

**Two-body-operator matrix element factorization technique in  $U(n) \downarrow S_N$  unitary bases.  
II. Raising-lowering operators**

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A detailed exposition of explicit formulas used in the evaluation of raising-lowering forms of two-body-operator matrix elements is presented. The methods are based on the use of the unitary group distinct row table and graphical representation of the many-particle basis. All matrix elements are expressible in terms of scalar and simple matrix factors. In order to facilitate the derivations of simple, computationally efficient forms for the matrix factors, we utilize a recently developed calculus based on elementary graphs. The methods are applicable to systems of particles involving spins greater than  $\frac{1}{2}$  and reduce to previously known results for the case of spin  $\frac{1}{2}$ .

**I. INTRODUCTION**

In a recent series of papers<sup>1-5</sup> we have introduced methods for representing the many-particle,  $S_N$  adapted bases of  $U(n)$ . We also proposed methods for evaluating the matrix elements of one- and two-body operators expressed in terms of the  $U(n)$  generators,  $E_{\mu\nu}$ . The representations, alternatively referred to as the distinct row table (DRT) or graphical unitary group approach (GUGA), are  $SU(n)$  generalizations of schemes developed for  $SU(2)$  [actually,  $U(2n) \supset U(n) \otimes SU(2)$ ] by Shavitt<sup>6,7</sup> based on the earlier  $\Delta ABC$  tableau technique of Paldus.<sup>8</sup> With respect to matrix element evaluation we developed a graphical formalism<sup>3,4</sup> which was used to deduce factorized expressions for the matrix elements of one- and two-body operators as well as a calculus<sup>5</sup> for deriving those detailed expressions to be used for raising-raising (lowering-lowering) cases.

The purpose of this work is to complete the presentation of the calculus rules to be used for deriving detailed expressions for raising-lowering (lowering-raising) cases. Thus this paper should be read in conjunction with Ref. 5, the two being viewed as a sequel to Refs. 3 and 4. The latter references were intended to introduce the graphical techniques which permit the decomposition of the matrix element expressions into factorized forms. The graphical techniques by themselves, however, are insufficient to provide detailed algebraic results for the factors. In this respect the contents of this paper and Ref. 5 constitute a detailed clarification and amplification of general results first presented in Refs. 3 and 4.

Factorization techniques are important for several reasons. First, they enable a significant reduction in the amount of computation to be performed in a strictly algebraic sense by allowing one to cast the matrix element expressions in closed form. Second, they enable one to program the formulas on computers utilizing multiprocessors connected in parallel thereby permitting the simul-

taneous evaluation of the many factors which do arise. The techniques, therefore, suggest alternative software and hardware approaches to model calculations performed on computers. Finally, by studying the expressions for the various factors it is anticipated that a better understanding of the coupling schemes and interaction operators used to describe many-particle configurations might be achieved.

The paper is divided into five sections. Section II contains a brief description of the background theory necessary to obtain the results presented later. Section III deals with the raising-lowering (lowering-raising) type of two-body operators. This section is further subdivided into parts which deal with a variety of general and special subcases. In Sec. IV we present examples of calculations intended to demonstrate the application of the relevant formulas.

**II. BACKGROUND THEORY**

We present a brief description of the generalized DRT-GUGA formalism. A more detailed description of the construction and generation of the DRT is provided in Refs. 1-5. It is to be noted that Ref. 5 introduced a more explicit, simplified notation, which is used herein, than was presented in earlier references.

The DRT, originally developed by Shavitt<sup>6,7</sup> based on work of Paldus,<sup>8</sup> is essentially a compact representation of the Clebsch-Gordan (CG) decomposition of the permutation symmetry,  $S_N$ , adapted irreducible representations of  $U(n)$  [or  $SU(n)$ ] formed by considering the subduction chain

$$U_{p_n}(n) \supset U_{p_{n-1}}(n-1) \supset \dots \supset U_{p_\mu}(\mu) \supset \dots \supset U_{p_1}(1) \supset U_{p_0}(0), \quad (2.1)$$

where the labels  $p_\mu = \{p_{\mu k} | p_{\mu k} \geq 0; k=0, 1, \dots, L\}$  are the integer partitions of  $N_\mu$  which label the  $U(\mu) \downarrow S_{N_\mu}$  ir-

reducible representations (irreps),  $N_\mu$  being the number of particles described by labels  $1, 2, \dots, \mu$  already compiled within a particular many-particle state.

As in previous work the  $p_{\mu k}$  describe the number of rows of length  $k$  in a Weyl-Young tableau (WYT) after the removal of all boxes containing labels greater than  $\mu$  (alternatively,  $p_{\mu k}$  is equal to the number of times the integer  $k$  appears in the  $\mu$ th row of the corresponding Gel'fand tableau). A single set of labels,  $p_\mu$ , describes only a Young frame shape while a complete set of labels,  $\{p\} = \{p_\mu; \mu=0, \dots, n\}$ , can be used to deduce the number of particles with label  $\mu$ , say, as well as the positions of these in a WYT. The parameter  $L$  is the maximum row length of the complete Young frame for a given irrep.

The DRT is a table whose entries are organized, hierarchically, first into subgroup levels  $\mu=n, n-1, \dots, 0$ . Within each level  $\mu$  are  $J_\mu$  (the total number of irreps at level  $\mu$ ) row entries arranged in lexical order by the  $p_\mu$  labels [see (2.7) of Ref. 5]. Each row entry contains, in addition to  $p_\mu$ , a variety of labels significant to a particular problem under consideration.<sup>1,2,7</sup>

The DRT can also be represented as a two-rooted, planar hierarchical digraph comprised of nodes and links. The irreps  $p_n$  and  $p_0 \equiv 0$  are represented by the head and tail nodes, respectively. At level  $\mu$  the irreps  $p_\mu$  are represented as nodes ordered lexically from left to right.

Links between nodes at successive levels  $\mu$  and  $\mu \pm 1$  can be labeled explicitly in such a way as to uniquely denote the particular subduction chain in the CG decomposition (2.1) [see (2.5) and (2.6) of Ref. 5].

