Two-body-operator matrix-element factorization technique in $U(n)\downarrow S_N$ unitary bases: Raising-raising operators

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A detailed exposition of explicit formulas used in the evaluation of raising-raising forms of two-body-operator matrix elements is presented. The methods are based on the use of the unitary-group distinct-row tabular-graphical representation of the many-particle basis. All matrix elements are expressible in the form of scalar and 2×2 matrix factors. In order to facilitate the derivations of simple, computationally efficient forms for the matrix factors we develop a 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

The application of unitary-group methods to the analysis of many-body problems has been studied in considerable depth since the pioneering work of Gel'fand and Zetlin.[1] Gel'fand and Zetlin demonstrated that the irreducible representations (irreps) of an N-particle system under unitary symmetry $U(n)$ are the permutational symmetry-adapted unitary groups $U(n)\downarrow S_N$ whose basis states are referred to as Gel'fand-Zetlin tableaux (GZT's). Biedenharn and co-workers[2-4] and Ciftan[5] further developed the basic theory into the tensor operator calculus (generalized Racah-Wigner calculus) based on techniques from substitutional analysis.[6] Moshinsky and co-workers[7] utilized certain aspects of the method in applications to nuclear physics. For an excellent review of the state of the art of the unitary-group approach up to 1970 the reader is referred to the paper of Louck.[8]

More recently, commencing with the work of Harter and Patterson[9] and Paldus,[10] there has been a focus on the case of $U(2n)\supset U(n)\otimes SU(2)$ which describes electronic spin-orbital configurations. An important aspect of the work of Harter and Patterson is the development of simplified computational techniques for the evaluation of elementary group generators using two-column Weyl-Young tableau[11] (WYT) representations of the basis states of each irrep. The advantages of this approach over earlier methods based on GZT's were that the states were described in a more compact notation which afforded a visually intuitive, easily implemented algorithm for matrix-element calculations.

It is seen through the literature on the unitary-group approach that the path that has been followed by most workers has been to determine methods which either lead to a more fundamental understanding of the connection between the physics and the mathematics or to improve upon existing methods for performing computations.[12-30]

In two recent papers[31,32] we have presented general results pertaining to the evaluation of one- and two-body-operator matrix elements in $U(n)\downarrow S_N$-adapted bases, that is, unitary bases of N-particle systems. Examples of such bases include the Gel'fand tableaux, Weyl-Young tableaux, and the distinct-row table formulation developed by Paldus[10] and Shavitt[14] for SU(2) and recently generalized to $SU(n)$ by us.[27,28] In particular, it is to be noted that the results are applicable to N-particle states made up from single-particle wave functions describing spins greater than $\frac{1}{2}$ as well as the spin-$\frac{1}{2}$ case.

A number of ambiguities may arise as a consequence of the manner in which results were presented in Refs. 31 and 32. The purpose of that work was to present a general graphical formalism which could be applied to the deduction of factorized expressions for two-body operators. The lack of detail can understandably lead to some confusion, however, which can only be dealt with effectively by presenting the method in expanded form, accounting for both general and special cases.

The purpose of the present paper is to present a coherent exposition of the algebraic expressions involved in our scheme together with a detailed treatment of special cases which do arise. In order to facilitate this we develop a simplified calculus based on elementary subgraphs introduced in Ref. 31.

The analysis and results of this paper differ from Refs. 31 and 32 not only in their being more coherent but also in that they utilize a notationally very precise, purely algebraic exposition of our methods. Thus they become more immediately amenable to implementation on a computer.

The paper is divided into four sections. Section II contains a brief description of the background theory necessary to obtain the results presented later. Section III deals with the raising-raising (lowering-lowering) type of two-body operators. This section is further subdivided into parts which deal with a variety of general and special subcases.

II. BACKGROUND THEORY

We present a brief description of the generalized distinct-row table (DRT), or graphical symmetric unitary-group approach (GSUGA), formalism. A more detailed description of the construction and generation of the DRT is provided in Refs. 27 and 28.

The DRT, originally developed by Shavitt[14] based on work of Paldus,[10] is essentially a compact representation of the Clebsch-Gordan (CG) decomposition of the permutation symmetry-adapted irreps $U(n)$ [or $SU(n)$] formed by adapting $U(\mu)$ at each stage in the subduction

$$U(n)\supset U(n-1)\supset\cdots\supset U(\mu)\supset\cdots\supset U(1) \tag{2.1}$$

to the chain

$$S_N\supset S_{N-1}\supset\cdots\supset S_1\ . \tag{2.2}$$

We introduce partition labels $p_\mu=\{p_{\mu k};k=0,\ldots,N\}$, $0\le\mu\le n$, satisfying conditions that $p_{\mu k}$ are *non-negative* integers and

$$\sum_{k=0}^{N} p_{\mu k}=\mu\ , \tag{2.3a}$$

$$\sum_{k=0}^{N} kp_{\mu k}=N_\mu,\quad N_n\equiv N \tag{2.3b}$$

where N_μ is the number of particles described by labels less than or equal to μ. (We note that in Ref. 31 and 32 we utilized the notation $\{p\}_\mu$ which has been abbreviated to the current p_μ.) Thus the CG decomposition of p_n can be expressed as

$$U_{p_n}(n)\supset U_{p_{n-1}}(n-1)\supset\cdots\supset U_{p_\mu}(\mu)\supset\cdots\supset U_{p_1}(1)\supset U_{p_0}(0)\ , \tag{2.4}$$

where we have added, formally, the group $U_{p_0}(0)$ ($p_{0k}=0$ $\forall k$) describing zero particles (vacuum state) as an artifice in order to generate a complete DRT and a corresponding graph.

In practice the actual number of labels, p_μ, required will be less than N, the number of particles in the system. Thus we define $L=\max\{k|p_{nk}\rangle 0;k=0,\ldots,N\}$ which we refer to as the maximum row length (due to its visual interpretation as the maximum row length of the corresponding WYT). The upper limits N in the summations (2.3) are, therefore, replaced by L and we refer henceforth to the set of labels $p_{\mu k}$, $k=0,\ldots,L$.

The $p_{\mu k}$ describe the number of rows of length k in a WYT after the removal of all boxes containing labels greater than μ. Thus a single set of labels p_μ describes only a Young frame shape, while a complete set of labels $\{p_\mu;\mu=0,\ldots,n\}$ can be used to deduce the number of particles with label μ, say, as well as the positions of these in a WYT. Alternatively, $p_{\mu k}$ is equal to the number of times the integer k appears in the μth row of the corresponding Gel'fand tableau. Also, for the SU(2) case,[10] the connection with the so-called Paldus, or *ABC*, tableau entries is $p_{\mu 0}=c_\mu$, $p_{\mu 1}=b_\mu$, and $p_{\mu 2}=a_\mu$.

