Young operator methods for fermion systems

Yaxiong Yu, Pancracio Palting, Ying-Nan Chiu
Department of Chemistry, The Catholic University of America, Washington DC 20064, USA

Summary. Alternative methods to the standard Young technique for the construction of Fermion wave functions in the spin orbital formalism are presented and shown to be equivalent to the standard technique. To develop these methods: (i) the starting or primitive function is factored into spin and spatial parts, (ii) the conjugacy feature required to satisfy the antisymmetry principle is exploited, (iii) the necessary commutation relations with the Fermion antisymmetrizer are shown to hold and (iv) the one-to-one correspondence between the independent picture of the Young tableaux and the independent Slater determinants is used. This last feature has the advantage of reducing all three methods to rapid efficient graphical procedures. Each method is analyzed to consider the amount of labor involved to carry it out. Several examples of the methods are given for constructing both electronic wave functions and spin functions.

1. Introduction

It is well known that the Slater determinants provide the proper antisymmetry for electronic wave functions when expressed as a product of spin–orbitals. The rather small interaction between the spatial and spin parts of the wave function permits their separation into factors, and the overall antisymmetry constraint is met by requiring that the spatial and spin factors transform according to conjugate partners of conjugate partitions (or irreducible representations) of the symmetric group of the electrons. In this way the antisymmetric partition is ensured to be contained in the decomposition of the product [1]. It may be obtained by simply projecting it with the antisymmetric projector of the symmetric group.

Since each factor (space or spin) is associated with a conjugate partner of a conjugate irreducible representation, each may be associated with a Young tableau (YT). There exist a variety of methods to obtain these associations [2–5]. The traditional way is to apply the Young projector [6, 7],

$$N^{[\lambda]_r} = Q^{[\lambda]_r} P^{[\lambda]_r}, \tag{1a}$$

to the YT. Here $[\lambda]$ specifies the partition of the symmetric group and τ the partner or Yamanouchi symbol [8]. The column – antisymmetrizer $Q^{(\lambda]_\tau}$ includes all possible permutations (accompanied by their parity factors) within the columns of the Young tableau, viz.,

$$Q^{[\lambda]_\tau} = \sum_{q \in \text{column}} (-)^q \, q \tag{1b}$$

which the row-symmetrizer is a symmetric operator for the permutations within the rows of the YT, as its name implies. Explicitly,

$$P^{[\lambda]_\tau} = \sum_{p \in \text{row}} p. \tag{1c}$$

The application of the Young operators to the Young tableaux and the subsequent perfunctory antisymmetrization gives rise to the linear combinations of Slater determinants sought. For example, consider a Fermion system of identical particles and the two conjugate partners, $[\lambda]_\tau$ and $[\tilde{\lambda}]_{\tau'}$, and define the corresponding Young tableaux as

$$\boxed{\quad} = [\lambda]_\tau = \text{YT}(\Phi^{[\lambda]_\tau})$$

and

$$\boxed{\cdots kl \cdots} = [\tilde{\lambda}]_{\tau'} = \text{YT}(\Omega^{[\tilde{\lambda}]_{\tau'}}),$$

where the k in $[\lambda]_\tau$ refers to the orbital ϕ_k, while the k in $[\tilde{\lambda}]_{\tau'}$ refers to its associated spin function α_k. The conjugacy of the Young tableaux requires that the object in the rth row and sth column in $[\lambda]_\tau$ be changed to the sth row and rth column in $[\tilde{\lambda}]_{\tau'}$. Under this definition the sum of the Yamanouchi symbols of the Young tableaux should give $\tau + \tau' = d^{[\lambda]} + 1 = d^{[\tilde{\lambda}]} + 1$, where the d's denote the dimensions of the irreducible representations.

It is quite important to notice that each conjugate pair of Young tableaux corresponds uniquely to a single Slater determinant. The symmetry projections with the Young operators will generate a linear combination of Slater determinants.