A complete many-particle state is represented by a walk, or traversal, from the head (top row of the DRT) to the tail (bottom row of the DRT) along allowed links. A complete, unique specification of a given state can be written as  $|\{p\}\rangle$ , where  $\{p\}$  denotes a list of  $p_\mu$  labels,  $\mu=0, 1, \dots, n$ . All such walks (states) form an orthonormal basis [see (2.9) of Ref. 5].

The  $U(n)$  group generators  $E_{\mu,\nu}$  are Hermitian matrices which satisfy the Lie algebra commutator relationship

$$E_{\mu,\nu} E_{\alpha,\beta} - E_{\alpha,\beta} E_{\mu,\nu} = \delta_{\alpha,\nu} E_{\mu,\beta} - \delta_{\mu,\beta} E_{\alpha,\nu}. \quad (2.2)$$

Matrix elements of the elementary one-step raising generators  $E_{\mu-1,\mu}$  (a lowering generator would be  $E_{\mu,\mu-1}$ ) can be expressed in the form

$$\langle \{p'\} | E_{\mu-1,\mu} | \{p\} \rangle = \Delta_0^{\mu-2} \Delta_\mu^n B_\mu(\lambda_{\mu-1}) A_{\mu-1}(\lambda_{\mu-1}), \quad (2.3)$$

where the factors  $\Delta$ ,  $A$ , and  $B$  were defined in Ref. 5; for completeness and ease of reference we repeat these definitions below, however:

$$\Delta_\alpha^\beta = \prod_{\tau=\alpha}^{\beta} \left[ \prod_{k=0}^L \delta(p_{\tau k}, p'_{\tau k}) \right], \quad (2.4)$$

$$B_\mu(\lambda; p_\mu p_{\mu-1} p'_{\mu-1}) = \Gamma_B(\lambda, \mu) \cdot D_{\mu-1}(\lambda) \prod_{k=0}^L \left[ \delta_{0,p_{\mu k}} + (1 - \delta_{0,p_{\mu k}}) \left( \frac{h_\mu(\lambda, k)}{\hat{h}_\mu(\lambda, k)} \right)^{1/2} \right], \quad (2.5)$$

and

$$A_\mu(\lambda; p_\mu p'_{\mu-1}) = \Gamma_A(\lambda, \mu) \cdot D_\mu(\lambda) \prod_{k=0}^L \left[ \delta_{0,p_{\mu k}} + (1 - \delta_{0,p_{\mu k}}) \left( \frac{\hat{h}_\mu(\lambda, k)}{h_\mu(\lambda, k)} \right)^{1/2} \right]. \quad (2.6)$$

The parameter  $\lambda$  above is referred to as a *pivot* index and denotes the position of labels,  $p_{\mu\lambda}$  and  $p_{\mu\lambda-1}$ , which differ between bra and ket states.

The quantities  $h$  and  $\hat{h}$  are referred to as hooklengths and are defined by

$$h_\mu(\lambda, k) = h_\mu(\lambda, k; p_\mu) = |k+1-\lambda| + \sum_{j=\min(\lambda, k)}^{\max(\lambda, k)-1} p_{\mu j} \quad (2.7)$$

and

$$\hat{h}_\mu(\lambda, k) = \hat{h}_\mu(\lambda, k; p_\mu p_{\mu-1}) = h_\mu(\lambda, k) + \epsilon_{\lambda k} \nu_\mu(\lambda, k), \quad (2.8)$$

where  $\epsilon_{\lambda\xi} = \text{sgn}(\lambda - \xi)$ .

The quantity  $\nu_\mu(\lambda, k)$ , whose value represents the number of boxes, in a WYT, containing the label  $\mu$  in a row of length  $k$  after the removal of all boxes containing labels greater than  $\mu$ , is defined as

$$\begin{aligned} \nu_\mu(\lambda, k) &= \nu_\mu(\lambda, k; p_\mu p_{\mu-1}) \\ &= \left[ 1 - \delta \left[ \sum_{j=k}^N (p_{\mu j} - p_{\mu-1 j}) \right] \right] \{ (k - k_{\max}) [(1 - \delta_{0, k_{\max}}) + \delta_{0, k_{\max}} (1 - \delta_{0, p_{\mu-10}})] + [1 - h_\mu(\lambda, k)] \delta_{0, k_{\max}} \delta_{0, p_{\mu-10}} \}, \end{aligned} \quad (2.9)$$

where  $k_{\max} = \max\{j(1 - \delta_{0, p_{\mu-1j}}); j=0, \dots, k-1\}$ . It should be noted that when calculating the ratio of  $h_\mu$  to  $\hat{h}_\mu$  in

(2.5) or (2.6) one should calculate  $v_\mu$  first, since if  $v_\mu=0$  then the ratio is 1 automatically; if all boxes in the WYT row (including “row” 0) are labeled  $\mu$  then  $\hat{h}_\mu \equiv 1$ ; otherwise, it is necessary to perform the complete calculation of (2.7)–(2.9).

Finally, we refer the reader to Eqs. (2.20)–(2.22) of Ref. 5 for the definitions of the  $D_\mu(\lambda)$ ,  $\Gamma_B(\lambda, \mu)$ , and  $\Gamma_A(\lambda, \mu)$  factors. These factors subject the triplet of labels  $p_\mu p_{\mu-1} p'_{\mu-1}$  ( $p_\mu p'_\mu p_{\mu-1}$ ), in the case of  $B_\mu$  ( $A_\mu$ ), to a consistency check; that is,  $\Gamma_B(\lambda, \mu)$  checks that  $p_{\mu-1}$  and  $p'_{\mu-1}$  are each valid subdivisions of  $p_\mu$  and  $D_\mu(\lambda)$  checks that  $p_{\mu-1}$  and  $p'_{\mu-1}$  are compatible in the sense that  $B_\mu$  is nonzero [and similarly for  $D_\mu(\lambda)$  and  $\Gamma_A(\lambda, \mu)$  with regard to  $A_\mu$ ]. In this respect these coefficients play roles similar to selection rules as do the triangularity conditions of Racah-Wigner  $6-j$  coefficients.