The irreps $U_{p_{\mu\pm1}}(\mu\pm1)$ are generated from $U_{p_\mu}(\mu)$ using a linear step operator

$$p_{\mu\pm1}=S_t^{\pm}p_\mu=p_\mu\pm d_t\ , \tag{2.5}$$

where the difference labels $d_t(t=0,\ldots,2^L-1)$ are defined by the relations

$$|d_{tk}|\le1,\quad 0\le\sum_{k=0}^{q} d_{tk}\le1\quad\forall q\le L\ , \tag{2.6a}$$

$$t=\sum_{k=0}^{L}[\delta(d_{tk},1)-\delta(d_{tk},-1)]2^k-1\ . \tag{2.6b}$$

Starting from the $U(n)$ irrep labels p_n one applies the step operators to p_μ, for each generating up to 2^L irreps $p_{\mu-1}$, subject to conditions (2.3). To distinguish the irreps p_μ a final row index is added, hence $p_{\mu-1\,R}$ (upper case is used to distinguish the row label from the element label k used previously—complete labeling is of the form $p_{\mu k\,R}$). Finally, a lexical ordering of the irreps, $p_{\mu R}<p_{\mu R'}$ ($R<R'$), is defined by the relations

$$p_{\mu q\,R}>p_{\mu q\,R'},\quad p_{\mu k\,R}=p_{\mu k\,R'}\quad\forall k>q \tag{2.7}$$

where q is the largest index value for which (2.7) holds.

The complete DRT is a table whose entries are organized first into subgroup levels $\mu=n,n-1,..,0$. Within each level μ are J_μ (the total number of irreps at level μ) row entries $p_{\mu R}$ ($R=1,\ldots,J_\mu$) in lexical order. Appended to each row entry are sets of associated labels such as linkage or chaining indices $k_{\mu t\,R}$ which give for a particular $p_{\mu-1\,R}$ the irrep $p_{\mu k_{\mu t\,R}}$ generated upon application of S_t^-, and various weight indices $y_{\mu t\,R}$ which are used to enumerate the many-particle states of the system.[14,27,28] Additional information, such as multiplicities of each irrep and other symmetry labels,[15,24] may also be included as part of each row entry.

The DRT can also be represented as a two-rooted, planar hierarchical digraph comprised of nodes and links. The irreps p_n and $p_0=0$ are represented by the head and tail nodes, respectively. At level μ the irreps $p_{\mu R}$ are represented as nodes ordered from left to right by the index R. Links between successive levels μ and $\mu\pm1$ can be either labeled explicitly (by the appropriate linkage label value t) or drawn in a way which assigns lines of unique slope and length for each linkage value. In the remaining discussion of matrix-element calculations we shall not require the row index R so it will be omitted. When the occasion arises where we must refer to two or more sets of labels (graph nodes) at level μ we shall distinguish these through the use of primes or some other label.

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. Since p_n is unique to each irrep of S_N then a complete, unique specification of a given state can be written as $|p_n\{T\}\rangle$, where $\{T\}$ is the set of all step operator indices t_μ which generate allowed irreps in the chain (2.4), namely,

$$|p_n\{T\}\rangle\equiv\prod_{\mu=1}^{n} S_{t_\mu}^{-}p_n\ , \tag{2.8}$$

and where the product of step operators is ordered left to

right. Further, the states form an orthonormal basis

$$\langle p'_n\{T'\}|p_n\{T\}\rangle=\delta(p_n,p'_n)\delta(\{T\},\{T'\}) . \tag{2.9}$$

It is to be noted that the orthogonality of these states requires, in general, some constraints on the manner of their construction.[33] We assume herein that the states are constructed by coupling particles, one at a time, to the many-particle system. In terms of the WYT, as a particle labeled μ is added to an intermediate tableau it is always placed in the lowest row, furthest-left column position allowed, consistent with the resultant final arrangement of labels. Each of our states (2.8) is equivalent to a WYT state constructed by drawing the Young frame corresponding to p_1 and filling the boxes with 1's, then adding boxes consistent with p_2 into which are placed 2's, and so on, up to p_n. The orthogonality of the WYT basis thus ensures (2.9).

Alternatively and equivalently, a state is represented by a list of labels $|\{p_n p_{n-1}\cdots p_1\}\rangle$ which can either be read from the complete DRT, proceeding from level to level, or generated recursively from p_n by application of the step operators in (2.8). In any case, for the purposes of evaluating matrix elements of the group generators, as will be seen below, it is necessary to use the partition labels explicitly.

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

$$E_{\mu,\nu}E_{\alpha,\beta}-E_{\alpha,\beta}E_{\mu,\nu}=\delta_{\alpha,\nu}E_{\mu,\beta}-\delta_{\mu,\beta}E_{\alpha,\nu} \tag{2.10}$$

and have the Hermitian property

$$\langle p_n\{T'\}|E_{\mu,\nu}|p_n\{T\}\rangle^*=\langle p_n\{T\}|E_{\nu,\mu}|p_n\{T'\}\rangle . \tag{2.11}$$

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

$$\langle p_n\{T'\}|E_{\mu-1,\mu}|p_n\{T\}\rangle = \Delta_0^{\mu-2}\Delta_\mu^n B_\mu(\lambda_{\mu-1})A_{\mu-1}(\lambda_{\mu-1}) , \tag{2.12}$$

where the factors Δ, A, and B are defined below. The subgraph identity product symbol Δ_α^β is defined as

$$\begin{aligned}\Delta_\alpha^\beta&=\Delta_\alpha^\beta(p,p')\\&=\prod_{\tau=\alpha}^{\beta}\left[\prod_{k=0}^{N}\delta(p_{\tau k},p'_{\tau k})\right]\\&=\left[\prod_{k=0}^{N}\delta(p_{\beta k},p'_{\beta k})\right]\left[\prod_{\tau=\alpha+1}^{\beta}\delta(t_\tau,t'_\tau)\right] .\end{aligned} \tag{2.13}$$

We find the latter form to be more efficient in computer applications.

The elementary subgraph factors B_μ and A_μ are defined as

$$B_\mu(\lambda)=B_\mu(\lambda;p_\mu p_{\mu-1}p'_{\mu-1})=\Gamma_B(\lambda,\mu)D_{\mu-1}(\lambda)\prod_{k=0}^{L}\left[\delta_{0,p_{\mu k}}+(1-\delta_{0,p_{\mu k}})\left[\frac{h_\mu(\lambda,k)}{\hat{h}_\mu(\lambda,k)}\right]^{1/2}\right] \tag{2.14}$$

and

$$A_\mu(\lambda)=A_\mu(\lambda;p_\mu p'_\mu p_{\mu-1})=\Gamma_A(\lambda,\mu)D_\mu(\lambda)\prod_{k=0}^{L}\left[\delta_{0,p_{\mu k}}+(1-\delta_{0,p_{\mu k}})\left[\frac{\hat{h}_\mu(\lambda,k)}{h_\mu(\lambda,k)}\right]^{1/2}\right] . \tag{2.15}$$

We note that (2.14) and (2.15) are written in a different form than expressions (3.8) and (3.9) of Ref. 31. Although the current expressions appear more complicated than those previously defined they prove to be more useful in subsequent derivations; however, they are equivalent.

