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Particle-hole formulation of the unitary group approach to the many-electron correlation problem. II. Matrix element evaluation

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Graphical methods of spin algebras are used to derive the expressions for the matrix elements of the total particle-number-conserving operators in the basis of hole-particle states, adapted to the chain $U(n'+n'') \supset U(n') \otimes U(n'')$, where n' and n'' designate dimensions of particle and hole subspaces, respectively. The matrix elements are expressed as a product of segment values, each associated with one orbital level as in the particle formalism, and of an additional segment value, representing a linkage of the hole and particle subspaces. It is shown that the particle formalism segment values can be used throughout except for the link segment, whose possible values are derived. An example of hole-particle bases and of their graphical representations is given and the advantages of the hole-particle formalism in shell-model calculations are outlined. An extension of this formalism to particle-number-nonconserving operators, needed in applications involving the mp-nh propagators with $m \neq n$, m, $n = 0$, 1, and 2, is discussed.

I. INTRODUCTION

The fundamental ideas of the unitary group approach (UGA) to the many-body problem were originally set forth by Moshinsky.[1] This approach becomes particularly suitable and simple when applied to the many-electron correlation problem as follows from the basic formalism and expressions for the construction of $U(n)$ spin-adapted bases, and the evaluation of the matrix elements of a spin-independent Hamiltonian in these bases developed by one of us.[2] These results were further extended by Shavitt[3] who proposed a highly suitable representation of the electronic Gelfand-Tsetlin (GT) basis[2] and a direct evaluation of nonelementary generator matrix elements based on their factorization as a product of contributions, each associated with a single orbital level.

A similar factorization was also achieved by Gouyet *et al.*[4] (GSS), Drake and Schlesinger[5] (DS), and Sasaki,[6] although in a different manner based on the SU(2) approach via the classical angular-momentum theory. Drake and Schlesinger,[5] in particular, showed that the matrix elements of products of two generators could also be factorized directly. A number of these results have been exploited in the meantime in several very diverse and most promising implementations,[7-9] based essentially on the idea of a so-called direct configuration-interaction (CI) approach.[10]

The present paper is the fourth in a series of papers dealing with the application of the graphical methods of spin algebras[11-13] in the UGA to the many-electron correlation problem. In the first paper[14] we described a general diagrammatic approach, based on the generalized Wick theorem[15] and graphical methods of spin algebras,[11-13] for the construction of geminally antisymmetric states[16] and for the evaluation of matrix elements of particle number-preserving operators between such states. In a subsequent paper[17] these ideas, together with those of the matrix-element factorization of Shavitt[3] and the evaluation of matrix elements of two-electron operators of Drake and Schlesinger,[5] were applied to obtain the particle-formalism UGA based expressions for one- and two-electron spin-independent operator matrix elements. These matrix elements were expressed as the product of segment values, each associated with a single orbital level. The various segment types needed were enumerated, all nonzero values for each segment type were tabulated, and various aspects of this formalism which will further simplify CI calculations were explicitly indicated. Since the results of this paper build upon those of Ref. 17, we present in the next section a brief review of the particle formalism.

Finally, the preceding paper[18] (referred to as I) and this paper deal with the extension of these particle-formalism results to the hole-particle formalism. The first hole-particle formulation of the UGA was made by Flores and Moshinsky.[19] However, as pointed out in I, our approach differs significantly from theirs. In I we outlined the general theory, identifying the structure of the necessary unitary group irreducible representations (irreps) and discussing the Yamanouchi-Kotani (YK)-type basis of particle-hole states. In this paper, the YK basis is explicitly constructed, and the expressions which yield the matrix elements of single generators and products of generators are derived. We also briefly discuss a generalization of this formalism to particle number-nonconserving systems.

II. REVIEW OF THE PARTICLE FORMALISM

We are interested in providing an efficient algorithm for the evaluation of the matrix elements of the spin-independent many-electron model Hamiltonian

$$H=\sum_{i,j}\langle i|h|j\rangle\sum_{m}X^{\dagger}_{im}X_{jm}+\tfrac{1}{2}\sum_{i,j,k,l}\langle ij|v|kl\rangle\sum_{m,m'}X^{\dagger}_{im}X^{\dagger}_{jm'}X_{lm'}X_{km}\,, \quad (1)$$

where $X^{\dagger}_{im}$ and X_{jm} are the creation and annihilation operators associated with the orthonormal spin orbitals $|im\rangle$, $i=1,2,\ldots,n$; $m=\pm\frac{1}{2}$. The generators E_{ij} of the unitary group U(n),

$$E_{ij}=\sum_{m}X^{\dagger}_{im}X_{jm}\,, \quad (2)$$

satisfy the commutation relations

$$[E_{ij},E_{kl}]_{-}=\delta_{jk}E_{il}-\delta_{il}E_{kj}\,, \quad (3)$$

and may be used to rewrite the Hamiltonian (1) as[17]

$$H=\sum_{i,j}\langle i|h|j\rangle E_{ij}+\tfrac{1}{2}\sum_{i,j,k,l}\langle ij|v|kl\rangle N[E_{ik}E_{jl}]\,, \quad (4)$$

where $N[\cdots]$ designates the normal product[15] defined with respect to the true vacuum state $|0\rangle$ ($X_{im}|0\rangle=0$ for all i and m).

The general spin-nonadapted N-electron states may be considered as belonging to the irrep $[1^N0]$ of U($2n$). A basis of spin-adapted N-electron states may then be obtained by adapting to the subgroup chain[1,20]

$$\mathrm{U}(2n)\supset\mathrm{U}(n)\otimes\mathrm{U}(2)\,. \quad (5)$$

The resulting basis of spin-adapted N-electron states of total spin S may be taken to be the set of canonical GT states for the irrep $[2^{N/2-S}1^{2S}0]$ of U(n). Since only two-columned U(n) irreps are necessary, the Gelfand tableaux notation may be considerably simplified.[2] In fact, by defining the intermediate notations of the ABC tableau,[2] an $n\times3$ array whose ith row (a_i,b_i,c_i) records the number of twos, ones, and zeros, respectively, in the ith row of the corresponding Gelfand tableau, and the ΔAC tableau derived from it, whose ith row $(\Delta a_i,\Delta c_i)$ is determined by $\Delta a_i=a_i-a_{i-1}$, $\Delta c_i=c_i-c_{i-1}$, (where we define $a_0=c_0=0$), we ultimately arrive at the step number vector $\underline{d}=(d_1,\ldots,d_n)$, whose ith entry d_i is determined as the binary value

$$d_i=(\Delta a_i\Delta\bar{c}_i)_{(2)},\quad \Delta\bar{c}_i=1-\Delta c_i\,. \quad (6)$$

The sequence of intermediate spins $\underline{S}=(S_1,\ldots,S_n)$, where S_i is the resultant spin of all electrons occupying the first i orbitals of the given state, is determined by the entries b_i of the ABC tableau via

$$b_i=2S_i\,, \quad (7)$$

and along with the sequence of orbital occupancies $\underline{n}=(n_1,\ldots,n_n)$ completely determines the state, and is thus equivalent to the step number vector $\underline{d}$. This relationship is given by

$$d_i=\begin{cases}0 & n_i=0\quad S_i=S_{i-1}\,,\\ 1 & n_i=1\quad S_i=S_{i-1}+\frac{1}{2}\,,\\ 2 & n_i=1\quad S_i=S_{i-1}-\frac{1}{2}\,,\\ 3 & n_i=2\quad S_i=S_{i-1}\,,\end{cases} \quad (8)$$

where $S_0\equiv0$ and $S_n\equiv S$.

Alternatively, an equivalent basis (up to phase) of spin-adapted N-electron states may be constructed using SU(2) coupling techniques, by successively coupling together the spins associated with the electrons in each orbital. In Ref. 17, we showed that this may be accomplished by setting

$$|\underline{d}\rangle=\phi\sum_{\{M_i\}}\sum_{\{m_i\}}\Big(\prod_{i=1}^{n}\langle S_{i-1}M_{i-1}s_im_i|S_iM_i\rangle\mathfrak{A}^{\dagger}_i(n_i)\Big)|0\rangle\,, \quad (9)$$

where $|0\rangle$ is the physical vacuum state, $\langle S'M'S''M''|SM\rangle$ designates the usual Clebsch-Gordan (CG) coefficient, S_i are the intermediate spins given by (8), M_i are the corresponding magnetic quantum numbers ($M_n=M, M_0=0$),

$$\begin{aligned}&s_i=m_i=0 \quad \text{if} \quad n_i=0,2\,,\\ &s_i=\tfrac{1}{2},\quad m_i=\pm\tfrac{1}{2} \quad \text{if} \quad n_i=1\,,\end{aligned} \quad (10)$$

and

$$\mathfrak{A}^{\dagger}_i(n_i)=\begin{cases}I, & \text{if} \quad n_i=0\,,\\ X^{\dagger}_{i,m_i}, & \text{if} \quad n_i=1\,,\\ X^{\dagger}_{i,1/2}X^{\dagger}_{i,-1/2}, & \text{if} \quad n_i=2\,.\end{cases} \quad (11)$$

The set of all such states for fixed n, N, and S is called the Yamanouchi-Kotani (YK) basis.[21] Moshinsky and Seligman[22] have shown that the GT and YK bases are equivalent up to a phase. This equivalence was also studied in considerable detail by Wormer[23] (cf. also Ref. 24). Thus, we may apply the entire apparatus of the unitary group approach to label the states (9); combined with the fact that the matrix elements of single generators and products of generators may be evaluated directly, as has been shown by GSS[4] and DS,[5] we obtain a compact and powerful formalism for the determination of matrix elements needed in CI calculations.

It is particularly convenient to employ the graphical methods of spin algebras[11-13] to represent the CG coefficients of (9) graphically, yielding (cf. Ref. 14)

$$|d\rangle = 2^{-N_2/2} \sum_{\{m_i\}} d_s(G_s) D_{so}(G_o) |0\rangle , \tag{12}$$

where G_o and G_s are the appropriate orbital and spin diagrams (cf. Ref. 17),

$$D_{so}(G_o) = \Big(\prod_{i(n_i=1)} X^{\dagger}_{im_i} \Big) \Big(\prod_{i(n_i=2)} X^{\dagger}_{im'_i} X^{\dagger}_{im''_i} \Big) , \tag{13}$$

$d_s(G_s)$ is the product of a phase and normalization factor with the value of the appropriate spin diagram [Figs. 1(a) and 1(b) of Ref. 17], and N_i represents the number of orbitals with occupancy i. A similar formula may be derived for bra states.

The use of YK states permits a direct calculation of matrix elements of single generators and products of generators, as we have shown in Ref. 17. Let us now give a brief outline of the work contained there. Considering first the matrix element $\langle \tilde{d} | E_{ij} | \underline{d} \rangle$ of a single generator E_{ij}, we obtained Eq. (35) of Ref. 17, in which the matrix element is expressed as a product of the values of the two spin graphs associated with $\langle \tilde{d} |$ and $|\underline{d}\rangle$, a vacuum mean value, and various phase and normalization factors. The vacuum mean value is evaluated using Wick's theorem,[15] or more simply, by means of orbital diagrams.[15,17] The matrix element thus reduces to a product of phase and normalization factors and the value of a spin diagram, which is given in Figs. 4(a) and 4(b) of Ref. 17 for raising and lowering generators, respectively. This spin diagram is then separated over two or three lines into n components or segments, and the phase and normalization factor factored and associated with the individual segments in such a way that the various contributions may be classified into a small number of general formulas, into which the quantities associated with the individual levels are substituted. In fact, one can see that the general formula for the contribution of the rth level is determined solely by the relationship between r and the generator indices, i.e., the position of the rth level in the spin diagram. This relationship determines the *segment type* of the rth-level segment; the various segment types necessary for single generator matrix elements are defined in Table I. (The contributions of segments outside the generator range are always unity and hence ignorable.) The contribution of the rth segment is written

$$W_r = W(Q_r; d_r \tilde{d}_r, \Delta b_r, b_r) , \tag{14}$$

where $Q_r \equiv Q_r(E_{ij})$ is the rth-level segment type defined by E_{ij}, $b_r = 2S_r$, and $\Delta b_r = 2S_r - 2\tilde{S}_r$. The matrix element may now be expressed as[3,17]

$$\langle \tilde{d} | E_{ij} | \underline{d} \rangle = \prod_{r \in \Omega} W_r = \prod_{r \in \Omega} W(Q_r(E_{ij}); d_r \tilde{d}_r, \Delta b_r, b_r) , \tag{15}$$

where $\Omega = \Omega(E_{ij}) = \{i, i \pm 1, \ldots, j\}$ is the generator range.

An analogous formula holds true[5,17] for the matrix element $\langle \tilde{d} | E_{ij} E_{kl} | \underline{d} \rangle$ of the generator product $E_{ij} E_{kl}$. However, the derivation is more complex since several complications arise from the possibility that the generator ranges overlap. First of all, the resulting spin diagram is not separable in the overlap range without the introduction of intermediate summation since the levels are connected by four lines. This problem is avoided by precoupling the spins of the two electrons[5] in the overlap range to X, $X = 0$, 1, thereby introducing an overall summation over X into the final result, and an X dependence into the formulas for the overlap range segment values.[17]

Secondly, new segment types are necessary for segments in the overlap range.[17] The new segment types $Q_r(E_{ij}E_{kl})$ are given in Table II and are determined by the pair of segment types $Q_r(E_{ij})$ and $Q_r(E_{kl})$ obtained by considering r as being in the range of each single generator separately. In addition, two segments denoted B'^R and B'^L are necessary for the so-called exchange terms, for which the generator lines in the spin diagram cross.

Finally, the possibility of noncommuting generators must be considered. E_{ij} and E_{kl} do not com-

TABLE I. Single generator segment types.

Level	Raising $E_{ij}(i<j)$	Lowering $E_{ji}(i<j)$
$r=j$	A_R	A_L
$i<r<j$	C'	C'
$r=i$	A^R	A^L

TABLE II. "Multiplication table" for generator product segment types. The notation for the segment type defined by a product of two generators is determined by the two single generator segment types (listed in the top row and the first column) obtained by considering the segment to be in the range of each generator separately (cf. Table I).