As shown in Ref. 5 the  $A_\mu$  and  $B_\mu$  factors are fundamental to the derivation of explicit algebraic expressions for the more complex subgraphs which arise in the raising-raising (RR) matrix element expressions and, as will be demonstrated below, in raising-lowering (RL) expressions as well.

From (2.3) above and (2.23) of Ref. 5 we express the result of a multistep raising generator,  $E_{\mu, \nu}$  ( $\mu < \nu$ ), operating on an arbitrary state  $|\{p\}\rangle$  as

$$E_{\mu, \nu} |\{p\}\rangle = \sum_{\substack{\lambda_\tau=1 \\ \mu \leq \tau < \nu}}^L B_\mu(\lambda_{\nu-1}; p_\nu p_{\nu-1} p_{\nu-1} + \partial_{\nu-1} \lambda_{\nu-1}) \\ \times \prod_{\kappa=\mu+1}^{\nu-1} T_\kappa(\lambda_\kappa, \lambda_{\kappa-1}; p_\kappa p_\kappa + \partial_{\kappa\lambda_\kappa} p_{\kappa-1} p_{\kappa-1} + \partial_{\kappa-1} \lambda_{\kappa-1}) A_\mu(\lambda_\mu; p_\mu p_\mu + \partial_{\mu\lambda_\mu} p_{\mu-1}) \left| \{p\} + \sum_{\substack{\lambda_\alpha=1 \\ \mu \leq \alpha < \nu}} \partial_{\alpha\lambda_\alpha} \right\rangle, \quad (2.10)$$

where the summation is for each label  $\lambda_\tau$  in the range from  $\tau=\mu$  to  $\nu-1$ . The factor  $T_\kappa$  is defined as [see also (2.24), (2.33), and (2.34) of Ref. 5]

$$T_\kappa(\lambda_\kappa, \lambda_{\kappa-1}; p_\kappa p_\kappa + \partial_{\kappa\lambda_\kappa} p_{\kappa-1} p_{\kappa-1} + \partial_{\kappa-1} \lambda_{\kappa-1}) \\ = A_\kappa(\lambda_\kappa; p_\kappa p_\kappa + \partial_{\kappa\lambda_\kappa} p_{\kappa-1}) \cdot B_\kappa(\lambda_{\kappa-1}; p_\kappa + \partial_{\kappa\lambda_\kappa} p_{\kappa-1} p_{\kappa-1} + \partial_{\kappa-1} \lambda_{\kappa-1}) \\ - A_\kappa(\lambda_\kappa; p_\kappa p_\kappa + \partial_{\kappa\lambda_\kappa} p_{\kappa-1} + \partial_{\kappa-1} \lambda_{\kappa-1}) \cdot B_\kappa(\lambda_{\kappa-1}; p_\kappa p_{\kappa-1} p_{\kappa-1} + \partial_{\kappa-1} \lambda_{\kappa-1}). \quad (2.11)$$

We define  $\partial_{\tau\lambda}$  to be a linear operator<sup>5,9</sup> which acts on the  $p_\tau$  labels according to the component relations

$$p'_{\tau k} = p_{\tau k} \pm \partial_{\tau\lambda k} = p_{\tau k} \pm (\delta_{\lambda, k} - \delta_{\lambda-1, k}) \quad \forall k \leq L \quad (2.12)$$

and where the label changes are performed at the index positions  $\lambda$  and  $\lambda-1$ . The plus (minus) sign denotes a raising (lowering) operation on the labels  $p_\tau$ . In terms of the graphical representation of states the effect of  $\partial_{\mu\lambda}$  is to shift the node  $p_\mu$  to the left (right) for raising (lowering) cases. The resultant node  $p'_\mu$  may or may not be consistent with nodes  $p_{\mu\pm 1}$ . Note that at most  $L$  states can be generated by application of  $E_{\mu-1, \mu}$ , whereas up to  $L^{|\nu-\mu|+1}$  states are generated using  $E_{\mu, \nu}$ .

Since lowering operations can be expressed in terms of raising operations using (2.3) we shall require the Hermitian conjugate forms of the  $A$ ,  $B$ , and  $T$  factors. These are expressed as follows, using  $p'_\tau = p_\tau + \partial_{\tau\lambda}$  ( $\tau = \mu, \kappa, \kappa-1$ ) to denote the bra state labels,

$$B_\mu^\dagger(\lambda; p_\mu p_{\mu-1} p_{\mu-1} + \partial_{\mu-1} \lambda) = B_\mu(\lambda; p'_\mu p'_{\mu-1} - \partial_{\mu-1} \lambda p'_{\mu-1}), \quad (2.13)$$

$$A_\mu^\dagger(\lambda; p_\mu p_\mu + \partial_{\mu\lambda} p_{\mu-1}) = A_\mu(\lambda; p'_\mu - \partial_{\mu\lambda} p'_\mu p'_{\mu-1}), \quad (2.14)$$

$$T_\kappa^\dagger(\lambda, \xi; p_\kappa p_\kappa + \partial_{\kappa\lambda} p_{\kappa-1} p_{\kappa-1} + \partial_{\kappa-1} \xi) = T_\kappa(\lambda, \xi; p'_\kappa - \partial_{\kappa\lambda} p'_\kappa p'_{\kappa-1} - \partial_{\kappa-1} \xi p'_{\kappa-1}) \\ = A_\kappa(\lambda; p'_\kappa - \partial_{\kappa\lambda} p'_\kappa p'_{\kappa-1} - \partial_{\kappa-1} \xi) \cdot B_\kappa(\xi; p'_\kappa p'_{\kappa-1} - \partial_{\kappa-1} \xi p'_{\kappa-1}) \\ - A_\kappa(\lambda; p'_\kappa - \partial_{\kappa\lambda} p'_\kappa p'_{\kappa-1}) \cdot B_\kappa(\xi; p'_\kappa - \partial_{\kappa\lambda} p'_{\kappa-1} - \partial_{\kappa-1} \xi p'_{\kappa-1}). \quad (2.15)$$

With respect to (2.13)–(2.15) we emphasize the importance of the order of the argument labels in performing computations where one must be careful to use the correct labels. Since many of the algebraic simplifications derived for the various subgraph factors rely on the relationship between hooklengths at adjacent subgroup levels it is vital that a standard reference state, or nodes, be

chosen in order to deduce the particular relationships required. Referring to the graphical representation we have established a convention where only the lexically greatest (rightmost) nodes are used to compute the  $A$  and  $B$ , and hence  $T$ , subgraphs. Clearly, alternate, equivalent conventions may be established.