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

$$h_\mu(\lambda,k)=h_\mu(\lambda,k;p_\mu)=|k+1-\lambda|+\sum_{j=\min(\lambda,k)}^{\max(\lambda,k)-1}p_{\mu j} \tag{2.16}$$

and

$$\hat{h}_\mu(\lambda,k)=\hat{h}_\mu(\lambda,k;p_\mu p_{\mu-1})=h_\mu(\lambda,k)+\epsilon_{\lambda k}\nu_\mu(\lambda,k) , \tag{2.17}$$

where

$$\epsilon_{\lambda\xi}=\begin{cases}1, & \lambda>\xi\\ -1, & \lambda<\xi .\end{cases} \tag{2.18}$$

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

$$\nu_\mu(\lambda,k)=\nu_\mu(\lambda,k;p_\mu p_{\mu-1})$$
$$=\left[1-\delta\left[0,\sum_{j=k}^{N}(p_{\mu j}-p_{\mu-1 j})\right]\right]\{(k-k_{\max})[(1-\delta_{0,k_{\max}})+\delta_{0,k_{\max}}(1-\delta_{0,p_{\mu-10}})]+(1-h_\mu(\lambda,k)]\delta_{0,k_{\max}}\delta_{0,p_{\mu-10}}\}\ , \tag{2.19}$$

where $k_{\max}=\max\{j(1-\delta_{0,p_{\mu-1j}});j=0,\ldots,k-1\}$. Note that expression (2.19) is much easier to evaluate than expression (3.12) of Ref. 31. The evaluation of the set $\{j(1-\delta_{0,p_{\mu-1j}});j=0,\ldots,k-1\}$ can be made more efficient by restricting attention to the subcases $0\le j\le k-1$ when $k<\lambda$ and $\lambda\le j\le k-1$ when $k\ge\lambda$. Practically speaking, however, the search for a maximum index j involves only a few comparison operations in typical cases of interest. This search problem is anticipated to become significant only in rather esoteric applications (for example, in biological situations where the number of particles is very large). Further, it should be noted that in calculating the ratio of h_μ to $\hat{h}_\mu$ in (2.14) or (2.15) one should calculate ν_μ first, since: if $\nu_\mu=0$ then the ratio is 1 automatically; if all boxes in the WYT row are labeled μ then $\hat{h}_\mu=1$; otherwise, a nontrivial ratio exists.

Finally, we define the quantities

$$D_\mu(\lambda)=D_\mu(\lambda;p_\mu p'_\mu)$$
$$=\prod_{k=0}^{\lambda-2}\delta(p_{\mu k},p'_{\mu k})\prod_{k=\lambda+1}^{N}\delta(p_{\mu k},p'_{\mu k})\delta(p_{\mu\lambda}+1,p'_{\mu\lambda})\delta(p_{\mu\lambda-1}-1,p'_{\mu\lambda-1})\ , \tag{2.20}$$

$$\Gamma_B(\lambda,\mu)=\Gamma_B(\lambda,\mu;p_\mu p_{\mu-1}p'_{\mu-1})=\begin{cases}1, & p_{\mu-1}=S_t^- p_\mu \text{ and } p'_{\mu-1}=S_{t'}^- p_\mu\\ 0, & p_{\mu-1}\neq S_t^- p_\mu \text{ or } p'_{\mu-1}\neq S_{t'}^- p_\mu\end{cases} \tag{2.21}$$

$$\Gamma_A(\lambda,\mu)=\Gamma_A(\lambda,\mu;p_\mu p'_\mu p_{\mu-1})=\begin{cases}1, & p_{\mu-1}=S_t^- p_\mu \text{ and } p_{\mu-1}=S_{t'}^- p'_\mu\\ 0, & p_{\mu-1}\neq S_t^- p_\mu \text{ or } p_{\mu-1}\neq S_{t'}^- p'_\mu\end{cases} \tag{2.22}$$

for some t,t' consistent with the conditions (2.5) and (2.6). The factor $D_\mu(\lambda)$, together with the Γ factors, subjects the triplet of labels $p_\mu p_{\mu-1}p'_{\mu-1}$ ($p_\mu p'_\mu p_{\mu-1}$), in the case of B_μ (A_μ), to a consistency check and in this respect plays a role similar to a selection rule as do the triangularity conditions of Racah-Wigner (6-j) coefficients.

In cases where no ambiguity is likely to arise we shall suppress the p labels in the various function argument lists. However, we shall see below where, by retaining the explicit functional dependence on p, simplifications of the algebraic expressions can be easily derived. We shall take the expressions (2.13)–(2.22) to be *standard* in the sense that when the p arguments are omitted it is to be understood that the explicit arguments are those given above. Further, in our approach the actual evaluation of the numerical value of a matrix element of an operator is performed using only the ket labels; the combination of bra and ket labels is used to verify, using (2.20)–(2.22), whether the matrix element is nonzero. An immediate advantage to this is that Hermitian conjugation of matrix-element expressions is easily derived simply by interchanging primed and unprimed partition labels.

Note that a phase convention has been established in which all one-step operator matrix elements (labels $\mu-1$ changing to μ, or vice versa) are assumed positive. All subsequent phase information is derived from this basic assumption and the Lie bracket relations (2.10).

The matrix elements of *multi-step* generators $E_{\mu,\nu}$ and their products can, in principle, be calculated using the result obtained from (2.10),

$$E_{\mu,\nu}=E_{\mu,\mu\pm1}E_{\mu\pm1,\nu}-E_{\mu\pm1,\nu}E_{\mu,\mu\pm1}\ ,$$

applied recursively, accounting for all possible intermediate states. This involves performing extensive sparse matrix multiplication involving only the matrices of one-step generators (2.12) and is a very inefficient procedure, primarily due to the associated problem of properly enumerating all intermediate states. Alternatively, as shown by a number of workers[13,18,29] and especially Ref. 32, it is possible to reduce the computational complexity significantly by using factorized expressions in which the relevant factors corresponds to subgraphs defined in terms of labels at levels μ and $\mu-1$ only.

We express the matrix element of the generator $E_{\mu,\nu}$ as the product of factors

$$\langle p_n\{T'\}|E_{\mu,\nu}|p_n\{T\}\rangle$$
$$=\Delta_\nu^n B_\nu(\lambda_{\nu-1})\prod_{\tau=\mu+1}^{\nu-1}T_\tau(\lambda_\tau,\lambda_{\tau-1})A_\mu(\lambda_\mu)\Delta_0^\mu\ , \tag{2.23}$$

where λ_τ refers to the pivot index relevant to level τ.