	A^R	A_R	A^L	A_L	C'
A^R	A^{RR}	A^R_R	A^{RL}	A^R_L	B^R
A_R	A^R_R	A_{RR}	A^L_R	A_{RL}	B_R
A^L	A^{RL}	A^L_R	A^{LL}	A^L_L	B^L
A_L	A^R_L	A_{RL}	A^L_L	A_{LL}	B_L
C'	B^R	B_R	B^L	B_L	C''

mute if $j=k$, or $i=l$, or both. These cases are handled by the introduction of the order index Y, $Y=1,2$, as an argument of the rth-level segment where r is the repeated index which leads to the noncommutativity. For the case $E_{ij}E_{ji}$, both the ith- and j-th-level segments are Y dependent.

The corresponding expression for the matrix element of the generator product $E_{ij}E_{kl}$ may now be written[17]

$$\langle \underline{\tilde{d}}|E_{ij}E_{kl}|\underline{d}\rangle = \prod_{r\in\Omega_1} W^{(Y)}(Q_r; d_r\tilde{d}_r, \Delta b_r, b_r) \times \sum_{X=0}^{1} \prod_{r\in\Omega_2} W^{(Y)}(Q_r; d_r\tilde{d}_r, \Delta b_r, b_r; X), \tag{16}$$

where $\Omega_1=\Omega(E_{ij})\Delta\Omega(E_{kl})$, $\Omega_2=\Omega(E_{ij})\cap\Omega(E_{kl})$, $Y=1$ for W_r if $r=i=l$, and $Y=2$ for W_r if $r=j=k$. If we consider the matrix elements of $e_{ik,jl}=E_{ik}E_{jl}-\delta_{jk}E_{il}=N[E_{ik}E_{jl}]$, appearing in the two-electron operators, rather than those of $E_{ik}E_{jl}$, it can be shown that the $Y=1$ values must be used throughout.[17] The advantage of this formulation is that the matrix elements of both single generators and products of generators may be expressed directly via (15) and (16). In Tables III and VII of Ref. 17, we have listed all nonzero values for the 22 necessary segments, thus making a calculational scheme based on these results immediately possible.

III. YK STATES IN THE HOLE-PARTICLE FORMALISM

We propose, in this paper, to carry out an analysis similar to that of the last section but instead within the particle-hole formalism. The goal is to express the matrix elements of both single generators and products of generators directly in terms of contributions associated with the individual orbitals. An additional desideratum is that the required segment values be obtainable from the particle-formalism segment formulas; we shall see that our formulation of the particle formalism permits this extension.

The first step, then, is to construct a basis of YK h-p states. In I, we established the notation, and developed the necessary representation theory for the adaptation of a basis of hole-particle states with respect to the chain of subgroups

$$\begin{aligned} U(2n) &\equiv U(2n'+2n'') \supset U(2n')\otimes U(2n'') \supset [U(n')\otimes U(2)]\otimes[U(n'')\otimes U(2)] \\ &\approx [U(n')\otimes U(n'')]\otimes[U(2)\otimes U(2)] \supset [U(n')\otimes U(n'')]\otimes[U(2)\dot{\times} U(2)] \approx [U(n')\otimes U(n'')]\otimes U(2). \end{aligned} \tag{17}$$

This chain may be easily interpreted within the SU(2) formalism. By means of the first subduction, we restrict ourselves to carrier spaces of $U(2n')\otimes U(2n'')$ which are the direct product of particle and hole spaces. The second subduction is, in fact, a pair of parallel subductions $U(2n')\supset U(n')\otimes U(2)$ and $U(2n'')\supset U(n'')\otimes U(2)$, each of which is identical to the subgroup chain (5) of the particle formalism. In each case, we restrict ourselves to a subspace of spin-adapted vectors, where the particle (hole) subspaces have total spin S' (S''). The final subduction may be interpreted as the coupling together of the total particle and total hole spins to yield an overall total spin S.

In I, we derived a prescription that indicated which irreps of $U(n')\otimes U(n'')$ occur, having chosen the values of the total spin S and the particle-hole deficiency N_0. Let us now see how the SU(2) coupling techniques may be used to construct a basis of the carrier space of any such irrep. Let us consider, then, the irrep $[2^{a'}1^{b'}\dot{0}]\otimes[\dot{0}-1^{b''}-2^{a''}] \equiv \{a'b'|b''a''\}$, where $N''=2a''+b''$, $N'=2a'+b' = N''+N_0$, $S''=2b''$, and $S'=2b'$. According to our interpretation of the subgroup chain (17), we must first construct from the set of n' particle orbitals, a basis of particle states of total spin S' containing N' particles, and from the set of n'' hole orbitals, a basis of hole states of total spin S'', containing N'' holes. The total particle and hole spins may then be coupled together to yield the desired total spin S.

The particle state and the hole state may be constructed in a manner similar to that of the particle formalism. Denoting the particle and hole labels by ordered index sets $\Lambda'=\{1',2',\ldots,(n')'\}$ and $\Lambda''=\{1'',2'',\ldots,(n'')''\}$, respectively, (assuming the orbitals to be arranged in some arbitrary but fixed order), we first define the reference state in which all hole orbitals are occupied

$$|\Phi_0\rangle = X^{\dagger}_{1'',1/2}X^{\dagger}_{1'',-1/2}\cdots X^{\dagger}_{(n'')'',1/2}X^{\dagger}_{(n'')'',-1/2}|0\rangle, \tag{18}$$

where $|0\rangle$ is the true vacuum and $X^{\dagger}_{i,m_i}$ are the particle creation operators defined for the orbitals considered. We shall find it convenient to employ the particle-hole creation and annihilation operators $Y^{\dagger}_{im}$ and Y_{jm}, which are defined by

$$Y^{\dagger}_{i,m} = \begin{cases} X^{\dagger}_{i,m}, & i\in\Lambda' \\ (-)^{1/2-m}X_{i,-m}, & i\in\Lambda'' \end{cases} \tag{19a}$$

$$Y_{i,m} = \begin{cases} X_{i,m}, & i\in\Lambda' \\ (-)^{1/2-m}X^{\dagger}_{i,-m}, & i\in\Lambda'' \end{cases}. \tag{19b}$$

The operator $Y^{\dagger}_{im}$ creates a particle or a hole, according as whether i belongs to Λ' or Λ''; in the latter case, the creation of a hole with spin magnetic quantum number m is effected by the destruction of a particle which must therefore have magnetic quantum number $-m$. The additional phase factor $(-)^{1/2-m}$ makes these operators transform as the irreducible tensor operators.[25]

It is now possible to define the creation operators for the electrons occupying a single orbital; the definition depends on the orbital occupancy $n_{i'}$ and $n_{i''}$:

$$\mathfrak{y}^{\dagger}_{i'}(n_{i'})=\begin{cases} I, & n_{i'}=0, \\ Y^{\dagger}_{i',m_{i'}}, & n_{i'}=1, \\ Y^{\dagger}_{i',1/2}\,Y^{\dagger}_{i',-1/2}, & n_{i'}=2, \end{cases} \tag{20a}$$

$$\mathfrak{y}^{\dagger}_{i''}(n_{i''})=\begin{cases} I, & n_{i''}=0, \\ Y^{\dagger}_{i'',m_{i''}}, & n_{i''}=1, \\ Y^{\dagger}_{i'',-1/2}\,Y^{\dagger}_{i'',1/2}, & n_{i''}=2. \end{cases} \tag{20b}$$

For a given set of orbital occupancies $(n_{1'}, n_{2'}, \ldots, n_{n'})$ and $(n_{1''}, n_{2''}, \ldots, n_{n''})$ we now form linear combinations of the monomials

$$\left(\prod_{r=1}^{n'} \mathfrak{y}^{\dagger}_{r'}(n_{r'})\right)\left(\prod_{r=n''}^{1} \mathfrak{y}^{\dagger}_{r''}(n_{r''})\right)|\Phi_0\rangle \tag{21}$$

to construct an eigenstate of the total spin operator by successively coupling together the spins associated with the particle orbitals using CG coefficients, and similarly for the hole orbitals, and then finally coupling together the spins associated with the hole and particle parts to yield the desired total spin S. Different states with the same set of orbital occupancies are distinguished by the sequences of intermediate spins $(S_{1'}, S_{2'}, \ldots, S_{(n')'})$ for the particle section and $(S_{1''}, S_{2''}, \ldots, S_{(n'')''})$ for the hole section. These intermediate spins and the orbital occupancies may be concisely represented by the step number vectors $\underline{d}'$ (particles) and $\underline{d}''$ (holes), which are defined in the same way as the particle step number vector (8). Using this notation, a particle-hole state is represented by $|\underline{d}'\underline{d}''SM\rangle$ and may be written (defining $S_{0'}=M_{0'}=S_{0''}=M_{0''}=0$) up to a phase factor ϕ as

$$\begin{aligned}|\underline{d}'\underline{d}''SM\rangle=\phi \sum_{\{m_{r'}\}}\sum_{\{M_{r'}\}}\sum_{\{m_{r''}\}}\sum_{\{M_{r''}\}}\prod_{r=1}^{n'}\langle S_{(r-1)'}M_{(r-1)'}s_{r'}m_{r'}\,|\,S_{r'}M_{r'}\rangle \\ \times\prod_{r=1}^{n''}\langle S_{(r-1)''}M_{(r-1)''}s_{r''}m_{r''}\,|\,S_{r''}M_{r''}\rangle\langle S_{(n')'}M_{(n')'},S_{(n'')''}M_{(n'')''}\,|\,SM\rangle \\ \times\left(\prod_{r=1}^{n'}\mathfrak{y}^{\dagger}_{r'}(n_{r'})\right)\left(\prod_{r=n''}^{1}\mathfrak{y}^{\dagger}_{r''}(n_{r''})\right)|\Phi_0\rangle,\end{aligned} \tag{22}$$

where

$$\begin{aligned} &s_{r'}=m_{r'}=0 \text{ if } n_{r'}=0 \text{ or } 2, \\ &s_{r'}=\tfrac{1}{2},\quad m_{r'}=\pm\tfrac{1}{2} \text{ if } n_{r'}=1. \end{aligned} \tag{23}$$

The summations labeled $\{m_{r'}\}$ and $\{M_{r'}\}$ are over $m_{1'}, m_{2'}, \ldots, m_{(n')'}$ and $M_{1'}, M_{2'}, \ldots, M_{(n'-1)'}$, respectively, and similarly for the quantities related to hole orbitals.

We shall see in the next section that it is necessary to evaluate reference-state mean values of products of annihilation and creation operators. This is conveniently done using the particle annihilation and creation operators; we thus define

$$\mathfrak{x}^{\dagger}_{i'}(n_{i'})=\begin{cases} I, & \text{if } n_{i'}=0, \\ X^{\dagger}_{i',m_{i'}}, & \text{if } n_{i'}=1, \\ X^{\dagger}_{i',m^1_{i'}}X^{\dagger}_{i',m^2_{i'}}, & \text{if } n_{i'}=2, \end{cases} \tag{24a}$$

and

$$\mathfrak{x}_{i''}(n_{i''})=\begin{cases} I, & \text{if } n_{i''}=0, \\ X_{i'',m_{i''}}, & \text{if } n_{i''}=1, \\ X_{i'',m^2_{i''}}X_{i'',m^1_{i''}}, & \text{if } n_{i''}=2, \end{cases} \tag{24b}$$

and rewrite (22) as

$$|\underline{d}'\underline{d}''SM\rangle = \phi \sum_{\{m_{r'}\}} \sum_{\{M_{r'}\}} \sum_{\{m_{r''}\}} \sum_{\{M_{r''}\}} \prod_{r=1}^{n'} \langle S_{(r-1)'} M_{(r-1)'} s_{r'} m_{r'} | S_{r'} M_{r'} \rangle$$
$$\times \prod_{r(n_{r'}=2)} \langle \tfrac{1}{2} m_{r'}^1 \tfrac{1}{2} m_{r'}^2 | 00 \rangle$$
$$\times \prod_{r=1}^{n''} \langle S_{(r-1)''} M_{(r-1)''} s_{r''} - m_{r''} | S_{r''} M_{r''} \rangle$$
$$\times \prod_{r(n_{r''}=2)} \langle \tfrac{1}{2} - m_{r''}^1 \tfrac{1}{2} - m_{r''}^2 | 00 \rangle F \langle S_{(n')'} M_{(n')'} S_{(n'')''} M_{(n'')''} | SM \rangle$$
$$\times \left(\prod_{r=1}^{n'} \mathfrak{X}_{r'}^{\dagger}(n_{r'}) \right) \left(\prod_{r=n''}^{1} \mathfrak{X}_{r''}(n_{r''}) \right) | \Phi_0 \rangle . \tag{25}$$

In this result F is a phase and normalization factor associated with the transition to particle-formalism operators $X_{im}, X_{im}^{\dagger}$,

$$F = (-)^f 2^{-(N_2'+N_2'')/2},$$
$$f = N_2'' + \tfrac{1}{2} N_1'' + \sum_{r=1}^{n''} m_{r''}, \tag{26}$$

N_i' and N_i'' being the numbers of particle and hole orbitals with occupancy i.

We shall again exploit the graphical approach as in our analysis of the particle formalism.[17] The CG coefficients in (25) are first represented graphically, and then further converted to 3-jm symbols. This yields

$$|\underline{d}'\underline{d}''SM\rangle = \mathfrak{N}_{\underline{d}',\underline{d}''} w(G_o) \sum_{\{m_{r'}\}} \sum_{\{m_{r''}\}} d_s(G_s) D_{so}(G_o) | \Phi_0 \rangle , \tag{27}$$

where the new symbols in this equation have the following connotations. G_s is the spin diagram displayed in Fig. 1(a), while $d_s(G_s)$ is given by

$$d_s(G_s) = \tau \, \mathrm{Val}(G_s) . \tag{28}$$

$\mathrm{Val}(G_s)$ represents the algebraic factor associated with the diagram G_s and τ represents the phase and normalization factors from (26) and from the transition to the graphical notation

$$\tau = \phi(-)^t [S_{1'}, \ldots, S_{(n')'}, S, S_{(n'')''}, \ldots, S_{1''}]^{1/2},$$
$$t = N_2' + N_2'' + 2S_{(n')'} + 2S_{(n'')''} , \tag{29}$$

where

$$[S] = 2S+1 ,$$
$$[S_1, S_2, \ldots, S_k] = \prod_{i=1}^{k} [S_i] . \tag{30}$$

G_o is the orbital diagram shown in Fig. 1(b) and is similar enough to the corresponding spin diagram G_s that its use is generally unnecessary. $D_{so}(G_o)$ is the collection of particle-formalism operators associated with G_o:

$$D_{so}(G_o) = \left(\prod_{r=1}^{n'} \mathfrak{X}_{r'}^{\dagger}(n_{r'}) \right) \left(\prod_{r=n''}^{1} \mathfrak{X}_{r''}(n_{r''}) \right) . \tag{31}$$

The weight $w(G_o)$ and normalization factor $\mathfrak{N}_{\underline{d}',\underline{d}''}$ are[14,15]

$$w(G_o) = 2^{-(N_2'+N_2'')}, \quad \mathfrak{N}_{\underline{d}',\underline{d}''} = 2^{(N_2'+N_2'')/2} , \tag{32}$$

together they provide the overall factor $2^{-(N_2'+N_2'')/2}$, which already appears in (26). Finally, the summation extends over the set of all magnetic quantum numbers $\{m_{i'}, m_{i''}\}$ that label the particle and hole $\frac{1}{2}$ angular-momentum lines of G_s.