### III. RAISING-LOWERING OPERATORS

In this section we present the evaluation of the matrix elements of the symmetric product of two generators, namely,

$$\{E_{\mu,\nu}, E_{\alpha,\beta}\} = E_{\mu,\nu}E_{\alpha,\beta} + E_{\alpha,\beta}E_{\mu,\nu}. \quad (3.1)$$

It is possible to express any physical two-body operator in terms of linear combinations of symmetric products like (3.1) [see, for example, Eqs. (2.11) and (2.13) of Ref. 4].

In Ref. 5 we evaluated the matrix elements of the symmetric raising-raising generator products primarily because they led to symmetrical expressions in our factorization scheme. Further, it was possible, in general, to simplify the algebraic expressions for the various factors by taking into account the relationships between hook-lengths (2.16) and (2.17) at successive subgroup levels. We can describe those matrix element expressions schematically in the form

$$\langle \{p'\} | \{E_{\mu,\nu}, E_{\alpha,\beta}\} | \{p\} \rangle = \left[ \prod_{\substack{\tau \text{ not} \\ \text{in} \\ \text{over} \\ \text{lap} \\ \text{range}}} \phi_{\tau}^{(1)} \right] \left[ \prod_{\substack{\tau \text{ in} \\ \text{overlap} \\ \text{range}}} \phi_{\tau}^{(2)} \right], \quad (3.2)$$

where  $\phi_{\tau}^{(1)}$  and  $\phi_{\tau}^{(2)}$  refer to scalar and  $2 \times 2$  matrix factors, respectively, and where, in cases defined by index relations such as  $\mu < \alpha < \nu < \beta$ , for example, the overlap range refers to subgroup levels from  $\alpha$  to  $\nu$ .

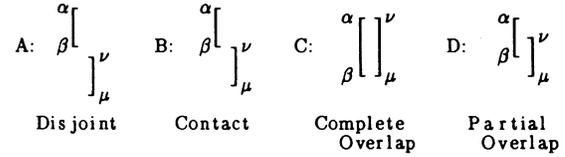
Similarly, for raising-lowering generator products we shall develop symmetrical expressions. The factors which arise in the overlap range, however, will no longer always be  $2 \times 2$ ; rather, they will be matrices of larger dimensions (indeed,  $\phi_{\tau}^{(2)}$  will be replaced, in general, by  $\phi_{\tau}^{(L)}$ , or  $L \times L$  matrices).

In the following treatment of the raising-lowering (RL) [lowering-raising (LR)] classes of operators we shall assume, without loss of generality, the relations on the elementary generator indices

$$\mu < \nu \text{ and } \alpha > \beta \quad (\mu > \nu \text{ and } \alpha < \beta).$$

The LR expressions are derived from these by finding the Hermitian conjugate of the matrix element expressions for the RL operators.

It is useful to decompose the RL products further into classes involving various degrees of overlap between the ranges of application of each generator in the symmetric product. The following diagrams serve to illustrate the ranges, and their overlap, of the operator indices. The various factors which are to be defined represent those subgraphs which arise completely in the overlap and nonoverlap ranges as well as the junctures of the two ranges.



In all the cases we consider  $\mu < \beta$ ; it is assumed that 0 and  $n$  are at the bottom and top of the diagrams, respectively. Remaining cases are easily derived from these either by conjugation or by renaming indices.

#### A. Case A: $\mu < \nu < \beta < \alpha$

Since the range of application of each generator is completely outside the range of the other the matrix element expression is found to be simply the product of two single generator matrix elements determined over restricted ranges of the state labels. Within the lowering range we employ the bra (primed) labels as reference labels for computing purposes [using (2.13)–(2.15)] thereby avoiding the need for alternate explicit expressions for  $A$ ,  $B$ , and  $T$  factors which differ only slightly from those already defined for the raising cases (which use the ket labels only).

#### B. Case B: $\mu < \nu = \beta < \alpha$

These cases are referred to as contact cases. The matrix element expression is similar to that of the nonoverlapping case and is given as

$$\begin{aligned} \langle \{p'\} | \{E_{\mu,\nu}, E_{\alpha,\beta}\} | \{p\} \rangle &= \Delta_{\alpha}^n B_{\alpha} (\xi_{\alpha-1}; p'_{\alpha} p'_{\alpha-1} p'_{\alpha-1} + \partial_{\alpha-1} \xi_{\alpha-1}) \\ &\times \prod_{\rho=\beta+1}^{\alpha-1} T_{\rho} (\xi_{\rho}; \xi_{\rho-1}; p'_{\rho} p'_{\rho} + \partial_{\rho} \xi_{\rho} p'_{\rho-1} p'_{\rho-1} + \partial_{\rho-1} \xi_{\rho-1}) \widehat{W}_{\nu} (\xi_{\nu}; \lambda_{\nu-1}; p_{\nu} p_{\nu} p'_{\nu-1} p'_{\nu-1}) \\ &\times \prod_{\tau=\mu+1}^{\nu-1} T_{\tau} (\lambda_{\tau}; \lambda_{\tau-1}; p_{\tau} p_{\tau} + \partial_{\tau} \lambda_{\tau} p_{\tau-1} p_{\tau-1} + \partial_{\tau-1} \lambda_{\tau-1}) A_{\mu} (\lambda_{\mu}; p_{\mu} p_{\mu} + \partial_{\mu} \lambda_{\mu} p_{\mu-1}) \Delta_0^{\mu-1}, \end{aligned} \quad (3.3)$$

where  $p'_{\nu} = p_{\nu} - \partial_{\nu} \xi_{\nu}$  and  $p'_{\nu-1} = p_{\nu-1} + \partial_{\nu-1} \lambda_{\nu-1}$  and where we have used  $\lambda_{\tau}$  and  $\xi_{\rho}$  to refer to those pivot indices operative within the ranges of the raising ( $\mu$  to  $\nu$ ) and lowering ( $\beta$  to  $\alpha$ ) generators, respectively. We define the factor  $\widehat{W}_{\nu}$  at the contact level  $\nu$  to be

$$\widehat{W}_v(\xi, \lambda; p_v, p'_v, p_{v-1}, p'_{v-1}) = A_v(\xi; p'_v, p_v, p_{v-1}) \cdot B_v(\lambda; p'_v, p_v, p_{v-1}) + A_v(\xi; p'_v, p_v, p'_{v-1}) \cdot B_v(\lambda; p_v, p_{v-1}, p'_{v-1}). \quad (3.4)$$