The starting (primitive) functions, Φ^0 and Ω^0, of the spatial and spin parts are thus symmetry adapted to the conjugate partners of the conjugate partitions in this fashion, i.e., with the aid of the Young tableaux. Explicitly,

$$\Phi^{[\lambda]_\tau} = N^{[\lambda]_\tau} \Phi^0, \tag{2a}$$

$$\Omega^{[\tilde{\lambda}]_{\tau'}} = N^{[\tilde{\lambda}]_{\tau'}} \Omega^0. \tag{2b}$$

It should be noted that in the above example conjugation has been defined in the traditional diagrammatic manner. Recently, it has been found that it may be defined mathematically by the parity operator π [1]. In this way the two Young

operators are seen to be related by conjugation. As a consequence,

$$\mathbf{N}^{[\tilde{\lambda}]_{\tau'}} = \pi \mathbf{N}^{[\lambda]_{\tau}} \pi$$

$$= \pi \mathbf{Q}^{[\lambda]_{\tau}} \pi \pi \mathbf{P}^{[\lambda]_{\tau}} \pi$$

$$= \pi \left[\sum_{\mathbf{q} \in \text{column}} (-)^{q} \mathbf{q} \right] \pi \pi \left[\sum_{\mathbf{p} \in \text{row}} \mathbf{p} \right] \pi$$

$$= \left[\sum_{\mathbf{q} \in \text{fow}} (-)^{q} \pi q \pi \right] \left[\sum_{\mathbf{p} \in \text{column}} \pi \mathbf{p} \pi \right]$$

$$= \left[\sum_{\mathbf{q} \in \text{row}} q \right] \left[\sum_{\mathbf{p} \in \text{column}} (-)^{p} \mathbf{p} \right]$$

$$= \mathbf{P}^{[\tilde{\lambda}]_{\tau'}} \mathbf{Q}^{[\tilde{\lambda}]_{\tau'}}, \tag{2c}$$

where Eqs. (1) have been used. Notice that in the third line the "column" and "row" refer to those of $[\lambda]_{\tau}$, whereas in the following lines they have been interchanged in order to refer to $[\lambda]_{\tau'}$ and thereby remain consistent with the traditonal graphic definition of conjugation. Equations (2c) also show that the same permutations for the columns (rows) of $[\lambda]_{\tau}$ are used for the rows (columns) of $[\lambda]_{\tau'}$. This result may have been expected.

If we now exploit the fact that these two disjoint kinematic spaces, orbital space and spin space, must transform as conjugate partners of conjugate irreducible representations of S_N in order for the resulting linear combination of Slater determinants to satisfy the antisymmetry principle, we have

$$\psi^{[\lambda]_{\tau}} = \mathbf{A}^{[1^N]} \Omega^{[\tilde{\lambda}]_{\tau'}} \Phi^{[\lambda]_{\tau}}, \tag{3}$$

where $\mathbf{A}^{[1^N]}$ is the antisymmetrizer. We have affixed the spatial labels to the result because it is related to the point-group symmetry, which is always shown by the symmetry of the orbital part.

The conjugacy constraint, expressed as $[\lambda] \otimes [\tilde{\lambda}]$, is seen to be a second rank inner direct product. The Young operator method will be shown to be representable in the following equivalent forms:

$$\Psi_{\lambda}^{[\lambda]_{\tau}} = \mathbf{A}^{[1^N]} (\mathbf{N}^{[\tilde{\lambda}]_{\tau'}} \otimes \mathbf{N}^{[\lambda]_{\tau}}) (\Omega^0 \otimes \Phi^0) = \mathbf{A}^{[1^N]} (\mathbf{N}^{[\tilde{\lambda}]_{\tau'}} \Omega^0 \otimes \mathbf{N}^{[\lambda]_{\tau}} \Phi^0), \tag{4a}$$

$$\psi^{[\lambda]_{\tau}} = \mathbf{A}^{[1^N]} (\mathbf{N}^{[\tilde{\lambda}]_{\tau'}} \otimes \mathbf{E}) (\Omega^0 \otimes \Phi^0) = \mathbf{A}^{[1^N]} (\mathbf{N}^{[\tilde{\lambda}]_{\tau'}} \Omega^0 \otimes \Phi^0), \tag{4b}$$

$$\psi^{[\lambda]_{\tau}} = \mathbf{A}^{[1^N]} (\mathbf{E} \otimes \mathbf{N}^{[\lambda]_{\tau}}) (\Omega^0 \otimes \Phi^0) = \mathbf{A}^{[1^N]} (\Omega^0 \otimes \mathbf{N}^{[\lambda]_{\tau}} \Phi^0), \tag{4c}$$

where $\mathbf{E}$ is the identity operator. These expressions indicate that the procedures may be carried out upon the factored products, and the results may be subsequently antisymmetrized. The antisymmetrization does not have to be carried out in reality. One merely indicates each term in the resulting linear combination as a Slater determinant.