Let us now establish some additional notation which will permit easy manipulation of the matrix elements considered in subsequent sections. First of all, the spin diagram of Fig. 1(a) may naturally be divided into three parts: The particle and hole sections, respectively, below and above the total spin line labeled S, and the S line and the vertex to which it is attached, which we call the *link section*. The ordering chosen for the p-h orbital creation operators in (21) is reflected by the linear ordering in the spin diagram G_s; for this reason, we call the ordering in which the hole labels appear in reverse order the *particle-hole* (p-h) *ordering*. However, for several reasons, it is useful to label the orbitals according to the *particle* (p) *ordering*, which is merely the sequential order of the orbitals in the spin diagrams, starting from the lowest orbital and omitting the link section. We shall indicate the position of an orbital in the p order by an index without single or double primes. The two orderings are related algebraically as follows:

$$i = \begin{cases} i', & i \in \Lambda' \\ n' + n'' + 1 - i'', & i \in \Lambda'' \end{cases} . \tag{33}$$

This relationship is also displayed in Table III.

The advantages of the p ordering are as follows: Firstly, it is the ordering that is suggested by the representation theory of paper I. In addition, the use of the p ordering permits a simpler formulation of the basic results and a concise definition of the segment types necessary for the matrix elements of a given generator or product of two generators; this latter task is somewhat cumbersome

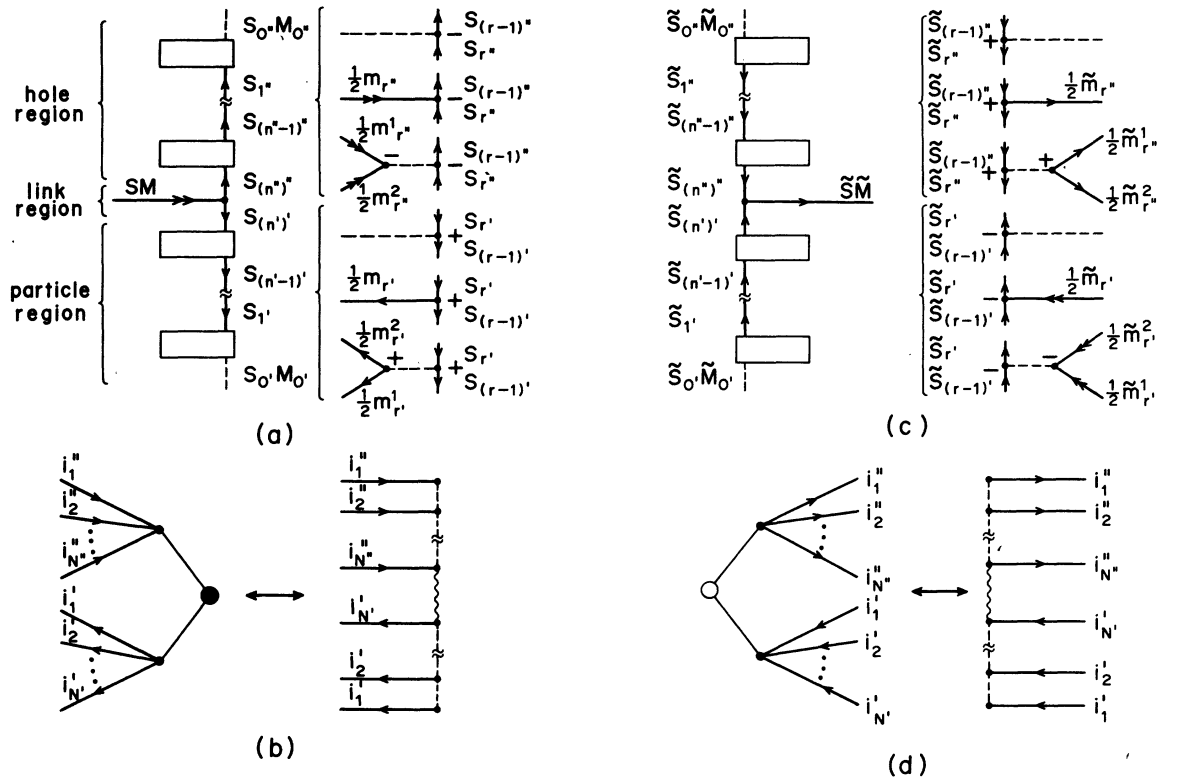

FIG. 1. Spin and orbital diagrams for bra and ket YK states. The spin and orbital diagrams for the YK ket state (27) are illustrated in diagrams (a) and (b), respectively. In diagram (a), the blank boxes represent the detailed coupling for each individual oribtal level. These depend on the orbital occupancy, and the three possibilities are displayed to the right of the diagram, corresponding to the occupancies $n_r = 0, 1$ or 2 (from the top) in both the particle and hole regions. In diagram (b), the two possible forms of the orbital diagram are shown, on the left-hand side is the Hugenholtz form, while on the right-hand side the Brandow-Goldstone form (cf. Refs. 14, 15, and 32). The corresponding spin and orbital diagrams for the YK bra state (35) are given in diagrams (c) and (d).

using the p-h ordering. In general, then, the p ordering is useful for the statement of the overall results, whereas the p-h ordering is more convenient for their derivation.

Using these ideas, we may concisely represent the p-h state using the total spin quantum number S and the step number vector $\underline{d} = (d_1, d_2, \ldots, d_n)$, whose indices are taken in the p order, and which is nothing more than the concatenation of the step number vectors $\underline{d}'$ and $\underline{d}''$ for the particle and hole sections, with the latter taken in reverse order. It must be remembered, however, that in this notation the b values are no longer obtained from this step number vector by the usual formula [Eq. (17) of Ref. 17], but are now defined by

$$b_i = \begin{cases} \sum_{k=1}^{i} [\delta(d_k, 1) - \delta(d_k, 2)], & 1 \le i \le n' \\ \sum_{k=i}^{n} [\delta(d_k, 1) - \delta(d_k, 2)], & n' < i \le n . \end{cases} \tag{34}$$

A general bra state may be represented by a formula derived from (27) by conjugation:

$$\langle \underline{\tilde{d}} \tilde{S} \tilde{M} | = \mathfrak{N}_{\underline{\tilde{d}}} w(\tilde{G}_o) \sum_{\{\tilde{m}_{r'}\}} \sum_{\{\tilde{m}_{r''}\}} \tilde{d}_s(\tilde{G}_s) \langle 0 | D^{\dagger}_{so}(\tilde{G}_o) , \tag{35}$$

where $\tilde{G}_s$ and $\tilde{G}_o$ are the spin and orbital diagrams

TABLE III. Relationship between the particle and particle-hole labeling schemes.

particle	: 1	2	⋯	$(n'-1)$	n'	$(n'+1)$	$(n'+2)$	⋯	$(n-1)$	n
particle-hole:	$1'$	$2'$	⋯	$(n'-1)'$	$(n')'$	$(n'')''$	$(n''-1)''$	⋯	$2''$	$1''$

given in Figs. 1(c) and 1(d),

$$\tilde{d}_s(\tilde{G}_s)=\tilde{\tau}\,\mathrm{Val}(\tilde{G}_s)\,, \tag{36}$$

$$\tilde{\tau}=\tilde{\phi}(-)^{\tilde{t}}[\tilde{S}_{1'},\ldots,\tilde{S}_{(n')'},\tilde{S},\tilde{S}_{(n'')''},\ldots,\tilde{S}_{1''}]^{1/2}\,,$$

$$\tilde{t}=\tilde{N}_2'+\tilde{N}_1''+\tilde{N}_2''+2\sum_{r=0}^{n'}\tilde{S}_{r'}+2\sum_{r=0}^{n''}\tilde{S}_{r''}\,, \tag{37}$$

$$\mathfrak{N}_{\tilde{g}}w(\tilde{G}_o)=2^{-(\tilde{N}_2'+\tilde{N}_2'')/2}\,. \tag{38}$$

(Quantities relating to the bra state are distinguished by tildes.)

Equations (27) and (35) express the YK basis states in the p-h formalism. For given values of the parameters N_0 and S then the basis may be constructed and stored in the following manner. The required irreps are first determined via the prescription given in I. Next, for each irrep, a distinct row table is created for the particle and hole sections separately; the p-h states for this irrep are then labeled by all possible pairs of step number vectors from the particle and hole sections. This provides an efficient means for the generation and storage of bases of YK states; we shall later show that the matrix elements of generators and products of generators in this basis may be directly obtained with a knowledge of the step number vectors of the two states involved being all that is necessary.

IV. AN EXAMPLE

Before continuing with an account of the evaluation of matrix elements with respect to the basis of h-p YK states, we first present an example of possible h-p bases for a simple four electron-four orbital case, employing two different reference states $|\Phi_0\rangle$. Rather than listing the basis vectors we shall employ Shavitt's graphical representation of the corresponding distinct row tables.[3] The vertices of these graphs represent distinct rows and the edges represent the pertinent step numbers. Instead of labeling individual vertices with the corresponding distinct rows of the ABC tableaux, Shavitt[3] places them on a rectangular grid with the vertical position indicating the orbital level (given by the sum of the ABC components in each row) and the horizontal position giving the values of a_i and b_i components [cf. Figs. 2(a) and 3(a)]. In this way the slope of the edges implies directly the corresponding step number, as shown in Figs. 2(a) and 3(a). We also recall that all possible walks between the top and bottom vertices uniquely define the canonical basis vectors of the

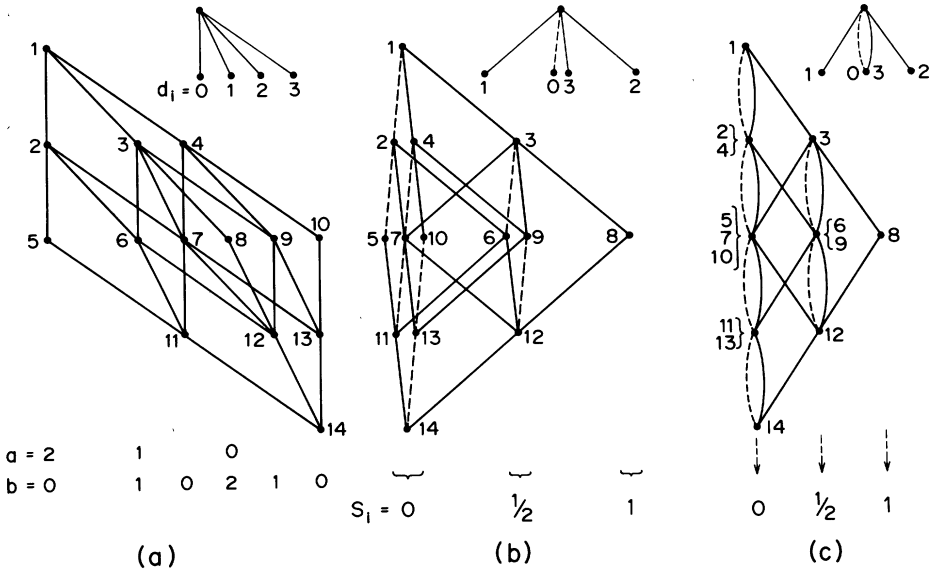

FIG. 2. Graphical representation of the canonical basis for the irrep $[2^2\,0^2]\equiv(202)\equiv\{20\}$ of U(4), yielding the spin-adapted basis for $n=4$, $N=4$, and $S=0$. Diagram (a) is a standard Shavitt graph (Ref. 3), while diagram (c), obtained as a superposition of an earlier graphical representation given in Ref. 2, may be regarded as an appropriate subgraph of a standard YK branching diagram. An intermediate graphical representation, which still represents uniquely the individual state vectors by distinct paths as the Shavitt graph (a), is given in diagram (b). In this graph the horizontal vertex position indicates the intermediate spin value, as in the branching diagram (c), while in the Shavitt graph (a) both a_r and b_r values are determined by the horizontal vertex position, as indicated at the bottom of the graph. The slope of the edges determines the pertinent step number in each case as indicated in the upper right-hand corner in each diagram (a)–(c). For greater convenience, the edges associated with unoccupied orbital levels ($d_r=0$) are represented by dashed lines in diagrams (b) and (c).

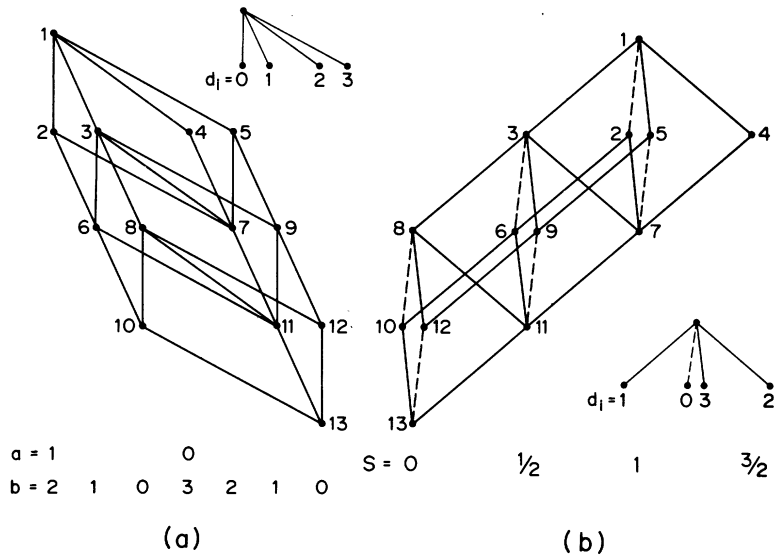

FIG. 3. Graphical representation of the canonical basis for the irrep $[2\ 1^2\ 0] \equiv (121) \equiv \{12\}$ of U(4), yielding the spin-adapted basis for $n=4$, $N=4$, and $S=1$. Diagram (a) is a standard Shavitt graph (Ref. 3) and diagram (b) a modified YK branching diagram. For details see caption to Fig. 2.

carrier space of the given irrep of U(n), uniquely labeled by the top row of the ABC tableaux (i.e., by the top vertex of Shavitt's graph).