Using the definitions of A (tail) and B (head) subgraph factors above we write[31] the (intermediate) subgraph factors $T_\gamma(\lambda,\xi)$,

$$T_\gamma(\lambda,\xi)=T_\gamma(\lambda,\xi;p_\gamma p'_\gamma p_{\gamma-1}p'_{\gamma-1})$$
$$=B_\gamma(\xi;p'_\gamma p_{\gamma-1}p'_{\gamma-1})A_\gamma(\lambda;p_\gamma p'_\gamma p_{\gamma-1})$$
$$-A_\gamma(\lambda;p_\gamma p'_\gamma p'_{\gamma-1})B_\gamma(\xi;p_\gamma p_{\gamma-1}p'_{\gamma-1})\ . \tag{2.24}$$

Due to the $\Gamma_A(\lambda,\gamma)$ and $\Gamma_B(\xi,\gamma)$ factors contained in the expression above [see (2.14) and (2.15)] it is often the case that only one of the two terms contributes to the evaluation of T_γ. In such cases the total amount of computation required is governed by the computations for each of A and B. When both terms contribute, however, it is possible to simplify the expression and thereby avoid the otherwise doubling of computation (actually, when computing with rational numbers, it is also necessary to include the computation which determines the difference of the two terms, a situation which is complicated by the necessary use of arbitrary precision arithmetic[34]).

First we note that the effect of the generator $E_{\mu-1,\mu}$ on the state $|p_n\{T\}\rangle$ is to alter only the labels $p_{\mu-1}$; leaving all other labels unaltered. Hence writing states in the form $|p_n\{T\}\rangle=|\{p\}\rangle=|\{p_np_{n-1}\cdots p_1\}\rangle$, we have that

$$E_{\mu-1,\mu}|\{p\}\rangle=\sum_{\{p'\}}\langle\{p'\}|E_{\mu-1,\mu}|\{p\}\rangle|\{p'\}\rangle$$
$$=\sum_{\lambda=1}^{L}\langle\{p_n\cdots p_{\mu-1}+\partial_{\mu-1\lambda}\cdots p_1\}|E_{\mu-1,\mu}|\{p\}\rangle|\{p_n\cdots p_{\mu-1}+\partial_{\mu-1\lambda}\cdots p_1\}\rangle\ , \tag{2.25}$$

where we define $\partial_{\tau\lambda}$ as an operator[35] which acts on the p_τ labels according to the component relations

$$p'_{\tau k}=p_{\tau k}+\partial_{\tau\lambda k}=p_{\tau k}+\delta_{\lambda,k}-\delta_{\lambda-1,k}\quad\forall k\le L \tag{2.26}$$

and where the label changes are performed at the index positions λ and $\lambda-1$. Note that, at most, L states can be generated by application of $E_{\mu-1,\mu}$.

Using (2.3a), (2.6a), (2.16)–(2.19), and (2.26) and assuming $p'_\tau=p_\tau+\partial_{\tau\lambda}$ and $p'_{\tau-1}=p_{\tau-1}+\partial_{\tau-1\xi}$, it is possible to derive the results

$$h_\tau(\xi,\lambda;p_\tau+\partial_{\tau\lambda})=h_\tau(\xi,\lambda-1;p_\tau)+\epsilon_{\lambda\xi}p_{\tau\lambda-1}\ , \tag{2.27}$$

$$\hat{h}_\tau(\xi,\lambda;p_\tau+\partial_{\tau\lambda}p_{\tau-1})=\begin{cases}\hat{h}_\tau(\xi,\lambda-1;p_\tau p_{\tau-1}), & p_{\tau\lambda-1}=1\\ h_\tau(\xi,\lambda;p_\tau+\partial_{\tau\lambda})-\epsilon_{\lambda\xi}, & p_{\tau\lambda-1}>1\end{cases} \tag{2.28}$$

$$h_\tau(\lambda,k_\xi;p_\tau p_{\tau-1}+\partial_{\tau-1\xi})=h_\tau(\lambda,k_\xi;p_\tau p_{\tau-1})\ , \tag{2.29}$$

$$\hat{h}_\tau(\lambda,k_\xi;p_\tau p_{\tau-1}+\partial_{\tau-1\xi})=\hat{h}_\tau(\lambda,k_\xi;p_\tau p_{\tau-1})-\epsilon_{\lambda\xi}\ , \tag{2.30a}$$

$$\hat{h}_\tau(\lambda,k_\xi;p_\tau p_{\tau-1})=h_\tau(\xi,\lambda;p_\tau+\partial_{\tau\lambda})\ , \tag{2.30b}$$

where $k_\xi=\min\{k\,[1-\delta(0,p_{\tau k})];k=\xi,\ldots,L\}$ is the length of a WYT row containing label τ in column ξ.

From (2.27) and (2.28) it follows that

$$B_\tau(\xi;p_\tau+\partial_{\tau\lambda}p_{\tau-1}p_{\tau-1}+\partial_{\tau-1\xi})=B_\tau(\xi;p_\tau p_{\tau-1}p_{\tau-1}+\partial_{\tau-1\xi})\left[\frac{h_\tau(\xi,\lambda-1)+\epsilon_{\lambda\xi}p_{\tau\lambda-1}}{h_\tau(\xi,\lambda-1)+\epsilon_{\lambda\xi}(p_{\tau\lambda-1}-1)}\right]^{1/2}. \tag{2.31}$$

Similarly, using (2.29) and (2.30) we find

$$A_\tau(\lambda;p_\tau p_\tau+\partial_{\tau\lambda}p_{\tau-1}+\partial_{\tau-1\xi})=A_\tau(\lambda;p_\tau p_\tau+\partial_{\tau\lambda}p_{\tau-1})\left[\frac{\hat{h}_\tau(\lambda,k_\xi;p_\tau p_{\tau-1}+\partial_{\tau-1\xi})-\epsilon_{\lambda\xi}}{\hat{h}_\tau(\lambda,k_\xi;p_\tau p_{\tau-1}+\partial_{\tau-1\xi})}\right]^{1/2}$$
$$=A_\tau(\lambda;p_\tau p_\tau+\partial_{\tau\lambda}p_{\tau-1})\left[\frac{h_\tau(\xi,\lambda-1)+\epsilon_{\lambda\xi}(p_{\tau\lambda-1}-1)}{h_\tau(\xi,\lambda-1)+\epsilon_{\lambda\xi}p_{\tau\lambda-1}}\right]^{1/2}. \tag{2.32}$$