When both terms in (3.4) are nonzero zero  $\widehat{W}_v$  can be expressed as

$$\widehat{W}_v(\xi, \lambda; p_v, p'_v, p_{v-1}, p'_{v-1}) = A_v(\xi; p'_v, p_v, p_{v-1}) \cdot B_v(\lambda; p_v, p_{v-1}, p'_{v-1}) 2 \left[ \frac{h_v(\xi, \lambda; p_v) + \epsilon_{\lambda\xi}}{h_v(\xi, \lambda; p_v)} \right]^{1/2}, \quad (3.5)$$

where it is to be noted that the hooklength  $h_v(\xi, \lambda)$  is evaluated using the ket state (unprimed) labels. By eliminating redundant evaluations of hooklengths (3.5) achieves greater efficiency than with (3.4).

By comparing (3.3)–(3.5) to Eqs. (3.2)–(3.5) of Ref. 5 it is evident that, although the relations are similar, the RL factor  $\widehat{W}$  cannot be derived directly from the RR factor  $W$  defined in Ref. 5. This point is relevant in practical computations where separate case identification criteria and formulas must be expressed (programmed).

### C. Case C: $\mu = \beta < \nu = \alpha$

It is necessary to recognize the variety of subcases which apply in this case. Included among these subcases

are diagonal and off-diagonal matrix elements for which the subgraph factors are expressible in terms of either scalars or matrices. This case affords one a good means to illustrate the fundamental differences between RR and RL classes of matrix elements. In particular, it will become evident why the RL class does not lend itself in all cases to representation in terms of only scalar and  $2 \times 2$  matrices.

We proceed by considering the effect of a RL generator product on an arbitrary state. Using  $\lambda$  and  $\xi$  to denote the raising and lowering pivot indices, respectively, and the relation between bra and ket state nodes,  $p'_\tau = p_\tau + \partial_{\tau\lambda_\tau} - \partial_{\tau\xi_\tau}$  in the overlap range, we find the result

$$\begin{aligned} E_{v,\mu} E_{\mu,v} |\{p\}\rangle &= \sum_{\substack{\xi_\tau=1 \\ \mu \leq \tau < \nu \leq \mu \leq \tau < \nu}}^L \sum_{\lambda_\tau=1}^L [B_v(\xi_{v-1}; p_v, p'_{v-1}, p'_{v-1} + \partial_{v-1\xi_{v-1}}) \cdot B_v(\lambda_{v-1}; p_v, p_{v-1}, p_{v-1} + \partial_{v-1\lambda_{v-1}})] \\ &\quad \times \prod_{\kappa=\mu+1}^{v-1} [T_\kappa(\xi_\kappa, \xi_{\kappa-1}; p'_\kappa, p'_\kappa + \partial_{\kappa\xi_\kappa} p'_{\kappa-1}, p'_{\kappa-1} + \partial_{\kappa-1\xi_{\kappa-1}}) \\ &\quad \quad \times T_\kappa(\lambda_\kappa, \lambda_{\kappa-1}; p_\kappa, p_\kappa + \partial_{\kappa\lambda_\kappa} p_{\kappa-1}, p_{\kappa-1} + \partial_{\kappa-1\lambda_{\kappa-1}})] \\ &\quad \times [A_\mu(\xi_\mu; p'_\mu, p'_\mu + \partial_{\mu\xi_\mu} p_{\mu-1}) \cdot A_\mu(\lambda_\mu; p_\mu, p_\mu + \partial_{\mu\lambda_\mu} p_{\mu-1})] \\ &\quad \times |\{p'\}\rangle \left\langle \{p'\} \middle| \{p\} + \sum_{\substack{\lambda_\alpha=1 \\ \mu \leq \alpha < \nu}}^L \partial_{\alpha\lambda_\alpha} - \sum_{\substack{\xi_\alpha=1 \\ \mu \leq \alpha < \nu}}^L \partial_{\alpha\xi_\alpha} \right\rangle. \end{aligned} \quad (3.6)$$

A similar result holds in the case of the generator product  $E_{\mu,v} E_{v,\mu}$ .

We shall consider three subcases, those for which (i) all bra and ket nodes in the overlap range differ,  $p'_\tau \neq p_\tau$  ( $\tau = \mu, \dots, \nu-1$ ), (ii) at least the head and tail nodes differ,  $p'_{v-1} \neq p_{v-1}$  and  $p'_\mu \neq p_\mu$ , some or all of the remaining nodes in the overlap range are identical, and (iii) all bra and ket nodes are identical, the diagonal cases in other words. The rationale of this approach is that it affords one the opportunity to gradually develop an understanding of the structure of the various factors (and the notation used to distinguish them) by proceeding from the simplest to the most complex.