Shavitt graphs for the case of the irreps (202) and (121) of U(4), associated with the singlets and triplets of the four-electron minimum basis set problem, are shown in Figs. 2(a) and 3(a), respectively. We would like to remark that these graphs may in fact be regarded as subgraphs of the general YK branching diagram.[21] This is easily seen if we distort these graphs in such a way that the horizontal position indicates the intermediate spin (i.e., the b_i value) as shown in Figs. 2(b) and 3(b). Here, for greater clarity, we use the dashed line to represent the zero step number ($d_i = 0$), associated with zero occupancy. Moreover, identifying the vertices associated with the same intermediate spin, we obtain the familiar YK branching diagram shown in Fig. 2(c) for the singlet case considered.

Clearly both forms (a) or (b) of Figs. 2 and 3 of these diagrams are equivalent and only differ in the slope of the edges associated with different step numbers. We also note that the branching diagram of Fig. 2(c) would result if we superimposed the graphical representations for individual states of the GT basis used earlier.[2] Since we rely in this work on the relationship between the U(n) and SU(2) approaches, we prefer to use a graphical representation which is intermediate to the U(n) based representation of Shavitt[3] and the SU(2) based YK branching diagrams, namely, the representation shown in Figs. 2(b) and 3(b).

Let us now describe the h-p form of the basis vectors of the irrep spaces considered in our example. We shall employ two distinct reference states $|\Phi_0\rangle$ or, equivalently, the following two distinct breakdowns of the orbital space into the hole and particle subspaces: (i) $n''=n'=2$ and (ii) $n''=1$, $n'=3$. In fact, these two cases are the only ones of interest, since the case $n''=3$, $n'=1$ is simply related to the case (ii) (by particle-hole inversion) and the cases $n''=4$, $n'=0$ and $n''=0$, $n'=4$ are equivalent to the particle formalism. The relevant irreps for cases (i) and (ii) for either singlets ($S=0$) or triplets ($S=1$) are easily found following the procedure outlined in I. For each such irrep we construct the distinct row table, or Shavitt-like graph, separately for the hole and the particle subspaces. These are given in Figs. 4–7, using a standard level ordering for the hole subspace, and a reversed one for the particle subspace. We could, of course, equally well reverse this ordering in both subspaces and identify the top and botton vertices. We could also reverse the vertical ordering of particle and hole subgraphs if desired.

We observe that, in fact, the graphs associated with different h-p irreps represent subgraphs of the p-formalism graphs. This is particularly easy to see for the case $S=0$, when the three different p-h irreps for case (ii), Fig. 5, are clearly associated with the three possible vertices at level one in the p-formalism graph, Fig. 2(b). However, there is no one-to-one correspondence between the basis vectors in particle only and p-h schemes,

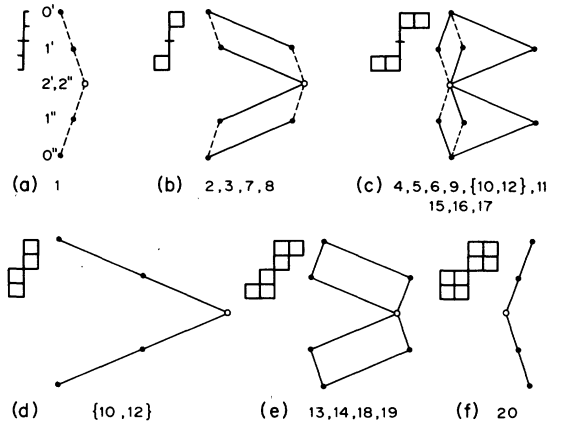

FIG. 4. Graphical representation of p-h states associated with different subproblems for the case $n=N=4$, $S=0$, and $|\Phi_0\rangle$, belonging to the irrep $[2^2]$ of U(2), i.e., $n'=n''=2$. The p-h irreps are represented by Young tableaux in the upper left-hand corner for each subspace, and the p-h basis vectors, yielding a noncanonical basis for $U(n)$ subduced to $U(n')\otimes U(n'')$, is represented by YK-type diagrams (b) of Figs. 2 and 3, drawn separately for the particle and hole subspaces and joined via an empty vertex. The orbital level ordering used is shown in diagram (a). Finally, the corresponding vectors from the particle formalism, Fig. 2, identified by their sequential number in a lexically ordered basis, are listed for each subproblem. A general linear combination of state vectors $k_1, k_2, \ldots, k_m$ is designated as $\{k_1, k_2, \ldots, k_m\}$. The representation of individual step numbers d_i for both particle and hole subspaces is shown in the upper right-hand corner of Fig. 5.

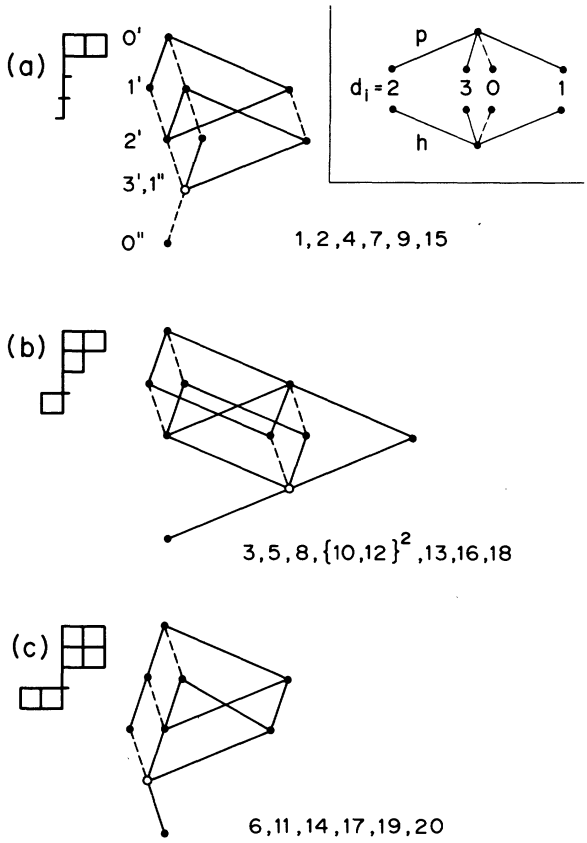

FIG. 5. Same as Fig. 4 for $|\Phi_0\rangle$ belonging to the irrep [2] of U(1), i.e., $n'=3$, $n''=1$.

except for those states which are uniquely determined by the orbital occupation numbers. This is illustrated by the list of p-formalism basis vectors (identified by their position in the lexically ordered canonical basis) given below each p-h formalism graph in Figs. 4–7. We see that in the case when more than one vector is associated with a given set of orbital occupancies (vectors 10 and 12 in the singlet case and 7, 9, and 12 in the triplet case), a linear combination of such vectors is obtained in the h-p version. Moreover, these linear combinations often occur in different h-p irreps. We shall discuss some advantages of these features of the h-p formalism in Sec. VIII.

V. THE GRAPHICAL METHOD

It now remains to demonstrate that an efficient and direct evaluation of the matrix elements of single generators and products of generators with respect to the basis of p-h YK states is possible just as in the particle formalism.[17] Let us begin then with some rather general considerations concerning the overall method and the different types of generators possible. From (27) and (35), the matrix elements of a single generator E_{ij} (whose indices are recorded in the p ordering and thus may refer either to hole or particle orbitals) may be written

$$\langle \underline{\tilde{d}}\tilde{S}|E_{ij}|\underline{d}S\rangle = 2^{-(N'_2+N''_2+\tilde{N}'_2+\tilde{N}''_2)/2}\sum_{\{m_{r'}\}}\sum_{\{m_{r''}\}}\sum_{\{\tilde{m}_{r'}\}}\sum_{\{\tilde{m}_{r''}\}}\tilde{\tau}\tau\,\mathrm{Val}(\tilde{G}_s)\,\mathrm{Val}(G_s)\sum_m\langle\Phi_0|D^\dagger_{so}(\tilde{G}_o)X^\dagger_{im}X_{jm}D_{so}(G_o)|\Phi_0\rangle, \quad (39)$$

where the generator has already been written in terms of particle-formalism operators.

The reference-state mean value contained in (39) may now be evaluated using Wick's theorem.[15] This is most easily done using the orbital diagrams in which the various contractions are represented by lines joining the bra and ket state orbital diagrams.[15] Each such line joins vertices at the same

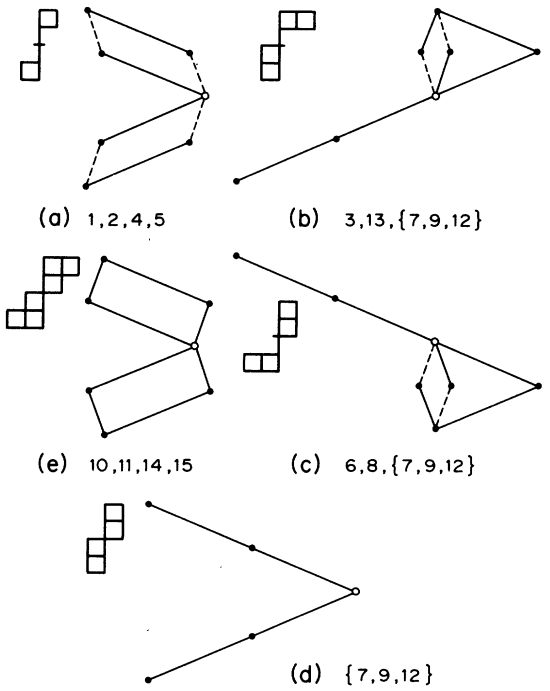

FIG. 6. Graphical representation of p-h states associated with different subproblems for the case $n=N=4$, $S=1$, and $|\Phi_0\rangle$ belonging to the irrep $[2^2]$ of U(2), i.e., $n'=n''=2$. See caption to Fig. 4 for details.

level except for one, due to the generator E_{ij}, which interconnects levels i and j. The side of the diagram to which this line is attached at the ith or jth level depends not only on whether that index is the first or second generator index but also on whether it refers to a particle or hole orbital; the various possibilities are examined separately below.

The resulting orbital diagram represents graphically the collection of products of pairs of Kronecker deltas involving the orbital and spin labels, respectively. When substituted into (39), the summation over one set of spin projections eliminates the Kronecker deltas involving the spin labels, while the remaining spin-projection summations are then represented graphically by joining identically labeled free-lines of the bra and ket spin diagrams, yielding the resulting spin diagram.[26] It is not hard to see that the arrangement of particle and hole lines in this resulting spin diagram is identical to that in the resulting orbital diagram. Thus this latter diagram is not really necessary at all; we may formulate rules which yield the resulting spin diagram directly from a knowledge of the particular generator or generators involved, without explicitly considering the relevant orbital diagrams.

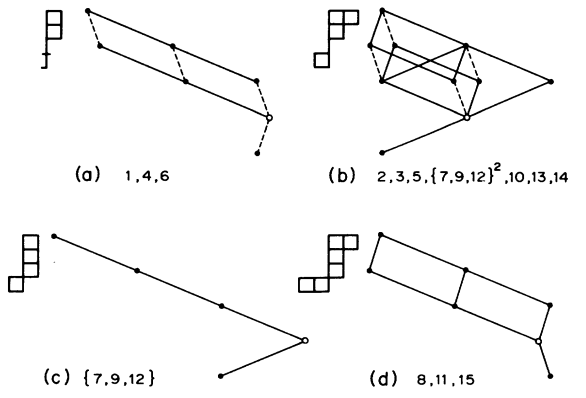

FIG. 7. Same as Fig. 6 for $|\Phi_0\rangle$ belonging to the irrep [2] of U(1), i.e., $n'=3$, $n''=1$.

Let us now consider the arrangement of particle and hole lines in the resulting spin diagram derived from (39). The most important difference which distinguishes the p-h from the p formalism is that for the hole-orbital operators the only nonzero contractions are of the form $:X^{\dagger}_{im}X_{im'}: = \delta_{m,m'}$, where the two operators appear in an order opposite to that for contractions of operators with particle indices[15] (note that the p-h formalism contractions are defined with respect to the Fermi vacuum $|\Phi_0\rangle$, Eq. (18), while the p-formalism contractions are defined with respect to the true vacuum state $|0\rangle$). This has the following implications for the resulting spin diagram of (39). First of all, for levels not equal to i or j, little is different from the p formalism; it is evident that the particle or hole lines must interconnect vertices at the same level. In addition, for doubly occupied levels, two contraction patterns are possible, each of which yields the same resulting spin diagram (this is true in general for any geminally antisymmetric spin functions; cf. Fig. 3 of Ref. 14). As in the p formalism, the doubly occupied levels may be converted, in the resulting spin diagram, to unoccupied levels,[17] as long as an extra factor of two is included.

The arrangement of lines at the ith and jth levels must be considered together due to the term $\sum_m X^{\dagger}_{im}X_{jm}$ in (39). If i refers to a particle orbital, then $X^{\dagger}_{im}$ is contracted with an annihilation operator from the bra state and the generator line thus terminates at the ith level on the left-hand side of the resulting spin diagram. If, however, i refers to a hole orbital, then $X^{\dagger}_{im}$ is contracted with an annihilation operator from the ket state and the generator line terminates at the ith level on the right-hand side. Similarly, the generator line terminates at the jth level on the right- or left-hand side, depending on whether j refers to a particle or hole level. Thus we may say in gener-

al that when a generator line terminates in the hole region, it is incident with the side of the resulting spin diagram which is opposite to that indicated for particle orbitals. Let us now enumerate the three possible distributions of generator indices among the particle and hole regions.

(1) Particle-particle (p-p) generators E_{ij}, $1 \leq i, j \leq n'$. When both indices of the generator refer to particle orbitals, the situation is exactly analogous to the p formalism. The two possible spin diagrams are represented schematically in Fig. 8(a) for a p-p raising generator ($i<j$) and Fig. 8(b) for a p-p lowering generator ($i>j$). The link segment is represented by a dotted line. It is clear that the same segment formulas as in the p formalism will apply, namely, A^R or A^L for the lower terminal segment and A_R or A_L for the upper terminal segment, for raising or lowering generators, respectively.