Since Young operators play a central role in constructing the basis functions of the different irreducible representations of the symmetric group S_N [8–14], and a drawback to their usefulness is that the number of permutations involved in them increases very rapidly with N, consequently, the Young operator method is a laborious procedure in the case of large N. Its simplification is essential if it is to be useful in such a situation.

2. New operator sets for fermion systems

The realization that each conjugate pair of Young tableaux corresponds to an independent Slater determinant in a one-to-one fashion means that the application of the Young operator to the YT gives rise to a linear combination of Slater determinants. This one-to-one correspondence, then, leads to a direct graphic method of producing the projected linear combinations of Slater determinants. This graphic approach is advantageous because it is both simple and rapid.

The most important feature in our method is that each independent picture (arrangement) of conjugate pair of Young tableaux corresponds to a single independent Slater determinant (one-to-one correspondence). In the resultant linear combination of Slater determinants the signs of the various terms are determined by the parity of the permutations which restore the determinant to its original order. In general, the results obtained in this way are not orthonormalized, but they may be made so by standard techniques, such as the Schmidt procedure of orthogonalization.

To achieve further understanding and simplifications we must consider the conjugate nature of the spin and space factors involved in the inner direct product. Write the primitive electronic wave function (it is the simple spin and space product of $[\lambda]_\tau$ and $[\tilde{\lambda}]_{\tau'}$) as

$$\boxed{ }\boxed{\cdots kl \cdots}\ \Big]\ \boxed{}\ \boxed{} = \cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots,$$

then consider the effect of a single permutation operator in freon space, say q_{kl} (see Eq. (1b)), on YT(Φ):

$$\boxed{}\boxed{\cdots kl \cdots}\ \Big]\ \Big((-)q_{kl}^{[\lambda]_\tau}\ \boxed{}\ \boxed{}\Big) = \cdots(-)\phi_l(\sigma_k)\phi_k(\sigma_l)\cdots. \qquad (5)$$

After antisymmetrization the right-hand side becomes

$$= |\cdots(-)\phi_l(\sigma_k)\phi_k(\sigma_l)\cdots|$$
$$= |\cdots \phi_k(\sigma_l)\phi_l(\sigma_k)\cdots|. \qquad (6)$$

If we take cognizance of the fact that $q_{kl}^{[\lambda]_\tau}$ is a column permutation operator and thus commutes with the antisymmetrizer, we may write this process as

$$(-)q_{kl}^{[\lambda]_\tau}|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots| = (-)|\cdots \phi_l(\sigma_k)\phi_k(\sigma_l)\cdots|$$
$$= |\cdots \phi_k(\sigma_l)\phi_l(\sigma_k)\cdots|. \qquad (7)$$

Similarly, a symmetric (row) operator in spin space, $p_{kl}^{[\tilde{\lambda}]_r}$ (see Eq. (1c)), acting on the spin function, represented by YT(Ω), will give

$$\left(p_{kl}^{[\tilde{\lambda}]_r}\ \boxed{\cdots kl \cdots}\ \right)\ \boxed{}\ \boxed{} \ = \ \cdots \phi_k(\sigma_l)\phi_l(\sigma_k)\cdots,$$

$$\Rightarrow |\cdots \phi_k(\sigma_l)\phi_l(\sigma_k)\cdots|. \tag{8}$$

after antisymmetrization. This process may be written as

$$p_{kl}^{[\tilde{\lambda}]_r}|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots| = |\cdots \phi_k(\sigma_l)\phi_l(\sigma_k)\cdots|. \tag{9}$$

Comparison of the Eqs. (6) and (8) (or the right-hand sides of Eqs. (7) and (9)) gives

$$p_{kl}^{[\tilde{\lambda}]_r}|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots| = (-)q_{kl}^{[\lambda]_r}|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots|. \tag{10a}$$

By similar reasoning it may be shown that

$$q_{kl}^{[\tilde{\lambda}]_r}|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots| = (-)p_{kl}^{[\lambda]_r}|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots|. \tag{10b}$$

Recalling the basic principle in the permutation group that an arbitrary permutation operator can always be represented as a product of transpositions, we will extend this result to more general cases. Performing the summation of Eqs. (1b) and (1c) in Eqs. (10) yields

$$\mathbf{P}^{[\tilde{\lambda}]_r}|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots| = \mathbf{Q}^{[\lambda]_r}|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots| \tag{11a}$$

and

$$\mathbf{P}^{[\lambda]_r}|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots| = \mathbf{Q}^{[\tilde{\lambda}]_r}|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots|. \tag{11b}$$