With the results (2.31) and (2.32) in (2.24), assuming both terms are nonzero and $p'_\tau=p_\tau+\partial_{\tau\lambda}$ and $p'_{\tau-1}=p_{\tau-1}+\partial_{\tau-1\xi}$, we find the simplified form

$$T_\tau(\lambda,\xi)=B_\tau(\xi;p_\tau p_{\tau-1}p'_{\tau-1})A_\tau(\lambda;p_\tau p'_\tau p_{\tau-1})C_\tau(\lambda,\xi;p_\tau)\ , \tag{2.33}$$

where

$$C_\tau(\lambda,\xi)=\epsilon_{\lambda\xi}\{[h_\tau(\xi,\lambda-1)+\epsilon_{\lambda\xi}(p_{\tau\lambda-1}-1)]\times[h_\tau(\xi,\lambda-1)+\epsilon_{\lambda\xi}p_{\tau\lambda-1}]\}^{-1/2}\ . \tag{2.34}$$

We note that the forms of T_γ and C_τ presented above differ from expressions (3.18′) and (3.19) presented in Ref. 31, but reduce to those special cases when $p_{\tau\lambda-1}=1$. The forms that we have chosen permit the numerical value of matrix elements of the $E_{\mu,\nu}$ operators to be determined solely from the ket (p) labels (recall that the selection rules require information about both states, however). Thus (2.33) is in standard form in this respect. In Refs. 31 and 32 we used a mixed notation in which both bra and ket labels were used. This can lead to some confusion, however, in the application of the results. [Indeed, there is an error in Eq. (3.19) of Ref. 31 which, in turn, led to an error in our second example numerical calculation in that paper.]

The generator product matrix elements that we shall be concerned with in Sec. III are those pertaining to the evaluation of the symmetric product of two generators, namely,

$$\{E_{\mu,\nu},E_{\alpha,\beta}\}=E_{\mu,\nu}E_{\alpha,\beta}+E_{\alpha,\beta}E_{\mu,\nu} .$$

We choose to evaluate these operator products primarily because they lead to rather symmetrical expressions in our factorization scheme. Further analysis of the *two-body*-operator matrix-element expressions is facilitated by considering subcases based on the relative values of the indices μ, ν, α, and β.

III. RAISING-RAISING OPERATORS

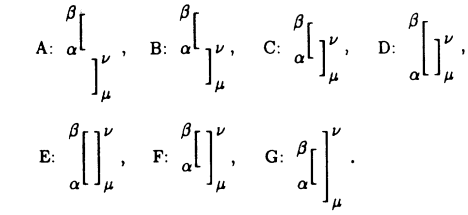
The raising-raising (RR) [lowering-lowering (LL)] subcases assume the relations on the elementary generator indices

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

The LL subcases are derived from these by finding the Hermitian conjugate of the matrix-element expressions for the RR subcases, hence

$$\langle T'|\{E_{\mu,\nu},E_{\alpha,\beta}\}|T\rangle^*=\langle T|\{E_{\nu,\mu},E_{\beta,\alpha}\}|T'\rangle .$$

It is useful to decompose the RR subcases into further subcases 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:



In all the cases we consider $\mu\le\alpha$; 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.

Before proceeding we state one further simplification in notation, namely, that states are written in the form $|T\rangle=|p_n\{T\}\rangle$.

Case A: $\mu<\nu<\alpha<\beta$. This case is referred to as *nonoverlapping,* or disjoint; the range of application of one generator, $E_{\mu,\nu}$, is completely out of the range of the other, $E_{\alpha,\beta}$. The matrix-element expression immediately reduces to the form

$$\langle T'|\{E_{\mu,\nu},E_{\alpha,\beta}\}|T\rangle=2\Delta_\beta^n B_\beta(\lambda_{\beta-1})\prod_{\rho=\alpha+1}^{\beta-1}T_\rho(\lambda_\rho,\lambda_{\rho-1})A_\alpha(\lambda_\alpha)\Delta_\nu^{\alpha-1}B_\nu(\lambda_{\nu-1})\prod_{\tau=\mu+1}^{\nu-1}T_\tau(\lambda_\tau,\lambda_{\tau-1})A_\mu(\lambda_\mu)\Delta_0^{\mu-1} . \tag{3.1}$$

Case B: $\mu<\nu=\alpha<\beta$. Cases in which one index, pertaining to one of the generators, is equal to an index pertaining to the other generator are referred to as *contact* cases. Thus this case involves nonoverlapping contact between the operator ranges:

$$\langle T'|\{E_{\mu,\nu}E_{\nu,\beta}\}|T\rangle=\Delta_\beta^n B_\beta(\lambda_{\beta-1})\prod_{\rho=\nu+1}^{\beta-1}T_\rho(\lambda_\rho,\lambda_{\rho-1})W_\nu(\lambda_\nu,\lambda_{\nu-1})\prod_{\tau=\mu+1}^{\nu-1}T_\tau(\lambda_\tau,\lambda_{\tau-1})A_\mu(\lambda_\mu)\Delta_0^{\mu-1} , \tag{3.2}$$

where the scalar factor $W_\gamma(\lambda,\xi)$ is similar to $T_\gamma(\lambda,\xi)$, differing only in the relative sign of the two terms below [see Eq. (2.24)], hence

$$W_\gamma(\lambda,\xi)=A_\gamma(\lambda;p_\gamma p'_\gamma p_{\gamma-1})B_\gamma(\xi;p'_\gamma p_{\gamma-1}p'_{\gamma-1})+A_\gamma(\lambda;p_\gamma p'_\gamma p'_{\gamma-1})B_\gamma(\xi;p_\gamma p_{\gamma-1}p'_{\gamma-1}) . \tag{3.3}$$

When both terms above are nonzero this simplifies to the form

$$W_\gamma(\lambda,\xi)=A_\gamma(\lambda;p_\gamma p'_\gamma p_{\gamma-1})B_\gamma(\xi;p_\gamma p_{\gamma-1}p'_{\gamma-1})\tilde{C}_\gamma(\lambda,\xi;p_\gamma p_{\gamma-1}) \tag{3.4}$$

[compare with (2.33)], where $\tilde{C}_\gamma(\lambda,\xi)$ is defined as

$$\begin{aligned}\tilde{C}_\gamma(\lambda,\xi)=&\{2[h_\gamma(\xi,\lambda-1)+\epsilon_{\lambda\xi}p_{\gamma\lambda-1}]-\epsilon_{\lambda\xi}\}\\&\times\{[h_\gamma(\xi,\lambda-1)+\epsilon_{\lambda\xi}(p_{\gamma\lambda-1}-1|)][h_\gamma(\xi,\lambda-1)+\epsilon_{\lambda\xi}p_{\gamma\lambda-1}]\}^{-1/2} .\end{aligned} \tag{3.5}$$