(2) Hole-hole (h-h) generators E_{ij}, $n'<i, j \leq n$. Since both indices belong to the hole region, the generator line is connected to the opposite side of the diagram than is usual for particle orbitals. Thus for a raising h-h generator ($i<j$), the schematic spin diagram is shown in Fig. 8(c), while 8(d) represents the schematic spin diagram for a lowering h-h generator. When we enquire as to the necessary segment types, we must remember that the p-h ordering for levels is used in Eq. (39), so that for the upper terminating segment for the h-h raising generator E_{ij}, $i<j$ [level j of Fig. 8(c)], the required segment type is A^R, and similarly, A_R is the type of the lower terminal segment. For the h-h lowering generator, the upper and lower terminating segment types are A^L and A_L, respectively. These are just the opposite of those which are indicated in the p formalism. Finally, due to the reversed contractions for hole operators, the contraction lines connected to the two operators comprising the generator cross, and an additional minus sign results.

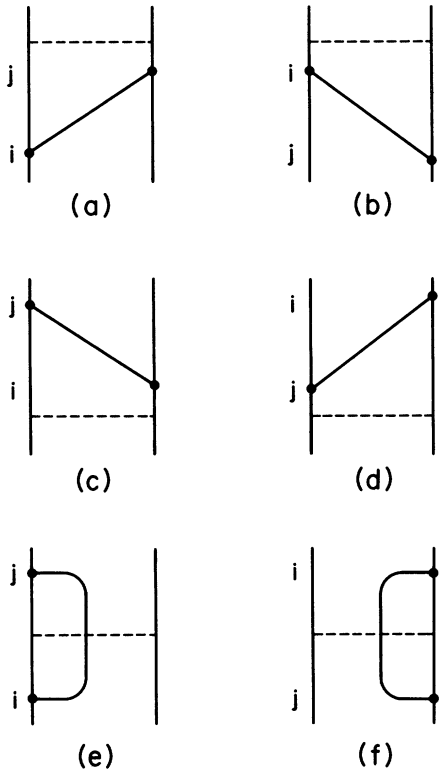

FIG. 8. Schematic resulting spin diagrams for single generators. The various types of resulting spin diagrams for a single generator are displayed. In each case, the dashed line locates the position of the link segment. The diagrams represent schematically the resulting spin diagrams for a p-p raising (a), p-p lowering (b), h-h raising (c), h-h lowering (d), p-h raising (e), and p-h lowering (f) generator.

(3) Particle-hole (p-h) generators E_{ij}, $1 \leq i \leq n' < j \leq n$, *or* $1 \leq j \leq n' < i \leq n$. As a result of the reversed contraction pattern for the hole operators, both ends of the generator line terminate on the same side of the spin diagram. Thus the schematic spin diagrams for p-h raising ($i<j$) and lowering ($i>j$) generators are shown in Figs. 8(e) and 8(f), respectively. In the former case, the necessary terminal segments are both of type A^R, while A^L is indicated for both terminating segments of a p-h lowering generator. In these two cases, for the segments in the hole region, we must again use the opposite segments that would be employed in the particle formalism (i.e., A^Q instead of A_Q and vice versa, for $Q=R, L$). The contraction lines associated with the generator creation and annihilation operators do not cross, and thus no additional minus sign is necessary as was the case for h-h generators.

Finally, there are two additional factors which arise from the evaluation of the reference-state mean value in (39). A factor of two from each doubly occupied level that is incident with the generator line (i.e., at the ith and jth levels), and $(-1)^p$ where p is the number of crossings of particle and hole lines in the resulting spin diagram.

It is instructive to note the following distinction between the p-h generators and the p-p and h-h generators. The latter transform states within the same irrep, while the former transform among different irreps. The p-h raising generator creates both a particle and a hole, thus increasing both N' and N'' by unity, while the p-h lowering generator destroys both a particle and a hole. Thus, the p-h generators are, in fact, the tensor operators,[27] which might be represented by appropriate double Gelfand tableaux with the highest weight (1 0 −1), which is common to both upper

and lower tableaux (the dot over the zero indicates repetition to a required length). The upper tableaux relates the two irreps involved, while the lower tableau structure represents the generator E_{ij} $(i \neq j)$ considered: The first component in each row equals 1 for the rows $k=i,\ i+1,\ldots,n$, and the last component equals -1 for the rows $k=j,\ j+1,\ldots,n$, all other entries being zero (cf. also Sec. IIIC and Fig. 3 of I). One could thus also exploit the tensor-operator formalism developed by Biedenharn, Louck, and others.[27,28] In fact, the case of generator matrix elements of the groups $U(n'+n'')$ in a noncanonical basis $U(n') \otimes U(n'')$, which is particularly relevant to the problem considered here, was very recently treated by Klimyk and Gruber.[29] [In their notation the two relevant Gelfand tableaux are written side by side rather than as a part of a $U(n'+n'')$ tableau, as the parts B and C in Fig. 3 of I.] Nevertheless, we find the SU(2) based approach exploiting the graphical techniques of spin algebras,[4,5,11-14,17] to be the most convenient and direct in the case of the irreps encountered in the many-electron problem considered here.

We may summarize this section by presenting the rules whereby the resulting spin diagram associated with (39) may be obtained directly.

(i) All particle and hole lines of the bra state spin diagram $\tilde{G}_s$ must be connected with the ket state particle and hole lines at the same level, with doubly occupied levels replaced by a dashed line signifying zero angular momentum, except for the generator line which connects an ith-level bra or ket line (depending on whether i refers to a particle or a hole orbital) to a jth-level ket or bra line (depending on whether j refers to a particle or a hole orbital). In addition, one must connect the lines labeled $S'_0M'_0$ and $\tilde{S}'_0\tilde{M}'_0$, $S''_0M''_0$ and $\tilde{S}''_0\tilde{M}''_0$, and S, M and $\tilde{S}, \tilde{M}$.

(ii) One must associate with this diagram the multiplicative factor

$$(-)^{p+\epsilon} 2^{N'_2+N''_2+\tilde{N}_2(i)+\tilde{N}_2(j)} [S]^{-1} \delta(S,\tilde{S}) \delta(M,\tilde{M}), \quad (40)$$

where p is the number of crossings of orbital lines in the resulting spin diagram, ϵ is one if $n' < i,\ j \leq n$ and 0 otherwise, and $\tilde{N}_2(r)$ is one if the rth orbital is doubly occupied and 0 otherwise. We note that the multiple of two included in (40) will substantially cancel with the first factor of (39), since $\tilde{N}_2(r) \equiv N_2(r)$ when $r \neq i, j$ and, in fact, the remaining multiplicative factor may be written $\lambda[S]^{-1}\delta(S,\tilde{S})\delta(M,\tilde{M})$, with

$$\lambda = (-)^{p+\epsilon} \left(\prod_{r \in \Lambda'} n_r \prod_{r \in \tilde{\Lambda}'} \tilde{n}_r \right)^{1/2}, \quad (41)$$

where Λ' and $\tilde{\Lambda}'$ are the sets of labels of orbitals incident with the generator lines in the ket and bra states, respectively (cf. Sec. 3(c) of Ref. 14).

VI. MATRIX ELEMENTS OF SINGLE GENERATORS

We are now in a position to derive the formulas which express the matrix elements of single generators and products of generators as a product of segment values associated with the individual levels as in the p formalism. An advantage of our choice for the segment values given in Ref. 17 is that the same formulas may be used in the p-h formalism. In order to see this, it is instructive to compare the formulas (27) and (35) for the p-h states with the corresponding formulas (25) and (32) of Ref. 17 in the p formalism. Considering first the particle portion of the state (27), which includes the particle section of the spin diagram G_s [Fig. 1(a)] and the corresponding part of the numerical factor, we note that it is formally identical to the entire p formalism state (25) of Ref. 17. A similar remark applies to the particle portion of the bra state (35) in relation to the entire p-formalism bra state (32) of Ref. 17. In order to compare the hole portions of these states to the p-formalism states, we view the appropriate portion of the spin diagram upside down. It can then be seen that the hole portion of the state (35) is formally identical to the p-formalism state (32) of Ref. 17, except that the hole lines are directed oppositely. The hole portion of the bra state (35) can also be seen to be formally identical to the p-formalism state (32) of Ref. 17, except for the hole lines being directed oppositely and the additional factor $(-)^{\tilde{N}''_1}$. This suggests that when matrix elements of generators between the states (27) and (35) are considered, both particle and hole portions of the resulting spin diagrams and numerical factors will be identical to expressions encountered in the p formalism, since the additional factor $(-)^{\tilde{N}''_1}$ may be used to reverse the directions of all hole lines. The factorization into a product of p-formalism segment values may then proceed.

Let us continue, then, with our calculation of the matrix elements of single generators. According to the development of the last section, the matrix element (39) may be written

$$\langle \underline{\tilde{d}}\tilde{S} | E_{ij} | \underline{d} S \rangle = \Psi \, \mathrm{Val}(G_r), \quad (42)$$

where G_r is the resulting spin diagram described in the last section in which the directions of all lines in the spine of the bra state have been reversed, yielding the factor $(-)^{2f}$, with $f = \sum_0^{n'} \tilde{S}_{r'} + \sum_0^{n''} \tilde{S}_{r''}$. The numerical factor Ψ is seen from (29), (37), and (41) to be

$$\Psi=\lambda\phi\tilde{\phi}(-)^{N_2'+N_2''+\tilde{N}_2'+\tilde{N}_2''+\tilde{N}_1''+2S_{n'}+2S_{n''}}\delta(S,\tilde{S})\delta(M,\tilde{M})[S_{1'},\ldots,S_{(n')'},S_{1''},\ldots,S_{(n'')''},\tilde{S}_{1'},\ldots,\tilde{S}_{(n')'},\tilde{S}_{1''},\ldots,\tilde{S}_{(n'')''}]^{1/2}. \tag{43}$$

It is convenient at this point to mention the three phase conventions of Ref. 17. Each convention is again utilizable in the p-h formalism; the corresponding choices of ϕ are as follows.

(i) YK phase convention:

$$\phi=(-)^{N_2'+N_2''}. \tag{44}$$

(ii) GT phase convention, implemented at the (a) *elementary generator level*:

$$\phi=(-)^{N_2'+N_2''+D},$$
$$D=\sum_{r\in\Theta_{23}'}2S_{(r-1)'}+\sum_{r\in\Theta_{23}''}2S_{(r-1)''}, \tag{45}$$

where Θ_{23}' and Θ_{23}'' are the index sets of levels r with $d_{r'}=2,3$ or $d_{r''}=2,3$, respectively; GT phase convention, implemented at the (b) *segment level*

$$\phi=(-)^{N_2'+N_2''}, \tag{46}$$

with additional factors analogous to (45) of Ref. 17.

Let us consider three examples of Eq. (42) in somewhat greater detail. The first case is that of a p-p raising generator E_{ij}, $1\leq i<j\leq n'$, whose resulting spin diagram is given in Fig. 9(a). The factor $(-)^{N_1''}$ in Eq. (43) is used to reverse the directions of all hole lines; at this point, both the hole and particle sections of the spin diagram resemble portions of diagrams encountered in the particle formalism. The diagram is now separated over pairs of lines labeled S_r and $\tilde{S}_r$ outside the generator range and over three lines inside the generator range, thus achieving the factorization into level contributions. At the same time, the factor Ψ is also split up into a product of terms which are associated with the individual spin diagrams obtained at each level.

The contributions of levels outside the generator range are all triangular deltas, and are thus equal to unity if the bra and ket states coincide at each such level. For levels inside the generator range, we may identify contributions derived from the segment formulas of the p formalism; of type A^R for level i, type A_R for level j, and type C' for levels $i+1$ through $j-1$. Each such contribution may be written $W(Q_r;\tilde{d}_r d_r,\Delta b_r,b_r)$, as in the p formalism. Finally, there is the contribution from the link segment, which is denoted $W(L)\equiv W(L;b_{n'},\Delta b_{n'},b_{n'+1},\Delta b_{n'+1},S)$. It is easily verified that for all three phase conventions mentioned above,

$$W(L)=1. \tag{47}$$

A similar development is possible for the matrix elements of a p-p lowering generator.

The second example is that of the h-h raising generator E_{ij}, $n'<i<j\leq n$. The pertinent spin diagram is displayed in Fig. 9(b). After a series of manipulations similar to those performed in the previous case, the matrix element of E_{ij} may be expressed as a product of $W(L)$ and segment values for levels in the generator range; of type A_R for level i, A^R for level j, and type C' for intermediate levels. Since $\epsilon=1$ in Eq. (41) for h-h generators, an additional minus sign is necessary. The matrix elements of a h-h lowering generator may be analyzed in a similar manner.