These results may be expressed in a more tractable form by using

$$|\cdots \phi_k(\sigma_k)\phi_l(\sigma_l)\cdots| = \mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0). \tag{12}$$

The final expressions are

$$(\mathbf{P}^{[\tilde{\lambda}]_r}\otimes \mathbf{E})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0) = (\mathbf{E}\otimes \mathbf{Q}^{[\lambda]_r})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0), \tag{13a}$$

$$(\mathbf{E}\otimes \mathbf{P}^{[\lambda]_r})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0) = (\mathbf{Q}^{[\tilde{\lambda}]_r}\otimes \mathbf{E})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0). \tag{13b}$$

We first make use of these equations to show that Eqs. (4b) and (4c) represent equivalent procedures which must lead to the same results.

$$(\mathbf{N}^{[\tilde{\lambda}]_r}\otimes \mathbf{E})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= (\mathbf{Q}^{[\tilde{\lambda}]_r}\mathbf{P}^{[\tilde{\lambda}]_r}\otimes \mathbf{E})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= (\mathbf{Q}^{[\tilde{\lambda}]_r}\otimes \mathbf{E})(\mathbf{P}^{[\tilde{\lambda}]_r}\otimes \mathbf{E})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= (\mathbf{Q}^{[\tilde{\lambda}]_r}\otimes \mathbf{E})(\mathbf{E}\otimes \mathbf{Q}^{[\lambda]_r})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= (\mathbf{E}\otimes \mathbf{Q}^{[\lambda]_r})(\mathbf{Q}^{[\tilde{\lambda}]_r}\otimes \mathbf{E})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= (\mathbf{E}\otimes \mathbf{Q}^{[\lambda]_r})(\mathbf{E}\otimes \mathbf{P}^{[\lambda]_r})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= (\mathbf{E}\otimes \mathbf{Q}^{[\lambda]_r}\mathbf{P}^{[\lambda]_r})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= (\mathbf{E}\otimes \mathbf{N}^{[\lambda]_r})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0). \tag{14}$$

The third line of this equation is a result of Eq. (13a). The fourth line is a consequence of the fact that the two prefactors with the Slater determinant commute, since they operate on different spaces. The fifth line results from Eq. (13b). Thus, Eqs. (4b) and (4c) are equivalent procedures. Of course, this means that the starting form represents the Young spin projector method, while the last result represents the Young orbital projector method. For obvious reasons they may both be called the Q–P method.

The importance of Eqs. (13) is that they allow us to develop even more equivalent methods, which may reduce the amount of labor required to generate the electronic wave functions. Let us consider

$$(\mathbf{E} \otimes \mathbf{N}^{[\lambda]_k})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= (\mathbf{E} \otimes \mathbf{Q}^{[\lambda]_k}\mathbf{P}^{[\lambda]_k})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= (\mathbf{E} \otimes \mathbf{Q}^{[\lambda]_k})\{(\mathbf{E} \otimes \mathbf{P}^{[\lambda]_k})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)\}$$

$$= (\mathbf{P}^{[\tilde\lambda]_{k'}} \otimes \mathbf{E})(\mathbf{E} \otimes \mathbf{P}^{[\lambda]_k})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= (\mathbf{P}^{[\tilde\lambda]_{k'}} \otimes \mathbf{P}^{[\lambda]_k})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= \mathbf{A}^{[1^N]}(\mathbf{P}^{[\tilde\lambda]_{k'}}\Omega^0 \otimes \mathbf{P}^{[\lambda]_k}\Phi^0) \tag{15}$$

To obtain the third line of Eq. (15) we made use of the fact that, since Eq. (13a) holds for a simple Slater determinant, it is also valid for a linear combination of Slater determinants, represented in the second line by the term in braces. We call this result the P–P method.