Case C: $\mu<\alpha<\nu<\beta$. These cases are referred to as *partial overlapping.* The matrix-element expressions are given as

$$\begin{aligned}\langle T'|\{E_{\mu,\nu},E_{\alpha,\beta}\}|T\rangle=&\Delta_\beta^n B_\beta(\lambda_{\beta-1})\prod_{\rho=\nu+1}^{\beta-1}T_\rho(\lambda_\rho,\lambda_{\rho-1})\tilde{F}_\nu(\lambda_\nu,\lambda_{\nu-1}^1,\lambda_{\nu-1}^2)\prod_{\kappa=\alpha+1}^{\nu-1}\tilde{T}_\kappa(\lambda_\kappa^1,\lambda_\kappa^2,\lambda_{\kappa-1}^1,\lambda_{\kappa-1}^2)\tilde{G}_\alpha(\lambda_\alpha^1,\lambda_\alpha^2,\lambda_{\alpha-1})\\&\times\prod_{\tau=\mu+1}^{\alpha-1}T_\tau(\lambda_\tau,\lambda_{\tau-1})A_\mu(\lambda_\mu)\Delta_0^{\mu-1} ,\end{aligned} \tag{3.6}$$

where the factors $\tilde{F}_\nu$, $\tilde{G}_\alpha$, and $\tilde{T}_\kappa$ will be defined below following case G. Factors $\tilde{F}$ and $\tilde{G}$ are two-element row and column vectors, respectively; $\tilde{T}$ is a 2×2 matrix. The two distinct pivot indices λ_τ^i, $i=1,2$, effective within the overlap range $\alpha-\nu$ are distinguished by an additional superscript. We assume $\lambda_\tau^1<\lambda_\tau^2$ in all cases; hence the operative nodes in the overlap region $\alpha-\nu$ are lexically ordered such that $p'_\tau<p_\tau^1<p_\tau^2<p_\tau$ (appearing as graph nodes in order from left to right; see Ref. 27).

Case D: $\mu=\alpha<\nu<\beta$:

$$\langle T'|\{E_{\mu,\nu},E_{\mu,\beta}\}|T\rangle=\Delta_\beta^n B_\beta(\lambda_{\beta-1})\prod_{\rho=\nu+1}^{\beta-1}T_\rho(\lambda_\rho,\lambda_{\rho-1})\tilde{F}_\nu(\lambda_\nu,\lambda_{\nu-1}^1,\lambda_{\nu-1}^2)\prod_{\kappa=\mu+1}^{\nu-1}\tilde{T}_\kappa(\lambda_\kappa^1,\lambda_\kappa^2,\lambda_{\kappa-1}^1,\lambda_{\kappa-1}^2)\tilde{A}_\mu(\lambda_\mu^1,\lambda_\mu^2)\Delta_0^{\mu-1}\ , \tag{3.7}$$

where the factor $\tilde{A}_\mu$, a column vector, is defined following case G.

Case E: $\mu=\alpha<\nu=\beta$;

$$\langle T'|E_{\mu,\nu}E_{\mu,\nu}|T\rangle=\Delta_\nu^n\tilde{B}_\nu(\lambda_{\nu-1}^1,\lambda_{\nu-1}^2)\prod_{\kappa=\mu+1}^{\nu-1}\tilde{T}_\kappa(\lambda_\kappa^1,\lambda_\kappa^2,\lambda_{\kappa-1}^1,\lambda_{\kappa-1}^2)\tilde{A}_\mu(\lambda_\mu^1,\lambda_\mu^2)\Delta_0^{\mu-1}\ , \tag{3.8}$$

where the factor $\tilde{B}_\nu$, a row vector, is defined following case G.

Case F: $\mu<\alpha<\nu=\beta$:

$$\langle T'|\{E_{\mu,\nu},E_{\alpha,\nu}|T\rangle=\Delta_\nu^n\tilde{B}_\nu(\lambda_{\nu-1}^1,\lambda_{\nu-1}^2)\prod_{\kappa=\alpha+1}^{\nu-1}\tilde{T}_\kappa(\lambda_\kappa^1,\lambda_\kappa^2,\lambda_{\kappa-1}^1,\lambda_{\kappa-1}^2)\tilde{G}_\alpha(\lambda_\alpha^1,\lambda_\alpha^2,\lambda_{\alpha-1})\prod_{\tau=\mu+1}^{\alpha-1}T_\tau(\lambda_\tau,\lambda_{\tau-1})A_\mu(\lambda_\mu)\Delta_0^{\mu-1}\ . \tag{3.9}$$

Case G: $\mu<\alpha<\beta<\nu$:

$$\langle T'|\{E_{\mu,\nu},E_{\alpha,\beta}|T\rangle=\Delta_\nu^n B_\nu(\lambda_{\nu-1})\prod_{\rho=\beta+1}^{\nu-1}T_\rho(\lambda_\rho,\lambda_{\rho-1})\tilde{F}_\beta(\lambda_\beta,\lambda_{\beta-1}^1,\lambda_{\beta-1}^2)\prod_{\kappa=\alpha+1}^{\beta-1}\tilde{T}_\kappa(\lambda_\kappa^1,\lambda_\kappa^2,\lambda_{\kappa-1}^1,\lambda_{\kappa-1}^2)\tilde{G}_\alpha(\lambda_\alpha^1,\lambda_\alpha^2,\lambda_{\alpha-1})\times\prod_{\tau=\mu+1}^{\alpha-1}T_\tau(\lambda_\tau,\lambda_{\tau-1})A_\mu(\lambda_\mu)\Delta_0^{\mu-1}\ . \tag{3.10}$$

In the cases C–G above the quantities $\tilde{A}_\gamma(\lambda,\xi)$, $\tilde{B}_\gamma(\lambda,\xi)$, $\tilde{F}_\gamma(\rho,\lambda,\xi)$, $\tilde{G}_\gamma(\rho,\lambda,\xi)$, and $\tilde{T}_\gamma(\lambda,\xi,\varphi,\psi)$ were introduced; they are defined below (using Q^T to denote the transpose of the matrix Q):

$$\tilde{B}_\gamma^T(\lambda,\xi)=\begin{bmatrix}B_\gamma(\xi;p_\gamma p_{\gamma-1}p_{\gamma-1}^1)B_\gamma(\lambda;p_\gamma p_{\gamma-1}^1p'_{\gamma-1})\\B_\gamma(\lambda;p_\gamma p_{\gamma-1}p_{\gamma-1}^2)B_\gamma(\xi;p_\gamma p_{\gamma-1}^2p'_{\gamma-1})\end{bmatrix}\ . \tag{3.11}$$

The notation p_τ^i used above refers to the use of the intermediate-state node derived from applying a raising operation, $p_\tau^i=p_\tau+\partial_{\tau\lambda}i$, *first* at the pivot point λ^i.