Finally we consider the matrix elements of a p-h raising generator E_{ij}, $1\leq i\leq n'<j\leq n$, whose resulting spin diagram is illustrated in Fig. 9(c). Unlike the diagrams of Figs. 9(a) and 9(b), the generator line crosses the link segment, thus necessitating a new link segment type which we denote L'. Upon separating the diagram, we may again express the matrix element of E_{ij} as a product of segment values over the range of the generator of types A^R for levels i and j, and of type C' for intermediate levels along with the link segment value $W(L')\equiv W(L';b_{n'},\Delta b_{n'},b_{n'+1},\Delta b_{n'+1},S)$. This latter value is given by

$$W(L')=\gamma(-)^{S+\tilde{S}_{(n'')''}+S_{(n')'}-1/2}[\tilde{S}_{(n')'},\tilde{S}_{(n'')''}]^{1/2}\begin{Bmatrix}S_{(n')'} & S_{(n'')''} & S\\ \tilde{S}_{(n'')''} & \tilde{S}_{(n')'} & \frac{1}{2}\end{Bmatrix}, \tag{48}$$

where

$$\begin{Bmatrix}j_1 & j_2 & j_3\\ l_1 & l_2 & l_3\end{Bmatrix}$$

is the usual $6j$ symbol, and γ depends on the phase convention used. For conventions (i) and (ii)(a), we may take $\gamma=1$, while for convention (ii)(b), $\gamma=\psi[\frac{1}{2}]$ for raising generators and $\gamma=\psi[-\frac{1}{2}]$ for lowering generators, where we defined

$$\psi[k]=(-)^{t_{(n')'}(k)+t_{(n'')''}(k)},$$
$$t_j(k)=2S_j\delta(S_j-\tilde{S}_j,k). \tag{49}$$

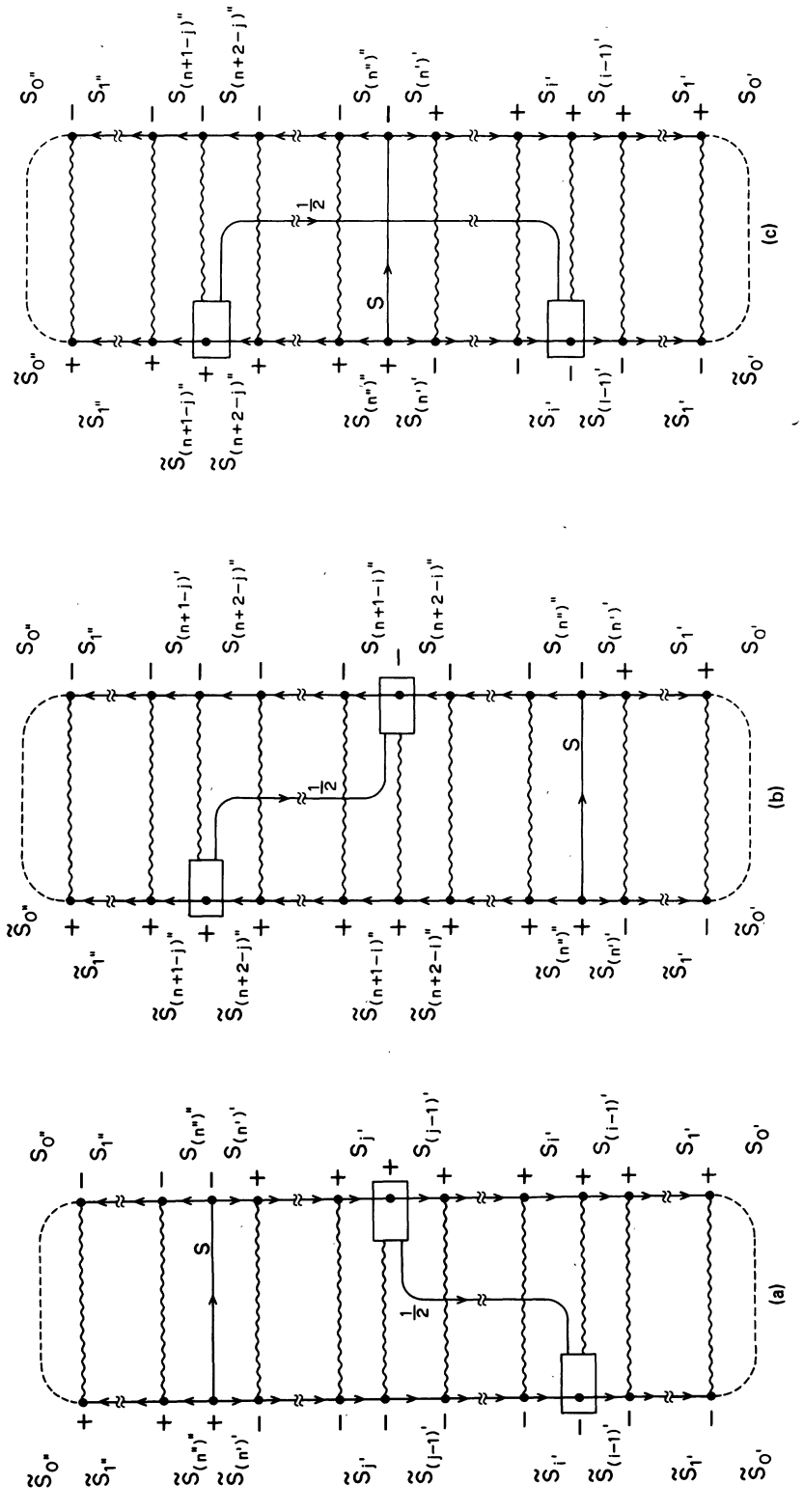

FIG. 9. Resulting spin diagrams for raising generators. The resulting spin diagrams for the cases of a p-p raising (a), h-h raising (b), and p-h raising (c) generator are displayed. In each diagram, the wavy line represents a zero or $\frac{1}{2}$ angular-momentum line, according to the orbital occupancy ($n_r = 0$, 2 and $n_r = 1$, respectively). The blank boxes represent one or two particle vertices as in Fig. 4 of Ref. 17.

The matrix elements of p-h lowering generators may be expressed in a similar manner with both terminal segments taken to be of type A^L.

The results of this section may be summarized in a single formula. However, due to the fact that the segment types necessary for hole levels are the inversions of those indicated by the p formalism (where by inversion we mean the exchange $A^Q \rightleftharpoons A_Q$, $Q=R,L$), we first define the barred segment types $\bar{Q}_r$, as in Table IV, for both one and two generator segment types. As can be seen, the effect of the bar is to reposition all superscripts as subscripts, and vice versa, when the segment refers to a hole orbital.

The matrix element of any single generator in the p-h formalism may now be written

$$\langle \tilde{d}S|E_{ij}|\underline{d}S\rangle = (-)^h W(L^{(m)}) \prod_{r\in\Omega} W(\bar{Q}_r) = (-)^h W(L^{(m)}; b_{n'}, \Delta b_{n'}, b_{n'+1}, \Delta b_{n'+1}, S) \prod_{r\in\Omega} W(\bar{Q}_r; \tilde{d}_r d_r, \Delta b_r, b_r), \tag{50}$$

where $\Omega=\Omega(E_{ij})=\{i, i\pm1, \ldots, j\}$ is the range of the generator, Q_r is the segment type of the rth level defined by E_{ij} based on the p-formalism definition, and h and m are the numbers of h-h and p-h generators, respectively, in the set $\{E_{ij}\}$.

VII. MATRIX ELEMENTS OF GENERATOR PRODUCTS

In this section, we derive a formula for the matrix elements of generator products in the p-h formalism. In the extension of the method just outlined for single generators to the case of generator products, several difficulties are encountered; among these are the problem of noncommuting generators, the appearance of direct and exchange terms and the possibility of overlap of the generator regions. These difficulties arose in a parallel fashion in the p formalism[17]; the methods for their disposal developed there are employed in the p-h formalism in more or less the same form. Thus in our discussion here, we shall concentrate on the minor differences and special considerations needed for the p-h formalism, and refer the reader to Ref. 17 for a more detailed account of the general procedures.

It is useful, first of all, to prepare a list of the possibilities for pairs of generators in the p-h formalism according to their type and the relationship between their ranges; this is done schematically in Fig. 10. The possibilities are primarily classified according to the number of p-h generators in the pair, since this number determines the type of the link segment. Diagrams 1–3 represent the patterns for pairs of generators which include no p-h generators. Since these cases are quite simple, the actual patterns are not given; instead we indicate with an encircled numeral the number of p-p or h-h generators present, according to the position of the numeral below or above the dotted line, respectively. Diagram 1 thus represents all pairs of two p-p generators; each of the diagrams of Fig. 6 of Ref. 17 may thus be inserted into the lower portion of this schematic diagram. Diagrams 4–7 of Fig. 10 represent the combination of a p-h generator and a p-p or h-h generator, where the latter generator is indicated by a numeral. Finally, all pairs of two p-h generators are listed individually in diagrams 8–20 of Fig. 10.

According to the results of Sec. IV, the matrix elements of the generator product $E_{ij}E_{kl}$ may be written

$$\langle \tilde{d}\tilde{S}|E_{ij}E_{kl}|\underline{d}S\rangle = \Psi \,\mathrm{Val}(G_r), \tag{51}$$

where G_r is the appropriate resulting spin diagram and Ψ is given by (43). G_r is then separated into segments, each of which is associated with a single orbital level. Before describing this procedure, however, we must first consider the possibility that the generators E_{ij} and E_{kl} do not commute. This is the case when $j=k$ or $i=l$ or both. In the

TABLE IV. Definition of barred segment types $\bar{Q}_r$ in terms of the p-formalism segment types Q_r, depending on whether the orbital referred to has hole ($1\leq r\leq n'$) or particle ($n'<r\leq n$) character. H and H' stands for either R or L.

Segment type	One-particle segments			Two-particle segments					
$Q_r (1\leq r\leq n)$	A^H	A_H	C'	$A^{HH'}$	$A^H_{H'}$	$A_{HH'}$	B^H	B_H	C''
$\bar{Q}_r$ $(1\leq r\leq n')$	A^H	A_H	C'	$A^{HH'}$	$A^H_{H'}$	$A_{HH'}$	B^H	B_H	C''
$\bar{Q}_r$ $(n'<r\leq n)$	A_H	A^H	C'	$A_{HH'}$	$A^{H'}_H$	$A^{HH'}$	B_H	B^H	C''

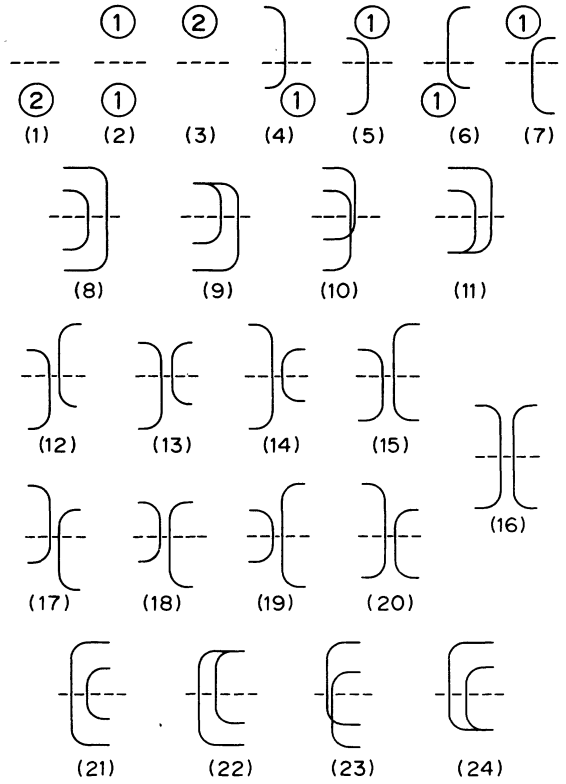

FIG. 10. Schematic resulting spin diagrams for generator products. The schematic resulting spin diagrams for generator products containing zero (1–3), one (4–7), or two (8–24) p-h generators are illustrated. In diagrams (1–7), the one and two p-p or h-h generator lines are indicated symbolically by an encircled numeral. We also note that diagrams (17–24) may be obtained by the bra-ket inversion from diagrams (12–15) and (8–11).

p formalism, the difference between the matrix elements of the two different orderings of generator products is that for one ordering, an additional contraction pattern is possible, in which a contraction occurs between two annihilation and creation operators contained within the generators themselves; thus the additional contraction pattern is possible for the ordering $E_{ij}E_{jl}$ but not for the ordering $E_{jl}E_{ij}$. The difference is accounted for in the segment formalism by recording two sets of values for the jth segment type, labeled by the additional index Y. The values corresponding to $Y=1$ are used for the latter order mentioned above, and those for $Y=2$ for the former order.

In the p-h formalism, a similar development is necessary. However, it must be remembered that the annihilation and creation operators referring to a hole orbital between which a nonzero contraction is possible, must occur in the opposite order to that for nonzero contractions of particle operators. Thus, it is the ordering $E_{jl}E_{ij}$ for which an additional contraction pattern is possible, when j refers to a hole orbital. We may summarize the Y index values which must be used for the jth segment according to

	$1 \leq j \leq n'$	$n' < j \leq n$
$E_{jl}E_{ij}$	$Y=1$	$Y=2$
$E_{ij}E_{jl}$	$Y=2$	$Y=1$

. (52)

For the special case $E_{ij}E_{ji}$, the appropriate values of the Y index must be used for both the ith and jth segments.

Having now accounted for the possibility of noncommuting generators, we may now continue with the separation of the resulting spin diagram G_r of (51). The main difficulty at this point is that the ranges of the two generators may overlap, thus making a separation into levels impossible without the introduction of intermediate summation variables at each overlap region level. However, this difficulty is easily avoided, as in the p formalism, by first precoupling the spins of the particles in the overlap region to X. Each segment in the overlap region thereby becomes dependent on X and in the final formula a summation over $X=0,1$ must be carried out.

Evidently, a new type of link segment is encountered when separating the spin diagrams for the generator products corresponding to diagrams 8–20 of Fig. 10. This segment, through which two generator lines (or one X line) pass, is denoted L'', and its value is given by the formula

$$W^{(X)}(L'')=\Gamma(-)^{X-S-\tilde{S}_{(n'')''}-S_{(n')'}}[\tilde{S}_{(n')'},\tilde{S}_{(n'')''}]^{1/2}\begin{Bmatrix} S_{(n')'} & S_{(n'')''} & S \\ \tilde{S}_{(n'')''} & \tilde{S}_{(n')'} & X \end{Bmatrix}, \tag{53}$$

where $\Gamma=1$ for phase conventions (i) and (ii)(a) and $\Gamma=\psi[0]$ for raising-raising and lowering-lowering generator products and $\Gamma=\psi[+1]\psi[-1]$ for raising-lowering generator products, where $\psi[k]$ is defined by Eq. (49).

The final problem in calculating the matrix elements of generator products is associated with the appearance of direct and exchange terms. The relationship between these terms is displayed schematically in Fig. 11, where each subfigure

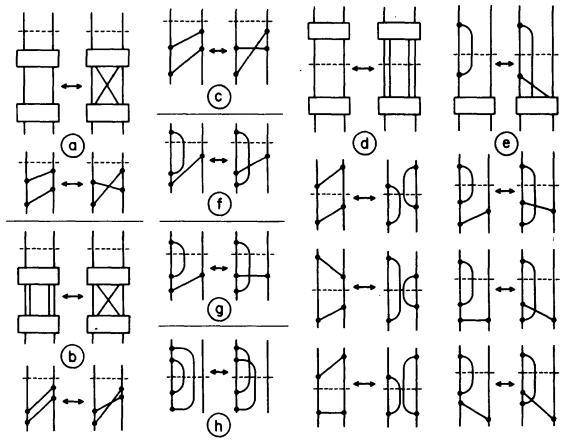

FIG. 11. Relationship between direct and exchange term diagrams. The resulting spin diagrams for direct and exchange generator product terms are illustrated schematically. Diagrams (a), (b), and (c) represent the possibilities for two p-p generators, diagram (d) for the combination of a p-p and h-h generator, diagrams, (e), (f), and (g) for a p-p and p-h raising generator, and diagram (h) for two p-h raising generators. Other possibilities are similar to one of these cases. In diagrams (a), (b), (d), and (e), the general form is given first, with typical examples beneath, although only one such is given for (a) and (b) since these are the same as in Fig. 8 of Ref. 17. In each case the direct and corresponding exchange terms are displayed to the left and right of the doubled arrow.

contains just a single specific schematic diagram or a general diagram along with some typical cases. In each diagram, the dashed line locates the position of the link segment, and the direct and corresponding exchange terms appear to the left and the right of the double arrow, respectively. Figures 11(a), 11(b), and 11(c) refer to the case with two p-p generators and thus may be found in Fig. 8 of Ref. 17. The diagrams for two h-h generators may be obtained by shifting the dashed line to a position below the generator lines. For the combination of one p-p and one h-h generator, Fig. 11(d) applies. The diagrams for one p-h generator and one p-p or h-h generator are given in Figs. 11(e), 11(f), and 11(g), which illustrate the possibilities for the particular case of a p-h raising generator and a p-p generator. Finally, Fig. 11(h) represents the case of two p-h raising generators; those for two p-h lowering generators are the reflections of these about a vertical line.