Equation (15) is derived from Eq. (4c). One may equally obtain the P–P method from Eq. (4b), i.e.,

$$(\mathbf{N}^{[\tilde\lambda]_{k'}} \otimes \mathbf{E})\mathbf{A}^{[1^N]}(\Omega^0 \otimes \Phi^0)$$

$$= \mathbf{A}^{[1^N]}(\mathbf{N}^{[\tilde\lambda]_{k'}}\Omega^0) \otimes \Phi^0$$

$$= \mathbf{A}^{[1^N]}(\mathbf{P}^{[\tilde\lambda]_{k'}}\Omega^0 \otimes \mathbf{P}^{[\lambda]_k}\Phi^0) \tag{16}$$

We will use a slightly different way to reach this result: beginning with $\Omega^0 = \alpha_1\alpha_2 \cdots \alpha_m\beta_{m+1} \cdots \beta_N$ and $\Phi^0 = a_1 b_2 c_3 \cdots f_N$, we have

$$\mathbf{N}^{[\tilde\lambda]_{k'}}\Omega^0\phi^0$$

$$= (\mathbf{Q}^{[\tilde\lambda]_{k'}}\mathbf{P}^{[\tilde\lambda]_{k'}}\Omega^0)\phi^0$$

$$= [(1 - q_{kl} + \cdots)(1 + p_{ij} + \cdots)\Omega^0]\phi^0$$

$$= [(1 - q_{kl} + \cdots + p_{ij} + \cdots - q_{kl}p_{ij} + \cdots)\Omega^0]\phi^0 \tag{17a}$$

and

$$\mathbf{A}^{[1^N]}(\mathbf{Q}^{[\tilde\lambda]_{k'}}\mathbf{P}^{[\tilde\lambda]_{k'}}\Omega^0)\phi^0$$

$$= |\Omega^0\phi^0| - |q_{kl}\Omega^0\phi^0| + \cdots + |p_{ij}\Omega^0\phi^0| + \cdots(-)|q_{kl}p_{ij}\Omega^0\phi^0| + \cdots. \tag{17b}$$

Comparing it to the P–P operator method (the Method D in the Table 1):

$$(\mathbf{P}^{[\tilde\lambda]_{k'}}\Omega^0)(\mathbf{P}^{[\lambda]_k}\phi^0)$$

$$= [(1 + p_{ij} + \cdots)\Omega^0][(1 + p_{kl} + \cdots)\Phi^0]$$

$$= [\Omega^0 + p_{ij}\Omega^0 + \cdots][\Phi^0 + p_{kl}\Phi^0 + \cdots]$$

$$= \Omega^0\phi^0 + p_{ij}\Omega^0\Phi^0 + \cdots + \Omega^0 p_{kl}\Omega^0 + \cdots + p_{ij}\Omega^0 p_{kl}\Phi^0 + \cdots$$

$$= \Omega^0\phi^0 + \Omega^0 p_{kl}\phi^0 + \cdots + p_{ij}\Omega^0\phi^0 + \cdots + p_{ij}\Omega^0 p_{kl}\phi^0 + \cdots, \tag{18a}$$

and, making use of the conjugate property of two Young operators for the spin and space parts (see Eq. (7) and the discussion following), we get

$$\mathbf{A}^{[1^N]}(\mathbf{P}^{[\tilde{\lambda}]_r}\Omega^0)(\mathbf{P}^{[\lambda]_r}\phi^0)$$

$$= |\Omega^0\phi^0| + |\Omega^0 p_{kl}\phi^0| + \cdots + |p_{ij}\Omega^0\phi^0| + \cdots + |p_{ij}\Omega^0 p_{kl}\phi^0| + \cdots$$

$$= |\Omega^0\phi^0| - |q_{kl}\Omega^0\phi^0| + \cdots + |p_{ij}\Omega^0\phi^0| + \cdots - |q_{kl}p_{ij}\Omega^0\phi^0| + \cdots. \quad (18b)$$

The results, i.e., (17b) and (18b), from two different operators are exactly the same in the form of the Slater-type functions.

All of the six equivalent methods are collected in Table 1.

Even though we have demonstrated that these six methods are equivalent, this does not mean that the amount of labor involved in each of them is the same. In fact, the work entailed in the $Q-P$ method is much greater than that of the others. These striking similarities and differences are graphically illustrated in Table 1. The blank areas indicate where no labor is involved. Horizontal (vertical) bars indicate those areas where row symmetrization (column antisymmetrization) is required, and the cross hatched areas show where both of these operations are to be performed.

Notice, from the expressions of the wave functions, that one does not actually have to perform the antisymmetrization. Instead it is only necessary to carry out the calculations indicated within the braces and simply designate the Slater determinants of the results by the conventional bar notation.