In cases where both elements above are nonzero (two intermediate states exist) (3.11) can be simplified. In addition to (2.27)–(2.30) we require the results

$$B_\tau(\xi;p_\tau p_{\tau-1}+\partial_{\tau-1\lambda}p_{\tau-1}+\partial_{\tau-1\lambda}+\partial_{\tau-1\xi})=B_\tau(\xi;p_\tau p_{\tau-1}p_{\tau-1}+\partial_{\tau-1\xi})\left[\frac{h_{\tau-1}(\xi,\lambda-1)+\epsilon_{\lambda\xi}p_{\tau-1\lambda-1}}{h_{\tau-1}(\xi,\lambda-1)+\epsilon_{\lambda\xi}(p_{\tau-1\lambda-1}+1)}\right]^{1/2}\ , \tag{3.12}$$

$$A_\tau(\xi;p_\tau+\partial_{\tau\lambda}p_\tau+\partial_{\tau\lambda}+\partial_{\tau\xi}p_{\tau-1})=A_\tau(\xi;p_\tau p_\tau+\partial_{\tau\xi}p_{\tau-1})\left[\frac{h_\tau(\xi,\lambda-1)+\epsilon_{\lambda\xi}(p_{\tau\lambda-1}-1)}{h_\tau(\xi,\lambda-1)+\epsilon_{\lambda\xi}p_{\tau\lambda-1}}\right]^{1/2}\ , \tag{3.13}$$

and, recalling that $\lambda^1<\lambda^2$,

$$h_{\tau-1}(\lambda^1,\lambda^2-1)+p_{\tau-1\lambda^2-1}=h_{\tau-1}(\lambda^2,\lambda^1-1)-p_{\tau-1\lambda^1-1}\ . \tag{3.14}$$

From (3.12)–(3.14) it follows that (abbreviating $\rho=\lambda^1$ and $\sigma=\lambda^2$)

$$\tilde{B}_\tau^T(\rho,\sigma)=B_\tau(\rho;p_\tau p_{\tau-1}p_{\tau-1}^1)B_\tau(\sigma;p_\tau p_{\tau-1}p_{\tau-1}^2)[h_{\tau-1}(\rho,\sigma-1)+p_{\tau-1\lambda-1}]^{1/2}\begin{bmatrix}[h_{\tau-1}(\rho,\sigma-1)+p_{\tau-1\lambda-1}-1]^{-1/2}\\[h_{\tau-1}(\rho,\sigma-1)+p_{\tau-1\lambda-1}+1]^{-1/2}\end{bmatrix}\ . \tag{3.15}$$

Similarly,

$$\tilde{A}_\gamma(\lambda,\xi)=\begin{bmatrix}A_\gamma(\xi;p_\gamma p_\gamma^1p_{\gamma-1})A_\gamma(\lambda;p_\gamma^1p'_\gamma p_{\gamma-1})\\A_\gamma(\lambda;p_\gamma p_\gamma^2p_{\gamma-1})A_\gamma(\xi;p_\gamma^2p'_\gamma p_{\gamma-1})\end{bmatrix}\ . \tag{3.16}$$

In cases where both terms in the matrix are nonzero this simplifies to the form (again with $\rho=\lambda^1$ and $\sigma=\lambda^2$)

$$\tilde{A}_\tau(\rho,\sigma)=A_\tau(\rho;p_\tau p_\pi^1 p_{\tau-1})A_\tau(\sigma;p_\tau p_\pi^2 p_{\tau-1})[h_\tau(\rho,\sigma-1)+p_{\tau\lambda-1}]^{-1/2}\begin{bmatrix}[h_\tau(\rho,\sigma-1)+p_{\tau\lambda-1}+1]^{1/2}\\ [h_\tau(\rho,\sigma-1)+p_{\tau\lambda-1}-1]^{1/2}\end{bmatrix}. \tag{3.17}$$

The individual matrix elements of the $\tilde{F}_\gamma(\rho,\lambda,\xi)$ matrices are defined as

$$\tilde{F}^{\,i}_\gamma(\rho,\lambda,\xi)=B_\gamma(\xi;p_\gamma p_{\gamma-1}p^i_{\gamma-1})T_\gamma(\rho,\lambda;p_\gamma p'_\gamma p^i_{\gamma-1}p'_{\gamma-1})+B_\gamma(\lambda;p'_\gamma p^i_{\gamma-1}p'_{\gamma-1})T_\gamma(\rho,\xi;p_\gamma p'_\gamma p_{\gamma-1}p^i_{\gamma-1}), \tag{3.18}$$

where $i=1,2$ for the first and second elements, respectively. Due to the treatment of the symmetrized product of generators being considered the sums above contain terms which cancel. In general, these expressions reduce to the forms

$$\begin{aligned}\tilde{F}^{\,i}_\gamma(\rho,\lambda,\xi)=&\,B_\gamma(\xi;p'_\gamma p_{\gamma-1}p^i_{\gamma-1})B_\gamma(\lambda;p^i_\gamma p'_{\gamma-1})A_\gamma(\rho;p_\gamma p'_\gamma p_{\gamma-1})\\ &-B_\gamma(\xi;p_\gamma p_{\gamma-1}p^i_{\gamma-1})B_\gamma(\lambda;p_\gamma p^i_{\gamma-1}p'_{\gamma-1})A_\gamma(\rho;p_\gamma p'_\gamma p'_{\gamma-1}),\end{aligned} \tag{3.19}$$

which can be rewritten in terms of the $\tilde{B}_\gamma$ matrices as

$$\tilde{F}_\gamma(\rho,\lambda,\xi)=A_\gamma(\rho;p_\gamma p'_\gamma p_{\gamma-1})\tilde{B}_\gamma(\lambda,\xi;p'_\gamma p_{\gamma-1}p^1_{\gamma-1}p^2_{\gamma-1})-A_\gamma(\rho;p_\gamma p'_\gamma p'_{\gamma-1})\tilde{B}_\gamma(\lambda,\xi;p_\gamma p_{\gamma-1}p^1_{\gamma-1}p^2_{\gamma-1}). \tag{3.20}$$

Additional simplification of the expressions can be derived in cases where both terms are nonzero. For instance, depending on the relative values of the indices ρ and λ and ξ we find from (2.32) (recall that $p'_\gamma=p_\gamma+\partial_{\gamma\rho}$ and $p'_{\gamma-1}=p_{\gamma-1}+\partial_{\gamma-1\lambda}+\partial_{\gamma-1\xi}$)

$$A_\gamma(\rho;p_\gamma p'_\gamma p'_{\gamma-1})=A_\gamma(\rho;p_\gamma p'_\gamma p_{\gamma-1})\left[\frac{h_\gamma(\rho,\lambda-1)+\epsilon_{\lambda\rho}(p_{\gamma\lambda-1}-1)}{h_\gamma(\rho,\lambda-1)+\epsilon_{\lambda\rho}p_{\gamma\lambda-1}}\,\frac{h_\gamma(\rho,\xi-1)+\epsilon_{\xi\rho}(p_{\gamma\xi-1}-1)}{h_\gamma(\rho,\xi-1)+\epsilon_{\xi\rho}p_{\gamma\xi-1}}\right]^{1/2}. \tag{3.21}$$

Similarly, the two $\tilde{B}_\gamma$ matrices appearing in (3.20) are related by a simple multiplicative factor

$$\tilde{B}_\gamma(\rho;p'_\gamma p_{\gamma-1}p'_{\gamma-1})=\tilde{B}_\gamma(\rho;p_\gamma p_{\gamma-1}p'_{\gamma-1})\left[\frac{h_\gamma(\xi,\rho-1)+\epsilon_{\rho\xi}p_{\gamma\rho-1}}{h_\gamma(\xi,\rho-1)+\epsilon_{\rho\xi}(p_{\gamma\rho-1}-1)}\,\frac{h_\gamma(\lambda,\rho-1)+\epsilon_{\rho\lambda}p_{\gamma\rho-1}}{h_\gamma(\lambda,\rho-1)+\epsilon_{\rho\lambda}(p_{\gamma\rho-1}-1)}\right]^{1/2} \tag{3.22}$$

such that the final form of $\tilde{F}_\gamma$ involves, at most, the multiplication of a coefficient, A_γ and the $\tilde{B}_\gamma$ subgraph factor (3.15).