#### 1. $p'_\tau \neq p_\tau; \tau = \mu, \dots, \nu-1$

From (3.6) (and its conjugate) it follows that the matrix element expression can be written in the form

$$\begin{aligned} \langle \{p'\} | E_{\mu,v} E_{v,\mu} + E_{v,\mu} E_{\mu,v} | \{p\} \rangle &= \Delta_v^n \widehat{B}_v(\lambda_{v-1}, \xi_{v-1}; p_v, p_{v-1}, p'_{v-1}) \\ &\quad \times \prod_{\tau=\mu+1}^{v-1} \widehat{T}_\tau(\lambda_\tau, \xi_\tau, \lambda_{\tau-1}, \xi_{\tau-1}; p_\tau, p'_{\tau-1}, p'_{\tau-1}) \widehat{A}_\mu(\lambda_\mu, \xi_\mu; p_\mu, p'_\mu, p_{\mu-1}) \Delta_0^{\mu-1}, \end{aligned} \quad (3.7)$$

where we define the factors introduced above as the matrices

$$\widehat{B}_v^T(\lambda; \xi; p_v, p_{v-1}, p'_{v-1}) = \begin{bmatrix} B_v(\xi; p_v, p_{v-1} - \partial_{v-1\xi} p_{v-1}) \cdot B_v(\lambda; p_v, p'_{v-1} - \partial_{v-1\lambda} p'_{v-1}) \\ B_v(\lambda; p_v, p_{v-1}, p_{v-1} + \partial_{v-1\lambda}) \cdot B_v(\xi; p_v, p'_{v-1}, p'_{v-1} + \partial_{v-1\xi}) \end{bmatrix}, \quad (3.8)$$

$$\widehat{A}_\mu(\lambda, \xi; p_\mu, p'_\mu, p_{\mu-1}) = \begin{bmatrix} A_\mu(\xi; p_\mu - \partial_{\mu\xi} p_\mu, p_{\mu-1}) \cdot A_\mu(\lambda; p'_\mu - \partial_{\mu\lambda} p'_\mu, p_{\mu-1}) \\ A_\mu(\lambda; p_\mu, p_\mu + \partial_{\mu\lambda} p_{\mu-1}) \cdot A_\mu(\xi; p'_\mu, p'_\mu + \partial_{\mu\xi} p_{\mu-1}) \end{bmatrix}, \quad (3.9)$$

and

$$\hat{T}_\tau(\lambda, \xi, \rho, \sigma; p_\tau p'_\tau p_{\tau-1} p'_{\tau-1}) = \begin{cases} T_\tau(\xi, \sigma; p_\tau p'_\tau p_{\tau-1} p'_{\tau-1}) & 0 \\ T_\tau(\xi, \sigma; p_\tau p'_\tau p_{\tau-1} p'_{\tau-1} + \partial_\xi p'_\tau p_{\tau-1} + \partial_\lambda p_\tau p'_{\tau-1} + \partial_\rho p'_\tau p_{\tau-1}) & 0 \end{cases}, \quad (3.10)$$

where  $\hat{B}^T$  denotes the transpose of  $\hat{B}$ . Also, in order to condense the notation somewhat, the subgroup label has been deleted from the  $\partial$  operator in (3.10).

We remark that the first (second) elements arise due to the first (second) generator product in (3.7). Further, in contrast to the analogous RR matrices,  $\hat{T}$  [see Eqs. (3.27) of Ref. 5],  $\hat{T}$  is diagonal, a property which derives from the fact that there are only two ways of proceeding from the nodal pair  $p_\tau p_{\tau-1}$  to  $p'_\tau p'_{\tau-1}$  using single raising and lowering operations as opposed to four ways using two raising (or lowering) operations.

Additional algebraic simplifications can be derived for factors (3.8)–(3.10). For example, when both terms in (3.8) are nonzero  $\hat{B}_\nu$  can be expressed in the form

$$\begin{aligned} \hat{B}_\nu^T(\lambda, \xi; p_\nu p_{\nu-1} p'_{\nu-1}) &= B_\nu(\lambda; p_\nu p_{\nu-1} p_{\nu-1} + \partial_{\nu-1} \lambda) \\ &\cdot B_\nu(\xi; p_\nu p_{\nu-1} - \partial_{\nu-1} \xi p_{\nu-1}) \\ &\times \left[ \begin{array}{c} \left( \frac{h_{\nu-1}(\lambda, \xi) - \epsilon_{\lambda\xi}}{h_{\nu-1}(\lambda, \xi)} \right)^{1/2} \\ \left( \frac{h_{\nu-1}(\lambda, \xi)}{h_{\nu-1}(\lambda, \xi) + \epsilon_{\lambda\xi}} \right)^{1/2} \end{array} \right], \end{aligned} \quad (3.11)$$

where we have used relations like (2.27)–(2.30) of Ref. 5. Similarly, when both terms in (3.9) are nonzero  $\hat{A}_\mu$  is expressible as

$$\begin{aligned} \hat{A}_\mu(\lambda, \xi; p_\mu p'_\mu p_{\mu-1}) &= A_\mu(\lambda; p_\mu p_\mu + \partial_{\mu\lambda} p_{\mu-1}) \\ &\cdot A_\mu(\xi; p_\mu - \partial_{\mu\xi} p_\mu p_{\mu-1}) \\ &\times \left[ \begin{array}{c} \left( \frac{h_{\mu-1}(\lambda, \xi) + \epsilon_{\lambda\xi}}{h_{\mu-1}(\lambda, \xi)} \right)^{1/2} \\ \left( \frac{h_{\mu-1}(\lambda, \xi)}{h_{\mu-1}(\lambda, \xi) - \epsilon_{\lambda\xi}} \right)^{1/2} \end{array} \right]. \end{aligned} \quad (3.12)$$

It is possible to obtain simplifications for  $\hat{T}$  also, but this involves a number of further subcategories. The importance of such results as (3.11) and (3.12) is seen in practical computations where one requires only single (instead of repeated) evaluations of each  $B$  (or  $A$ ) factor in addition to the more easily determined elements of the relatively simple matrices given.