TABLE V. Typical generator product segment sequences. The sequence of segment types necessary for the evaluation of the matrix elements of generator products represented by diagrams 8–16 of Fig. 10. The left-to-right order corresponds to the order from bottom to top in the diagram. Those for diagrams 17–24 of Fig. 10 are obtained by making the substitution $R \longleftrightarrow L$ in the sequence given for the diagram which is a reflection about a vertical line.

Diagram (Fig. 10)	Segment sequence
8	$A^R C' \cdots C' B^R C'' \cdots C'' B^R C' \cdots C' A^R$
9	$A^R C' \cdots C' B^R C'' \cdots C'' A^{RR}$
10	$A^R C' \cdots C' B'^R C'' \cdots C'' B^R C' \cdots C' A^R$
11	$A^{RR} C'' \cdots C'' B^R C' \cdots C' A^R$
12	$A^R C' \cdots C' B^L C'' \cdots C'' B^R C' \cdots C' A^L$
13	$A^R C' \cdots C' B^L C'' \cdots C'' A^{RL}$
14	$A^R C' \cdots C' B^L C'' \cdots C'' B^L C' \cdots C' A^R$
15	$A^{RL} C'' \cdots C'' B^R C' \cdots C' A^L$
16	$A^{RL} C'' \cdots C'' A^{RL}$

We may now state the final rule for the determination of the proper segments to be used in finding the matrix elements of a given generator product, namely, for exchange-type matrix elements in which the generator lines cross [Figs. 11(a), 11(b), 11(e), 11(f), and 11(h)] replace the B^Q segment by the B'^Q segment whose value is defined by Eq. (57) of Ref. 17. For cases corresponding to Fig. 11(h), it is thus necessary to use the primed segment values for the B^Q segment in one of the particle or hole regions; we have arbitrarily chosen to assign the primed B^Q segment to the particle region. As an illustration of these remarks, we list in Table V the sequences of segment types associated with the generator products represented by diagrams 8–16 of Fig. 10.

Our expression for the matrix elements of generator products in the p-h formalism may now be given

$$\langle \underline{\tilde{d}} S | E_{ij} E_{kl} | \underline{d} S \rangle = (-)^h \prod_{r \in \Omega_1} W^{(Y)}(\bar{Q}_r; \tilde{d}_r d_r, \Delta b_r, b_r) \times \sum_{X=0,1} \left\{ W^{(X)}(L^{(m)}; b_{n'}, \Delta b_{n'}, b_{n'+1}, \Delta b_{n'+1}, S) \prod_{r \in \Omega_2} W^{(Y)}(\bar{Q}_r; \tilde{d}_r d_r, \Delta b_r, b_r; X) \right\}, \quad (54)$$

where $\Omega_1 = \Omega(E_{ij}) \Delta \Omega(E_{kl})$, $\Omega_2 = \Omega(E_{ij}) \cap \Omega(E_{kl})$, $\bar{Q}_r$ are the barred segments defined in Table IV, h and m are the numbers of h-h and p-h generators, respectively, among the set $\{E_{ij}, E_{kl}\}$, and the appropriate values of Y are used for noncommuting generators according to (52).

There exists a close relationship between the matrix elements of the generator products corresponding to the direct and exchange terms, and they can often be evaluated simultaneously. By writing the expression on the right-hand side of Eq. (54) as $w_0 + w_1$, where w_i is the term corresponding to $X = i$, $i = 0, 1$, and w_0 is the entire term if $\Omega_2 = \emptyset$, we may establish the following relationships between the direct and exchange matrix elements. The pertinent relationship depends on the nature of the generators involved, and is indicated by the appropriate diagram of Fig. 11.

Case (1). b (p-p + p-p, h-h + h-h),

f (p-h + p-p, p-h + h-h; both raising or both lowering),

h (p-h + p-h, both raising or both lowering).

Direct term: $\langle \underline{\tilde{d}} S | E_{ij} E_{kl} | \underline{d} S \rangle = w_0 + w_1$.

Exchange term: $\langle \underline{\tilde{d}} S | E_{il} E_{kj} | \underline{d} S \rangle = w_0 - w_1$. (55)

Case (2). a (p-p + p-p, h-h + h-h),

d (p-p + h-h),

e (p-h + p-p, p-h + h-h).

Direct term: $\langle \underline{\tilde{d}} S | E_{ij} E_{kl} | \underline{d} S \rangle = w_0$.

Exchange term: $\langle \underline{\tilde{d}} S | E_{il} E_{kj} | \underline{d} S \rangle = -\frac{1}{2} w_0 + w_1$. (56)

Case (3). c (p-p + p-p, h-h + h-h),

g (p-h + p-p, p-h + h-h).

The direct and exchange terms may again be evaluated simultaneously, the only difference being that the A_R^R or A_L^L segment value in the direct-term expression is replaced by the matrix element of a weight generator in the exchange term expression.

We might add at this point, that for CI calculations, it is the matrix elements of the operator

$$e_{ij,kl} = E_{ij} E_{kl} - \delta_{jk} E_{il} = N[E_{ij} E_{kl}], \quad (57)$$

that are needed rather than those of the simple generator product. In the p-h formalism, the matrix elements of $e_{ij,kl}$ are given by the same formula (54), in which the values $Y = 1$ and 2 are used for any Y-dependent segment values located in the particle or hole sections, respectively.

VIII. DISCUSSION

We have presented algorithms for the evaluation of the matrix elements of the one and two particle parts of the Hamiltonian (4) within the p-h formalism. This method may be employed in conjunction with the generation and representation scheme for electronic p-h states based on the distinct row table, which is described in Sec. III and illustrated in Sec. IV.

In both the particle[17] and particle-hole formalisms, the required matrix elements were expressed in terms of the same segment values, a complete list of which is given in Ref. 17. It was possible to develop the p-h formalism in such a way that only three new segment formulas were necessary, namely, those given by Eqs. (47), (48), and (53) for the link segment. In order to complete the list of all nonzero segment values necessary for the p-h formalism, we list those for the link segments in Table VI. Even though different phase conventions may be employed, as in the particle formalism, the most natural convention to use in the p-h formalism is clearly that referred to as YK convention.

Let us now briefly discuss some of the advantages offered by this formalism when applied to the CI approach. The h-p formalism will not only avoid repetitious calculations for all diagonal and certain off-diagonal CI matrix elements which involve summations over the orbitals occupied in the reference configuration (which in fact can be avoided even in the p formalism when the Hamiltonian is appropriately repartitioned, as shown recently by Shavitt[30]), but it will also add to the flexibility in the configuration-selection process and avoid repetitious calculations in the handling of states with different spin multiplicities, since a considerable number of matrix elements will only differ in the central link segment. It also provides an automatic labeling and separation of configurations with different excitation levels. For example, considering only singly or doubly excited states out of an arbitrary singlet reference state (an extension to arbitrary multiplicity is straightforward) we immediately get a splitting into the four subproblems, labeled by the irreps $\{00|00\}$ $(N' = 0)$, $\{01|10\}$ $(N' = 1)$, $\{10|01\}$ and $\{02|20\}$ $(N' = 2)$ [e.g., in the case considered in Sec. IV the irreps of Figs. 4(a)–4(d)]. These irreps correspond directly to the V, D, S, and T classes introduced by Siegbahn.[8]

Since the particle-formalism full CI space is factored into the direct sum of subspaces, which may be labeled by their excitation level and spin coupling, we have an additional flexibility in the configuration-selection process when using the

TABLE VI. List of nonvanishing link-segment values in terms of the functions $T=S+\frac{1}{2}(x+y)$, $U=[(x+1)(y+1)]^{-1/2}$, and

$$V=\left[\frac{(x+1+\frac{1}{2}\Delta x)(y+1+\frac{1}{2}\Delta y)}{x(x+1)(x+2)y(y+1)(y+2)}\right]^{1/2},$$

where $x=b_{n'}$, $y=b_{n'+1}$, $\Delta x=\Delta b_{n'}$, and $\Delta y=\Delta b_{n'+1}$.

Q	X	Δx	Δy	$W(Q;x,\Delta x,y,\Delta y,S)$ or $W^{(X)}(Q;x,\Delta x,y,\Delta y,S)$
L		0	0	1
L'		−1	−1	$-U[(T+2)(T-2S+1)]^{1/2}$
		−1	1	$-U[(T-x)(T-y+1)]^{1/2}$
		1	−1	$U[(T-y)(T-x+1)]^{1/2}$
		1	1	$-U[(T+1)(T-2S)]^{1/2}$
L''	0	0	0	1
	1	−2	−2	$V[(T+2)(T+3)(T-2S+1)(T-2S+2)]^{1/2}$
		−2	0	$V[2(T+2)(T-2S+1)(T-x)(T-y+1)]^{1/2}$
		−2	2	$V[(T-x-1)(T-x)(T-y+1)(T-y+2)]^{1/2}$
		0	−2	$-V[2(T+2)(T-2S+1)(T-x+1)(T-y)]^{1/2}$
		0	0	$-\frac{1}{2}V[2S(2S+2)-x(x+2)-y(y+2)]$
		0	2	$V[2(T+1)(T-2S)(T-x)(T-y+1)]^{1/2}$
		2	−2	$V[(T-x+1)(T-x+2)(T-y-1)(T-y)]^{1/2}$
		2	0	$-V[2(T+1)(T-2S)(T-x+1)(T-y)]^{1/2}$
		2	2	$V[T(T+1)(T-2S-1)(T-2S)]^{1/2}$

distinct row table representation. This separation of the full space into subspaces labeled by h-p formalism irreps may thus be regarded as a "natural" row splitting introduced by Brooks and Schaefer.[7] This separation will further depend on the choice of the reference state $|\Phi_0\rangle$ or, equivalently, on the partitioning of the orbital space into the particle and hole subspaces. This is illustrated in Tables VII(a)–VII(c), where we give the breakdown of the full CI space into the p-h subspaces for the six-electronic case using different reference states. The actual dimensions are listed for the two choices of the orbital space which correspond to the minimum and double zeta basis sets. We also list for each subproblem the maximal number of independent spin states, i.e., the maximal number of states having the same orbital occupation numbers. These numbers indicate a distribution of independent spin states over the p-h subproblems and their sum for the subproblems associated with the same excitation level must equal the maximal number of independent spin states for each excitation type, as given by the Young-Yamanouchi branching diagram (unless some of them cannot be realized due to the limited dimensionality of either particle or hole subspaces). For example, in cases considered in Table VII, we obtain three doubly excited triplets and nine triply excited triplets in all cases considered, but their distribution into the individual p-h subspaces is different in each case. This feature should be beneficial, for example, in the implementation of a truncation scheme proposed by Lucchese and Schaefer.[31]

Let us also mention the possibility of choosing the reference state with m doubly occupied orbitals, where m equals the number of orbitals in the so-called active space. Then a zero excitation level subproblem will correspond to a full CI within the active space and one can limit appropriately the excitation level for the remaining subspaces (say, to the doubly excited states).

The h-p formalism, as developed in this and the preceding paper I, represents in fact a spin-adapted formulation of the usual h-p diagrammatic formalism, and may thus be employed in various problems in which the total particle number is conserved. Thus it may be directly used in the shell-model or CI calculations discussed above, in the coupled-cluster approach (note that the orthogonally spin-adapted formulation of this approach[32] exploits in fact the h-p YK or GT states used here, the only difference being in the phase convention used), or in calculations of p-h propagators. However, if we wish to have complete flexibility of the general h-p formalism, we must relax the condition of the total particle number conservation, so that we can also treat various electron attachment and detachment processes. This relaxation can be considered either in the p formalism or in the p-h formalism. Any operator relating the states with different particle numbers cannot, of course, be represented through U(n) generators and must be considered as a proper

TABLE VII. Irrep labels, their excitation levels, and maximal multiplicities for fixed spatial occupations and dimensions for the case $N=6$ and $S=0$ or 1.

(a) $N_0=2$, $n''=2$, $n'=4$ $(n=6)$, and $n'=10$ $(n=12)$

S	Irrep	Excitation level	Maximal multiplicity	Dimension $n'=4$ $(n=6)$	Dimension $n'=10$ $(n=12)$
0	{10|00}	0	1	10	55
	{11|10}	1	2	40	660
	{20|01}	2	2	60	2 475
	{12|20}	2	3 } 5	15	990
	{21|11}	3	10	40	6 600
	{30|02}	4	10	10	4 950
			Total dimension:	175	15 730
1	{02|00}	0	1	6	45
	{11|10}	1	2	40	660
	{03|10}	1	1 } 3	8	240
	{12|01}	2	3	45	2 970
	{20|20}	2	2	20	825
	{12|20}	2	3 } 9	15	990
	{04|20}	2	1	1	210
	{21|11}	3	10	40	6 600
	{13|11}	3	8 } 18	8	3 696
	{22|02}	4	18	6	6 930
			Total dimension:	189	23 166

(b) $N_0=0$, $n''=3$, $n'=3$ $(n=6)$, and $n'=9$ $(n=12)$

S	Irrep	Excitation level	Maximal multiplicity	Dimension $n'=3$ $(n=6)$	Dimension $n'=9$ $(n=12)$
0	{00|00}	0	1	1	1
	{01|10}	1	1	9	27
	{10|01}	2	1	36	270
	{02|20}	2	1 } 2	9	108
	{11|11}	3	4	64	1 920
	{03|30}	3	1 } 5	1	84
	{20|02}	4	4	36	3 240
	{12|21}	4	9 } 13	9	1 890
	{21|12}	5	25	9	5 670
	{30|03}	6	25	1	2 520
			Total dimension:	175	15 730
1	{01|10}	0	1	9	27
	{10|20}	1	1	18	135
	{02|20}	1	1 } 3	9	108
	{02|01}	1	1	18	216
	{11|11}	2	4	64	1 920
	{11|30}	2	2	8	240
	{03|11}	2	2 } 9	8	672
	{03|30}	2	1	1	84
	{20|21}	3	6	18	1 620
	{12|02}	3	6	18	3 780
	{12|21}	3	9 } 24	9	1 890
	{04|21}	3	3	0	378
	{21|12}	4	25	9	5 670
	{13|12}	4	20 } 45	0	3 024
	{22|03}	5	45	0	3 402
			Total dimension:	189	23 166

TABLE VII. (Continued)

(c) $N_0 = -2$, $n'' = 4$, $n' = 2$ ($n = 6$), and $n' = 8$ ($n = 12$).