Proceeding in a similar fashion we find for the $\tilde{G}_\gamma$ matrices the expressions

$$\tilde{G}_\gamma(\rho,\lambda,\xi)=B_\gamma(\rho;p'_\gamma p_{\gamma-1}p'_{\gamma-1})\tilde{A}_\gamma(\lambda,\xi;p_\gamma p^1_\gamma p^2_\gamma p_{\gamma-1})-B_\gamma(\rho;p_\gamma p_{\gamma-1}p_{\gamma-1})\tilde{A}_\gamma(\lambda,\xi;p_\gamma p^1_\gamma p^2_\gamma p'_{\gamma-1}). \tag{3.23}$$

When both terms are nonzero the following relations, derived using (2.31), can be used to further reduce the amount of computation:

$$B_\gamma(\rho;p_\gamma p'_\gamma p'_{\gamma-1})=B_\gamma(\rho;p_\gamma p'_\gamma p_{\gamma-1})\left[\frac{h_\gamma(\rho,\lambda-1)+\epsilon_{\lambda\rho}p_{\gamma\lambda-1}}{h_\gamma(\rho,\lambda-1)+\epsilon_{\lambda\rho}(p_{\gamma\lambda-1}-1)}\,\frac{h_\gamma(\rho,\xi-1)+\epsilon_{\xi\rho}p_{\gamma\xi-1}}{h_\gamma(\rho,\xi-1)+\epsilon_{\xi\rho}(p_{\gamma\xi-1}-1)}\right]^{1/2}, \tag{3.24}$$

$$\tilde{A}_\gamma(\rho;p'_\gamma p_{\gamma-1}p'_{\gamma-1})=\tilde{A}_\gamma(\rho;p_\gamma p_{\gamma-1}p'_{\gamma-1})\left[\frac{h_\gamma(\xi,\rho-1)+\epsilon_{\rho\xi}(p_{\gamma\rho-1}-1)}{h_\gamma(\xi,\rho-1)+\epsilon_{\rho\xi}p_{\gamma\rho-1}}\,\frac{h_\gamma(\xi,\rho-1)+\epsilon_{\rho\lambda}(p_{\gamma\rho-1}-1)}{h_\gamma(\lambda,\rho-1)+\epsilon_{\rho\lambda}p_{\gamma\rho-1}}\right]^{1/2}. \tag{3.25}$$

The greatest degree of computational complexity arises in the evaluation of the $\tilde{T}_\gamma$ matrices occurring in the overlap range of the generator product:

$$\begin{aligned}&\tilde{T}_\gamma(\lambda,\xi,\varphi,\psi)\\ &=\begin{bmatrix}T_\gamma(\xi,\varphi;p_\gamma p^1_\gamma p_{\gamma-1}p^1_{\gamma-1})T_\gamma(\lambda,\psi;p^1_\gamma p'_\gamma p^1_{\gamma-1}p'_{\gamma-1}) & T_\gamma(\xi,\psi;p_\gamma p^1_\gamma p_{\gamma-1}p^2_{\gamma-1})T_\gamma(\lambda,\varphi;p^1_\gamma p'_\gamma p^2_{\gamma-1}p'_{\gamma-1})\\ T_\gamma(\lambda,\varphi;p_\gamma p^2_\gamma p_{\gamma-1}p^1_{\gamma-1})T_\gamma(\xi,\psi;p^2_\gamma p'_\gamma p^1_{\gamma-1}p'_{\gamma-1}) & T_\gamma(\lambda,\psi;p_\gamma p^2_\gamma p_{\gamma-1}p^2_{\gamma-1})T_\gamma(\xi,\varphi;p^2_\gamma p'_\gamma p^2_{\gamma-1}p'_{\gamma-1})\end{bmatrix}.\end{aligned} \tag{3.26}$$

As might be expected from previous subgraph factors there are numerous simplifications which arise when we consider subcases. The worst case, in terms of computations, occurs when all four matrix elements are nonzero *and* when both terms of each T_γ factor are nonzero. In such cases (3.26) simplifies to the form

$$\tilde{T}_\gamma(\lambda,\xi,\varphi,\psi)=A_\gamma(\lambda;p_\gamma p^2_\gamma p_{\gamma-1})A_\gamma(\xi;p_\gamma p^1_\gamma p_{\gamma-1})B_\gamma(\varphi;p_\gamma p_{\gamma-1}p^2_{\gamma-1})B_\gamma(\psi;p_\gamma p_{\gamma-1}p^1_{\gamma-1})\tilde{M}_\gamma(\lambda,\xi,\varphi,\psi), \tag{3.27}$$

where the elements of the 2×2 matrix $\tilde{M}_\gamma(\lambda,\xi,\varphi,\psi)$ are comprised of simple combinations of hooklength ratios.

The results presented in this section are intended to demonstrate the techniques used for defining the graphical factors which arise in raising-raising matrix-element calculations as well as the application of fundamental rules, a calculus in other words, by which specific simplifications of these factors may be obtained. The fundamental quantities in this respect are the subgraphs A and B from which all other higher-order graphs are defined. Though the results presented herein are completely general we have not attempted to cover explicitly

all of the many special cases which do occur. These can be derived, however, by the use of the algebra based on expressions (2.27)–(2.32) and (3.12)–(3.14).

IV. CONCLUSIONS

We have presented a detailed exposition of the algebraic methods used to derive specific subgraph factors pertinent to the efficient evaluation of raising-raising matrix elements of the U(n) group generators. 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 use of 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.

As part of the presentation we have introduced a number of essential algebraic relations, notably expressions (2.27)–(2.32) and (3.12)–(3.14) which facilitate the derivations of simplified forms for higher-order graphical factors. As such, these relations form the basis for a calculus based on the graphical techniques of Ref. 31, in particular, the elementary subgraphs A and B.

The treatment of the raising-lowering (lowering-raising) operator matrix elements will be the subject of the next paper in this series.

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