \\ \lambda_{i-1} \end{matrix} \right\rangle_E \left\langle \begin{matrix} \lambda'_{i-1} \\ W'_{i-1} \end{matrix} \middle| E_{jk} \middle| \begin{matrix} \lambda_{i-1} \\ W_{i-1} \end{matrix} \right\rangle \right. \\ & \left. + \left\langle \begin{matrix} \lambda'_i \\ \lambda'_{i-1} \end{matrix} \middle| G \middle| \begin{matrix} \lambda_i \\ \lambda_{i-1} \end{matrix} \right\rangle_N \left\langle \begin{matrix} \lambda'_{i-1} \\ W'_{i-1} \end{matrix} \middle| N_{jk}^{(\kappa)} \middle| \begin{matrix} \lambda_{i-1} \\ W_{i-1} \end{matrix} \right\rangle \right\}, \end{aligned} \tag{116}$$

with κ fixed by the irreps λ'_{i-1} and λ_{i-1} (see also table 13). Again, following the level $\max\{j,k\}$, the MEs of E_{jk} and $N_{jk}^{(\kappa)}$ may possess a common factor (114) or (115) constituting to W^Q of the generic formula, eq. (109).

8. Conclusions

We have shown in this paper that within the orbital (or spin-free) $\mathrm{U}(n)$ formalism one can introduce vector operators $C_j^{\sigma\dagger}$ and corresponding conjugate (or contragredient) vector operators C_j^{σ} that have similar properties as the creation and annihilation operators of the second quantization formalism at the spin orbital $\mathrm{U}(2n)$ level. Roughly speaking, the operators $C_j^{\sigma\dagger}$ (C_j^{σ}) create (annihilate) a single box, labelled with j, in the σth column of the Weyl tableau when acting on any $\mathrm{U}(n)$ irrep state labelled by this tableau. They may thus be regarded as spin-free orbital equivalents of the second quantization creation and annihilation spin orbital operators $X_{j\mu}^{\dagger}$ and $X_{j\mu}$, respectively.

We have further shown that products of these operators yield various tensor operators that play a very useful role in calculating MEs of various one- and two-body operators in the GT basis. Thus, products of two creation-like and two annihilation-like operators form symmetric and antisymmetric tensors associated with the irreps (1, 0) and (0, 2), respectively, while products of creation and an annihilation operators, $C_i^{\sigma\dagger} C_j^{\tau}$ represent components of a U(n) adjoint tensor. In fact, a simple sum of diagonal (i.e. $\sigma = \tau$) components represents U(n) generators E_{ij}, that map any U(n) irrep module (a, b) into itself, while the off-diagonal ones ($\sigma \neq \tau$) represent shift operators that take an (a, b) module into the $(a-1, b+2)$ and $(a+1, b-2)$ modules, respectively (cf. eqs. (61a) and (61c)). The remaining possible linear combination of diagonal-type operators, corresponding to the other zero-shift component of a general adjoint tensor (assuming $b \neq 0$), is not, however, a simple difference of the operators representing E_{ij}, eq. (56). It is shown that a suitable choice for this zero-shift tensor operators results when the ratio of corresponding (irrep dependent) "coefficients" equals $b/(b+2)$. It is also shown that by appropriate scaling of all quantities by the corresponding RMEs we achieve a very simple, a-independent (i.e. only intermediate spin dependent given by the b-label) formalism, that also naturally leads to a convenient phase convention that corresponds to that chosen by Shavitt [4,11] (convention IIB of ref. [37]). All the segment values that are required for the evaluation of various one- and two-body MEs may then be easily expressed in terms of corresponding isoscalar factors (or reduced Wigner coefficients) and RMEs and their explicit form derived. With the scaling just mentioned, their form is extremely simple.

The introduction of vector operators such as $C_i^{\sigma\dagger}$ and C_i^{σ} may, in principle, be avoided in developing the U(n) formalism for the evaluation of various MEs that arise in quantum chemical applications, as is the case in all existing approaches to this problem. This is also true when spin-dependent operators [41] or various reduced density matrices [47] are considered. However, these operators not only provide a very useful counterpart of the second quantization formalism at the spin-adapted (or orbital) level and enable one of the simplest derivations of explicit expressions for various segment values, but also throw new light on the existing formalisms. In particular, it will be interesting to establish a detailed relationship of the formalism developed in this series with a very general Green–Gould approach, as well as to investigate the possible connection with the Clifford algebra UGA [39] and U(n) universal enveloping algebra formalism [25] that proved to be very helpful for a spin-adapted formulation of various many-body approaches employing the effective Hamiltonian formalism (see, e.g., ref. [48]). It would thus be worthwhile to examine more closely the algebra of these vector operators in their own right and to establish its relationship with existing formalisms.

In subsequent communications of this series, we shall thus show how to exploit this formalism when spin-dependent operators are present as well as when system partitioning is employed [46]. We shall also indicate [49] how this approach is related with the Green–Gould formalism, showing that $C_i^{\sigma\dagger}$ (C_i^{σ}) represent unique vector (contragredient vector) operators whose squared RMEs are equal to the characteristic roots of Green's polynomial identities [42], corresponding to a given U(n) irrep (a, b). Likewise, the close relationship between the zero-shift tensor $N_{ij}^{(0)}$ and the Δ_{ij} operator [41], represented by a second degree polynomial in U(n) generators, will be shown [49]. This operator plays a fundamental role in the UGA spin-dependent formalism [41] as well as in the theory of reduced density matrices [47] and is worthy of further inquiry providing new insight into its structure and role.

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