S	Irrep	Excitation level	Maximal multiplicity	Dimension $n'=2$ ($n=6$)	Dimension $n'=8$ ($n=12$)
0	{00|01}	0	1	10	10
	{01|11}	1	2	40	160
	{10|02}	2	2 } 5	60	720
	{02|21}	2	3 }	15	420
	{11|12}	3	10 } 14	40	3 360
	{03|31}	3	4 }	0	224
	{20|03}	4	10	10	3 360
	{12|22}	4	27	0	2 268
	{21|13}	5	70	0	4 032
	{30|04}	6	70	0	1 176
			Total dimension:	175	15 730
1	{00|20}	0	1	6	6
	{01|11}	1	2 } 3	40	160
	{01|30}	1	1 }	8	32
	{10|21}	2	3 }	45	540
	{02|02}	2	2 } 9	20	560
	{02|21}	2	3 }	15	420
	{02|40}	2	1 }	1	28
	{11|12}	3	10 }	40	3 360
	{11|31}	3	8 } 27	8	672
	{03|12}	3	5 }	0	1 120
	{03|31}	3	4 }	0	224
	{20|22}	4	18 }	6	2 016
	{12|03}	4	15 } 69	0	3 780
	{12|22}	4	27 }	0	2 268
	{04|22}	4	9 }	0	420
	{21|13}	5	70 } 126	0	4 032
	{13|13}	5	56 }	0	2 016
	{22|04}	6	126	0	1 512
			Total dimension:	189	23 166

tensor operator, as in fact, is the case of the p-h excitation operators within the hole and particle subspaces considered in this paper.

The particle number-nonconserving processes of ionization and electron attachment, which can be described by one-particle or one-hole propagators, were very recently studied by Shavitt and Born[33] within the p formalism. These authors showed how the U(n) tensor-operator formalism can be translated into the ABC tableaux or Shavitt-graph formalism and used in the evaluation of one-electron propagators. The key problem in these applications is an evaluation of matrix elements of various tensor operators, in particular, of the matrix elements of single creation or annihilation operators. This is equivalent to the problem of calculating one-electron coefficients of fractional parentage (CFP) in the U(n) or YK coupling scheme.

We would like to note how this problem and its generalization can be treated by the graphical methods of spin algebras, which were exploited in this and preceding[18] studies. In the p formalism, the desired matrix elements of a spin-adapted single creation or a single annihilation operator will be characterized by the spin graphs shown in Figs. 12(a) or 12(b), respectively. The irreps involved must clearly differ in one box in the first or the second column of their Young patterns. We also see immediately from the spin graphs of Figs. 12(a) or 12(b), that all the segment types needed in this case are identical with those needed in the single generator case, and that the range involved in the evaluation of a spin-adapted particle creation or annihilation operator for the ith orbital level is $i \leq r \leq n$, in agreement with the findings of Shavitt and Born.[33]

These results may also be easily generalized to the case of two-particle or two-hole propagators, in which case the matrix elements of spin-adapted products of two creation or of two annihilation operators will be needed. Again, the same segments

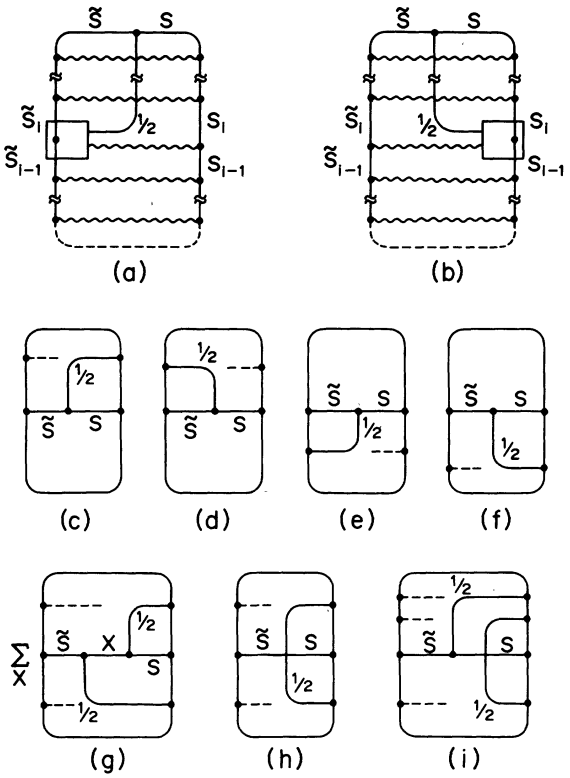

FIG. 12. Schematic resulting spin diagram for matrix elements of particle number-nonconserving operators. Diagrams (a) and (b) represent the resulting spin diagrams for a single spin-adapted (or reduced) creation and annihilation operators, respectively, in the p formalism or, equivalently, for the one particle CFP's. Correspondingly, single hole (c), (d), and single particle (e) and (f) creation and annihilation operator resulting spin diagrams are obtained in the h-p formalism. The relationship between a particle and hole annihilation operator product (g) and our p-h lowering generator (h); [cf. also, diagram (f) of Fig. 8], follows easily using the graphical orthogonality rule for the crossed lines (cf., e.g., Fig. 5 of Ref. 34). Finally, diagram (i) corresponds to the 1-p–2-h propagator case. See the text for more details.

as in the two-generator p-formalism case will be needed for the nth-level segment, which would be associated with a simple $6j$ coefficient

$$\begin{Bmatrix} \tilde{S} & S\pm\frac{1}{2} & S \\ \frac{1}{2} & \frac{1}{2} & X \end{Bmatrix},$$

where $X=0,1$ and $\tilde{S}=S$ or $S\pm1$.

We should also note that the h-p formalism as described here and in I can be generalized in the same way. Thus, the matrix elements involving a single particle or a single hole creation or annihilation will be given by diagrams shown schematically in Figs. 12(c)–12(f). Similar diagrams will result for more complex processes. For example, the evaluation of a 1-p–2-h propagator will require matrix elements of the type shown in Fig. 12(i). In fact, the 1-p–1-h or 2-p–2-h type tensor operators, considered in this paper, are simply related to these more general operators. Combining, for example, the processes characterized by diagrams (c) and (f) of Fig. 12, we obtain the diagram (g) of Fig. 12, which is clearly equivalent to the diagram (h) of Fig. 12 considered here (for the orthogonality rule for crossing lines see, e.g., Fig. 5 of Ref. 34). We find that in all the cases just mentioned we will only need the segment types derived earlier in the p formalism[17] except for the link segments. However, these are again given through simple $6j$ or $9j$ coefficients.

Finally, another useful extension of the h-p formalism developed here and in I would be obtained if the orbital space was partitioned into two or more subspaces, each spanned by orbitals characterizing a certain part of the system considered (cf. Refs. 35 and 36). In this case it would be convenient to consider the basis of $U(n)$ subduced to $U(k_1)\otimes U(k_2)\otimes\cdots\otimes U(k_m)$, where $n=k_1+k_2+\cdots+k_m$ $(m\geq 2)$. Such a formalism would enable a spin-adapted formulation of the group orbital method of McWeeny[37] as recently suggested by Wormer.[38]

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[1]M. Moshinsky, in *Many-Body Problems and Other Selected Topics in Theoretical Physics*, edited by M. Moshinsky, T. A. Brody, and G. Jacob (Gordon and Breach, New York, 1966), p. 289. Also published separately as *Group Theory and the Many-Body Problem* (Gordon and Breach, New York, 1968).

[2]J. Paldus, J. Chem. Phys. 61, 5321 (1974); Int. J. Quantum Chem. Symp. 9, 165 (1965); in *Theoretical Chemistry: Advances and Perspectives*, edited by H. Eyring and D. Henderson (Academic, New York, 1976), Vol. 2, pp. 131–290.
[3]I. Shavitt, Int. J. Quantum Chem. Symp. 11, 131 (1977); 12, 5 (1978).
[4]J.-F. Gouyet, R. Schranner, and T. H. Seligman, J. Phys. A 8, 285 (1975).
[5]G. W. F. Drake and M. Schlesinger, Phys. Rev. A 15, 1990 (1977).
[6]F. Sasaki, in *Progress Report* XI, *Research Group on Atoms and Molecules* (Department of Physics, Ochanomizu University, Tokyo, Japan, 1978), p. 1–3.
[7]B. R. Brooks and H. F. Schaefer III, J. Chem. Phys. 70, 5092 (1979); B. R. Brooks, W. D. Laidig, P. Saxe, N. C. Handy, and H. F. Schaefer III, Phys. Scr. 21, 312 (1980).
[8]P. E. M. Siegbahn, J. Chem. Phys. 70, 5391 (1979); 72, 1647 (1980).
[9]D. Hegarty and M. A. Robb, Mol. Phys. 38, 1795 (1979) and references therein.
[10]B. O. Roos and P. E. M. Siegbahn, in *Methods of Electronic Structure Theory*, edited by H. F. Schaefer III (Plenum, New York, 1977), pp. 277–318.
[11]A. P. Jucys, I. B. Levinson, and V. V. Vanagas, *Mathematical Apparatus of the Theory of Angular Momenta* (Israel Program for Scientific Translations, Jerusalem, 1962, and Gordon and Breach, New York, 1964); A. P. Jucys and A. A. Bandzaitis, *Theory of Angular Momentum in Quantum Mechanics*, (Mokslas, Vilnius, 1977), 2nd ed., in Russian.
[12]D. M. Brink and G. R. Satchler, *Angular Momentum*, (Clarendon, Oxford, 1968), 2nd ed., Chap. VII, p. 112.
[13]E. El Baz and B. Castel, *Graphical Methods of Spin Algebras* (Dekker, New York, 1972).
[14]J. Paldus and P. E. S. Wormer, Int. J. Quantum Chem. 16, 1321 (1979).
[15]See, e.g., J. Paldus and J. Čížek, Adv. Quantum Chem. 9, 105 (1975).
[16]K. Ruedenberg, Phys. Rev. Lett. 27, 1105 (1971); W. I. Salmon and K. Ruedenberg, J. Chem. Phys. 57, 2776 (1972).
[17]J. Paldus and M. J. Boyle, Phys. Scr. 21, 295 (1980).
[18]J. Paldus and M. J. Boyle, Phys. Rev. A 22, 2299 (1980); referred to as paper I.
[19]J. Flores and M. Moshinsky, Nucl. Phys. A 93, 81 (1967).
[20]For a recent introductory review of the unitary group approach, see, J. Paldus, in The Unitary Group for the Evaluation of Energy Matrix Elements (Proceedings of the Workshop on The Unitary Group for the Evaluation of Electronic Energy Matrix Elements, 1979, University of Bielefeld, Bielefeld, Germany), edited by J. Hinze (Springer, Berlin, 1980) (in press).
[21]T. Yamanouchi, Proc. Phys.-Math. Soc. Jpn. 19, 436 (1937); M. Kotani, A. Amemiya, E. Ishiguro, and T. Kimura, *Tables of Molecular Integrals* (Maruzen, Tokyo, 1963) 2nd ed.
[22]M. Moshinsky and T. H. Seligman, Ann. Phys. (N. Y.) 66, 311 (1971).
[23]P. E. S. Wormer, Ph.D. thesis, University of Nijmegen, The Netherlands, 1975 (unpublished).
[24]P. E. S. Wormer and J. Paldus, Int. J. Quantum Chem. (in press).
[25]See, e.g., B. L. Silver, *Irreducible Tensor Methods* (Academic, New York, 1976), p. 190.
[26]See, e.g., Sec. 2C and Fig. 4 of J. Paldus, B. G. Adams, and J. Čížek, Int. J. Quantum Chem. 11, 813 (1977).
[27]See, e.g., J. D. Louck, Am. J. Phys. 38, 3 (1970).
[28]G. E. Baird and L. C. Biedenharn, J. Math. Phys. 5, 1730 (1964); L. C. Biedenharn and J. D. Louck, Commun. Math. Phys. 8, 89 (1968); J. D. Louck and L. C. Biedenharn, J. Math. Phys. 11, 2368 (1970).
[29]A. U. Klimyk and B. Gruber, J. Math. Phys. 20, 1995 (1979); 20, 2011 (1979).
[30]I. Shavitt, Annual Report to the National Aeronautics and Space Administration, Battelle Columbus Laboratories, Columbus, Ohio, 1979 (unpublished).
[31]R. J. Lucchese and H. F. Schaefer III, J. Chem. Phys. 68, 769 (1978).
[32]J. Paldus, J. Chem. Phys. 67, 303 (1979); B. G. Adams and J. Paldus, Phys. Rev. A 20, 1 (1979).
[33]I. Shavitt and G. J. Born, Progress Report to the National Science Foundation, Battelle Columbus Laboratories, Columbus, Ohio, 1980 (unpublished).
[34]J. Paldus and P. E. S. Wormer, Phys. Rev. A 18, 827 (1978).
[35]P. E. S. Wormer and A. van der Avoird, J. Chem. Phys. 57, 2498 (1972).
[36]C. W. Patterson and W. G. Harter, Phys. Rev. A 15, 2572 (1977).
[37]See, e.g., R. McWeeny and B. T. Sutcliffe, *Methods of Molecular Quantum Mechanics* (Academic, New York, 1969).
[38]P. E. S. Wormer, in The Unity Group for the Evaluation of Energy Matrix Elements (see Ref. 20 for details) (in press).