In the Young operator for the irreducible representation $[N-p, p]$ there are a total of $2^p p!(N-p)!$ distinct permutations, of which 2^p permutations are in the column antisymmetrizer $\mathbf{Q}^{[N-p, p]}$ and $p!(N-p)!$ are in the row symmetrizer $\mathbf{P}^{[N-p, p]}$. For the conjugate irreducible representation $[2^p, 1^{N-2p}]$, there are again a total of $2^p p!(N-p)!$ distinct permutations. However, in this case the column antisymmetrizer now contains $p!(N-p)!$ permutations, while the row symmetrizer contains 2^p. Thus, method A is the most laborious procedure. Methods B–D are less tedious and each require the same amount of labor. Methods E and F are the most efficient procedures because they do not require the total number of permutations defined in $\mathbf{Q}$ and $\mathbf{P}$. These truncated column and row operators are denoted by the primes.

3. Applications

An interesting point in our methods is that the independent pictures of Young tableaux are in one-to-one correspondence with the Slater determinants. By applying the Young operator we permute the index numbers 1, 2, ... ; by the independent pictures we exchange the objects $a, b, \ldots$. Clearly, the permutations of the objects $a, b, \ldots$ and the index numbers 1, 2, ... are isomorphic. In other words, it does not matter how many operators are used in the different methods; the final results just show as many as possible different (independent) rearrangements in the Young tableaux. In a detailed problem, we may proceed either by using the Young operators (from Methods C to F, see Example 2) or just by the different pictures (see Examples 1 and 3 below).

Example 1. The construction of basis functions

Let us deal with a six-electron system with $S = 1$ and $M_S = 0$. The YD's for spin and spatial are [42] and $[2^2 1^2]$, respectively. From the traditional Young operator

Table 1. The six equivalent methods[a] for the construction of electronic wave functions by the young operator $N^{[\lambda]}$.

Method	Wave function	Young tableau

A(double Q–P) (Number of operators required = $[2^p p!(N-p)!]^b$:

$$\mathbf{A}^{[1^N]}\{(\mathbf{N}^{[\bar\lambda]}\Omega^0) \otimes (\mathbf{N}^{[\lambda]}\Phi^0)\} \equiv$$

B(spin Q–P) (Number of operators required = $2^p p!(N-p)!)^b$:

$$\mathbf{A}^{[1^N]}\{(\mathbf{Q}^{[\bar\lambda]}\mathbf{P}^{[\bar\lambda]}\Omega^0) \otimes \Phi^0) \equiv$$

C(space Q–P) (Number of operators required = $2^p p!(N-p)!)^b$:

$$\mathbf{A}^{[1^N]}\{\Omega^0 \otimes (\mathbf{Q}^{[\lambda]}\mathbf{P}^{[\lambda]}\Phi^0)\} \equiv$$

D(double P–P) (Number of operators required = $2^p p!(N-p)!)^b$:

$$\mathbf{A}^{[1^N]}\{((\mathbf{P}^{[\bar\lambda]}\Omega^0) \otimes (\mathbf{P}^{[\lambda]}\Phi^0)\} \equiv$$

E(Q'–Q') (Number of operators required = $2^p(N-p)!^b$:

$$\mathbf{A}^{[1^N]}\{(\mathbf{Q}'^{[\bar\lambda]}\Omega^0) \otimes (\mathbf{Q}'^{[\lambda]}\Phi^0)\} \equiv$$

Table 1. (Continued)

Method	Wave function	Young tableau

$F(P'-P')$ (Number of operators required $= 2^p(N-p)!)^b$:

$$A^{[1^N]}\{(\mathbf{P}'^{[\bar{\lambda}]},\Omega^0) \otimes (\mathbf{P}'^{[\lambda]},\Phi^0)\} \equiv$$

^{a} A)–D) apply to all Fermion systems; E) and F) apply to electronic systems (or nuclear systems with $I = 1/2$) only.
^{b} The formulas apply for spin-$\frac{1}{2}$ particles only. Here N stands for the total number of boxes in the Young tableau and p stands for the number of boxes in the second row of the Young tableau which are placed on the left.