2.  $p'_{\nu-1} \neq p_{\nu-1}$ ;  $p'_\mu \neq p_\mu$ ;  $p'_\tau = p_\tau$  for some, or all,  $\tau$  in  $\mu+1, \dots, \nu-2$

The matrix element expression for this case is essentially the same as (3.7), the major difference being in the definition of the intermediate factors,  $\hat{T}_\tau$ . If one applies a lowering (raising) operation first and then a raising

(lowering) operation with the result that the bra and ket nodes at level  $\tau$ , say, are identical then one must account for all ways of achieving this, up to  $L$  ways. In order to account properly for this we attach an additional (vector) index on the pivot indices, hence  $\lambda = \{\lambda^i; i=1, \dots, L\}$ , and similarly for  $\xi$ . As before, we distinguish the pivot

indices for raising ( $\lambda$ ) and lowering ( $\xi$ ) for the sake of clarity in the presentation but emphasize that  $\lambda^i = \xi^i$ . In practice, there will not always be  $L$  operative pivot indices and the size of the pivot index “vectors” is therefore less than  $L$  at each level  $\tau$ . The  $\hat{T}_\tau$  factor corresponding to (3.10) can be cast in the form

$$\hat{T}_\tau(\lambda, \xi, \rho, \sigma; p_\tau p'_\tau p_{\tau-1} p'_{\tau-1}) = \begin{pmatrix} \hat{T}_\tau^{\text{LR}}(\lambda, \xi, \rho, \sigma; p_\tau p'_\tau p_{\tau-1} p'_{\tau-1}) & 0 \\ 0 & \hat{T}_\tau^{\text{RL}}(\lambda, \xi, \rho, \sigma; p_\tau p'_\tau p_{\tau-1} p'_{\tau-1}) \end{pmatrix}, \quad (3.13)$$

where we note that the matrix is block diagonal.  $\hat{T}_\tau^{\text{LR}}$  and  $\hat{T}_\tau^{\text{RL}}$  are each  $L \times L$  matrices in general whose elements are defined as

$$\hat{T}_\tau^{\text{LR}}(\lambda^i, \xi^i, \rho^j, \sigma^j; p_\tau p'_\tau p_{\tau-1} p'_{\tau-1}) = T_\tau(\xi^i, \sigma^j; p_\tau - \partial_{\xi^i} p_\tau p_{\tau-1} - \partial_{\sigma^j} p_{\tau-1}) \cdot T_\tau(\lambda^i, \rho^j; p'_\tau - \partial_{\lambda^i} p'_\tau p'_{\tau-1} - \partial_{\rho^j} p'_{\tau-1}), \quad (3.14)$$

$$\hat{T}_\tau^{\text{RL}}(\lambda^i, \xi^i, \rho^j, \sigma^j; p_\tau p'_\tau p_{\tau-1} p'_{\tau-1}) = T_\tau(\xi^j, \sigma^j; p'_\tau + \partial_{\xi^j} p'_\tau p'_{\tau-1} + \partial_{\sigma^j}) \cdot T_\tau(\lambda^i, \rho^j; p_\tau p_\tau + \partial_{\lambda^i} p_{\tau-1} p_{\tau-1} + \partial_{\rho^j}), \quad (3.15)$$

using the pivot index labels to indicate the positions of each element within the appropriate submatrix. We have suppressed certain indices in (3.14) and (3.15) where no ambiguity is likely to arise.

We note that in Ref. 4 there exists some ambiguity with respect to the structure of the matrices (3.13). In particular Figs. 11 and 12 of Ref. 4 indicate off-diagonal blocks; these matrices are not incorrect for more general generator products than are considered herein, but for symmetric products (3.13)–(3.15) should clarify any ambiguity.

$$3. \quad p'_\tau = p_\tau; \tau = \mu, \dots, \nu - 1$$

The diagonal matrix elements form this subcase. Each of the head, tail, and intermediate factors are  $L$ -element matrices in general. One major simplifying feature which arises, however, is that all of the elements are rational numbers due to the fact that they are each the square of either a  $B$ ,  $A$ , or  $T$  factor. The head and tail factors are defined as

$$\hat{B}_\nu(\lambda, \xi; p_\nu p_{\nu-1}) = [\hat{B}_\nu^{\text{LR}}(\lambda, \xi; p_\nu p_{\nu-1}) \hat{B}_\nu^{\text{RL}}(\lambda, \xi; p_\nu p_{\nu-1})], \quad (3.16)$$

$$\hat{A}_\mu(\lambda, \xi; p_\mu p_{\mu-1}) = \begin{pmatrix} \hat{A}_\mu^{\text{LR}}(\lambda, \xi; p_\mu p_{\mu-1}) \\ \hat{A}_\mu^{\text{RL}}(\lambda, \xi; p_\mu p_{\mu-1}) \end{pmatrix}, \quad (3.17)$$

where

$$\hat{B}_\nu^{\text{LR}}(\lambda, \xi; p_\nu p_{\nu-1}) = B_\nu(\xi^i; p_\nu p_{\nu-1} - \partial_{\nu-1} p_{\nu-1})^2, \quad (3.18a)$$

$$\hat{B}_\nu^{\text{RL}}(\lambda, \xi; p_\nu p_{\nu-1}) = B_\nu(\lambda^i; p_\nu p_{\nu-1} p_{\nu-1} + \partial_{\nu-1} p_{\nu-1})^2, \quad (3.18b)$$

and

$$\hat{A}_\mu^{\text{LR}}(\lambda, \xi; p_\mu p_{\mu-1}) = A_\mu(\xi^i; p_\mu - \partial_{\mu-1} p_{\mu-1})^2, \quad (3.19a)$$

$$\hat{A}_\mu^{\text{RL}}(\lambda, \xi; p_\mu p_{\mu-1}) = A_\mu(\lambda^i; p_\mu p_\mu + \partial_{\mu-1} p_{\mu-1})^2. \quad (3.19b)$$

The intermediate factors, in conjunction with (3.13)–(3.15), are expressed as

$$\hat{T}_\tau^{\text{LR}}(\lambda^i, \rho^j; p_\tau p_{\tau-1}) = T_\tau(\lambda^i, \rho^j; p_\tau - \partial_{\lambda^i} p_\tau p_{\tau-1} - \partial_{\rho^j} p_{\tau-1})^2, \quad (3.20a)$$

$$\hat{T}_\tau^{\text{RL}}(\lambda^i, \rho^j; p_\tau p_{\tau-1}) = T_\tau(\lambda^i, \rho^j; p_\tau p_\tau + \partial_{\lambda^i} p_{\tau-1} p_{\tau-1} + \partial_{\rho^j})^2. \quad (3.20b)$$