method, a tableau belonging to the partition $[2^2 1^2]$ requires $2! * 4! = 48$ operators from the column-antisymmetrizer and $2! * 2! = 4$ from the row-symmetrizer. In all there are as many as $48 * 4 = 192$ operations. But, based on our proposed Method F, there are only two independent pictures for the spin part (here the dashed lines were used for the independent pictures of the Young tableaux)

$$\boxed{\begin{array}{|c|c|c|c|}\hline \alpha & \alpha & \alpha & \beta \\\hline \beta & \beta \\\cline{1-2}\end{array}} \rightarrow \begin{vmatrix} \alpha\alpha\alpha\beta \\ \beta\beta \end{vmatrix}; \quad \begin{vmatrix} \alpha\alpha\beta\alpha \\ \beta\beta \end{vmatrix} \tag{19}$$

$$\text{(A)} \qquad \text{(B)}$$

and four independent pictures for the orbital part of symmetry $[2^2 1^2]$:

$$\begin{array}{|c|c|}\hline a & b \\\hline c & d \\\hline e \\\cline{1-1} f \\\cline{1-1}\end{array} \rightarrow \begin{vmatrix} ab \\ cd \\ e \\ f \end{vmatrix} \begin{vmatrix} ba \\ cd \\ e \\ f \end{vmatrix} \begin{vmatrix} ab \\ dc \\ e \\ f \end{vmatrix} \begin{vmatrix} ba \\ dc \\ e \\ f \end{vmatrix} \tag{20}$$

$$\text{(a)} \quad \text{(b)} \quad \text{(c)} \quad \text{(d)}$$

Then the result is given in a very direct way using only the six pictures and the eight Slater determinants from their combinations. (A)–(a) gives rise to the determinant $|ace\bar{f}\bar{b}\bar{d}|$. (A)–(b) gives rise to the determinant $|bce\bar{f}\bar{a}\bar{d}|$ and finally, (B)–(d) gives rise to the determinant $|bd\bar{e}\bar{f}\bar{a}\bar{c}|$. The linear combination is

$$\psi_{10}^{[2^2 1^2]} = |ace\bar{f}\bar{b}\bar{d}| + |bce\bar{f}\bar{a}\bar{d}| + |ade\bar{f}\bar{b}\bar{c}| + |bde\bar{f}\bar{a}\bar{c}| + |ac\bar{e}\bar{f}\bar{b}\bar{d}|$$

$$+ |bc\bar{e}\bar{f}\bar{a}\bar{d}| + |ad\bar{e}\bar{f}\bar{b}\bar{c}| + |bd\bar{e}\bar{f}\bar{a}\bar{c}|$$

$$= -|a\bar{b}cde\bar{f}| + |\bar{a}bcde\bar{f}| - |a\bar{b}cd\bar{e}f| + |\bar{a}bcd\bar{e}f|$$

$$+ |\bar{a}bcd\bar{e}\bar{f}| - |a\bar{b}cd\bar{e}f| + |\bar{a}bcd\bar{e}\bar{f}|. \tag{21}$$

This is comparable with the interaction of the sp^2 hybrid of carbon (d_1, d_2, d_3) with three hydrogen in the case of CH_3, e.g., determinant $|d_1 \bar{H}_1 d_2 \bar{H}_2 d_3 \bar{H}_3|$ has $2^3 = 8$ terms.

It is necessary to emphasize that these new methods place no restriction on the orbitals. They can be used in both valence bond (VB) theory and molecular orbital (MO) theory. The case depends only on the choice of the orbitals. They may be either atomic or molecular orbitals. They can also be all different $(a, b, \ldots f$ stand for different orbitals) or partly the same (say $b = a$ or $d = c$, etc.). This allows us to make all kinds of basis functions for either a localized or a delocalized treatment.

Example 2. The comparison of different methods

For the construction of one component of the basis functions belonging to the partition $[2^2]$ in a four-electron system with $S = 0$ (the second component for this partition may be found by the same method by changing the order in both Young tableaux). Taking the first component as

$$\left| \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & 4 \\ \hline \end{array} \quad \begin{array}{|c|c|} \hline \alpha & \alpha \\ \hline \beta & \beta \\ \hline \end{array} \right\rangle * \left| \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 & 4 \\ \hline \end{array} \quad \begin{array}{|c|c|} \hline a & c \\ \hline b & d \\ \hline \end{array} \right\rangle, \tag{22}$$

while using the following operators for the spin part (see Eqs. (1))

$$\mathbf{N}^{[2^2]_1} = [E - (13) - (24) + (13)(24)][E + (12) + (34) + (12)(34)],$$