#### D. Case D: $\mu < \beta < \nu < \alpha$

These cases are referred to as *partial overlapping*. The matrix element expression is given as

$$\begin{aligned} \langle \{p'\} | \{E_{\mu, \nu}, E_{\alpha, \beta}\} | \{p\} \rangle &= \Delta_\alpha^n B_\alpha(\xi_{\alpha-1}) \prod_{\rho=\nu+1}^{\alpha-1} T_\rho(\lambda_\rho, \lambda_{\rho-1}) \hat{F}_\nu(\lambda_\nu, \lambda_{\nu-1}, \xi_{\nu-1}) \\ &\quad \times \prod_{\kappa=\beta+1}^{\nu-1} \hat{T}_\kappa(\lambda_\kappa, \xi_\kappa, \lambda_{\kappa-1}, \xi_{\kappa-1}) \cdot \hat{G}_\beta(\lambda_\beta, \xi_\beta, \lambda_{\beta-1}) \\ &\quad \times \prod_{\tau=\mu+1}^{\beta-1} T_\tau(\lambda_\tau, \lambda_{\tau-1}) \cdot A_\mu(\lambda_\mu) \Delta_0^{\mu-1}, \end{aligned} \quad (3.21)$$

where we define the factors  $\hat{F}$  and  $\hat{G}$  in analogy with (3.16) and (3.17), respectively. The elements of these are given as



Using the iterative approach based on the use of one-step generators we must first decompose the operator expression, using (2.2), into the form

$$\begin{aligned}
 E_{9,11}E_{12,10} + E_{12,10}E_{9,11} = & E_{9,10}E_{10,11}E_{12,11}E_{11,10} - E_{9,10}E_{10,11}E_{11,10}E_{12,11} \\
 & - E_{10,11}E_{9,10}E_{12,11}E_{11,10} + E_{10,11}E_{9,10}E_{11,10}E_{12,11} \\
 & + E_{12,11}E_{11,10}E_{9,10}E_{10,11} - E_{12,11}E_{11,10}E_{10,11}E_{9,10} \\
 & - E_{11,10}E_{12,11}E_{9,10}E_{10,11} + E_{11,10}E_{12,11}E_{10,11}E_{9,10} .
 \end{aligned} \tag{4.1}$$

Applying each term in (4.1), retaining only those intermediate terms which contribute to the matrix element value (note that in practice one would in fact include all intermediate terms, thereby increasing significantly the amount of computation), we find for the contributions from each term

$$\begin{aligned}
 [5^2(2^{16})]^{-1}[3(11)159\,791 - 3^2(7)11(9577) - 3(7^2)11(3373) + 2^3(3^2)7^2(11)179 + 3(11)159\,791 \\
 - 3^2(7)11(9577) - 3(7^2)11(3373) + 2^3(3^2)7^2(11)179] = [3(11)3901]/(2^{15})(5^2) .
 \end{aligned} \tag{4.2}$$

We remark that the symmetry between the first four and last four terms is fortuitous, occurring due to the specific states and operators which we have chosen for our example. Due to the intermediate states which arise on application of each generator in (4.1) the numbers of  $A$  and  $B$  factors which must be calculated (excluding those states which eventually prove not to contribute) are 68 respectively. (We note that even the value of 68 assumes certain obvious optimizations.) The eight terms in (4.2) were determined by combining the results from all of the intermediate states used for the corresponding generator product.

In addition to the calculation of  $A$  and  $B$  factors other issues relating to the efficiency of the computation involve the arithmetic combination of the different product terms in (4.1) which require determining square roots and, typically, the greatest common divisor of two numbers; none of these processes is displayed explicitly in (4.2) but they have been carried out. Thus optimizing the computation will involve reducing the actual numbers of factors as well as recognizing squares of  $A$  or  $B$  factors, each of which is expressible as the square root of a rational number.

Using the factorization technique corresponding to case D of Sec. III we find the following factors, namely,

$$B_{12} = \sqrt{4} , \tag{4.3}$$

$$\hat{F}_{11} = \left(\frac{231}{5}\right)^{1/2} \left(-\frac{85}{3584}, -\frac{105}{512}, -\frac{735}{4096}, -\frac{1155}{5120}, -\frac{15}{512}, -\frac{117}{1920}, -\frac{165}{1024}, \frac{429}{2560}\right) , \tag{4.4}$$

$$\hat{G}_{10}^T = \left(\frac{231}{5}\right)^{1/2} \left(\frac{429}{10880}, -\frac{5}{384}, -\frac{3}{560}, -\frac{1}{320}, -\frac{77}{3200}, -\frac{105}{6656}, -\frac{35}{2112}, -\frac{5}{1344}\right) , \tag{4.5}$$

$$A_9 = \left(\frac{1}{16}\right)^{1/2} . \tag{4.6}$$

Multiplication of the factors (4.3)–(4.6) yields the same result obtained in (4.2) as required.

The numbers of  $A$  and  $B$  factors required to calculate (4.3)–(4.6) are 25 each; the reduction by 43 of the total number of calculations for each type of factor, compared to using (4.1) and (4.2), is due to the elimination of redundant evaluations of  $B_{12}$  and  $A_9$ , an efficient accounting of intermediate states and the use of the previously described algebraic simplifications in the subgraph factors.

Although the comparison of efficiencies is purely empirical the results indicate that the factorization technique is the better one to use in practical computations. Preliminary, more rigorous analysis further bears this out and indicates even greater gains in efficiency when evaluations of overlap range  $\hat{T}$  factors are required.

## V. CONCLUSIONS

We have presented a detailed exposition of the algebraic methods used to derive specific subgraph factors pertinent to the efficient evaluation of raising-lowering matrix elements of the  $U(n)$  group generators. We have shown that the techniques employed yield factors which

are analogous to those found for raising-raising generator products with the important differences that in the overlap range the factors are expressed as matrices whose size is larger than  $2 \times 2$ , in general, and whose structure is block diagonal.

It is to be emphasized that the method is fully general with respect to the treatment of arbitrary  $S_N$  adapted irreps of  $U(n)$ , in other words, Weyl-Young tableaux of arbitrary shape (appropriate to  $n$  and  $N$ ). Thus the methods are likely to be of use to practitioners in diverse areas such as nuclear and elementary particle physics in addition to applications in the atomic and molecular domains to which the unitary group approach has been largely restricted heretofore.

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