$$\mathbf{Q}^{[2^2]_1} = E - (13) - (24) + (13)(24),$$

$$\mathbf{P}^{[2^2]_1} = E + (12) + (34) + (12)(34) \tag{23}$$

and the following operators for the space part

$$\mathbf{N}^{[2^2]_2} = [E - (12) - (34) + (12)(34)][E + (13) + (24) + (13)(24)]$$

$$\mathbf{Q}^{[2^2]_2} = E - (12) - (34) + (12)(34) \tag{24}$$

$$\mathbf{P}^{[2^2]_2} = E + (13) + (24) + (13)(24)$$

then taking $\alpha_1 \alpha_2 \beta_3 \beta_4$ and $a_1 b_2 c_3 d_4$ as the primitive functions, we have the same results shown below for all of the different methods.

Method A (double Q–P):

$$\psi = \{[E - (13) - (24) + (13)(24)][E + (12) + (34) + (12)(34)]\alpha_1 \alpha_2 \beta_3 \beta_4\}$$

$$\times \{[E - (12) - (34) + (12)(34)][E + (13) + (24) + (13)(24)]a_1 b_2 c_3 d_4\}$$

$$= \{[E + (12) + (34) + (12)(34) - (13) - (123) - (134) - (1234) - (24) - (142)$$

$$- (324) - (1432) + (13)(24) + (1423) + (13)(24) + (14)(32)]\alpha_1 \alpha_2 \beta_3 \beta_4\}$$

$$\times \{[E + (13) + (24) + (13)(24) - (12) - (132) - (124) - (1324) - (34) - (143)$$

$$- (234) - (1423) + (12)(34) + (1432) + (1234) + (14)(23)]a_1 b_2 c_3 d_4\}$$

$$= 4(\alpha\alpha\beta\beta - \beta\alpha\alpha\beta - \alpha\beta\beta\alpha + \beta\beta\alpha\alpha)$$

$$\times (abcd + cbad + adcb + cdab - bacd - bcad - dacb - cdba - abdc - cbda$$

$$- adbc - cdba + badc + bcda + dabc + dcba)$$

$$= 4[(ab\overline{cd} + cb\overline{ad} + ad\overline{cb} + cd\overline{ab} - ba\overline{cd} - bc\overline{ad} - da\overline{cb} - ab\overline{dc} - cb\overline{da}$$

$$- da\overline{bc} - ad\overline{bc} - cd\overline{ba} + ba\overline{cd} + bc\overline{da} + da\overline{bc} + dc\overline{ba}) + (\overline{abcd} + \overline{cbad} + \overline{adcb}$$

$$+ \overline{cdab} - \overline{bacd} - \overline{bcad} - \overline{dacb} - \overline{dabc} - \overline{abdc} - \overline{cbda} - \overline{adbc} - \overline{cdba} + \overline{badc}$$

$$+ \overline{bcda} + \overline{dabc} + \overline{dcba}) - (\overline{a}bc\overline{d} + \overline{c}ba\overline{d} + \overline{a}dc\overline{b} + \overline{c}da\overline{b} - \overline{b}ac\overline{d} - \overline{b}ca\overline{d} - \overline{d}ac\overline{b}$$

$$- \overline{d}ab\overline{c} - \overline{a}bd\overline{c} - \overline{c}bd\overline{a} - \overline{a}db\overline{c} - \overline{c}db\overline{a} + \overline{b}ad\overline{c} + \overline{b}cd\overline{a} + \overline{d}ab\overline{c} + \overline{d}cb\overline{a})$$

$$- (a\overline{bc}d + c\overline{ba}d + a\overline{dc}b + c\overline{da}b - b\overline{ac}d - b\overline{ca}d - d\overline{ac}b - d\overline{ab}c - a\overline{bd}c - c\overline{bd}a$$

$$- a\overline{db}c - c\overline{db}a + b\overline{ad}c + b\overline{cd}a + d\overline{ab}c + d\overline{cb}a)]$$

$$\mathbf{A}^{[1^N]}\psi = 16(|ab\overline{cd}| - |\overline{a}bc\overline{d}| - |a\overline{bc}d| + |\overline{abcd}|). \tag{I}$$

Method B (spin Q–P):

$$\psi = \{[E - (13) - (24) + (13)(24)][E + (12) + (34) + (12)(34)]\alpha_1\alpha_2\beta_3\beta_4\}$$

$$\times \{a_1 b_2 c_3 d_4\} = 4(\alpha\alpha\beta\beta - \beta\alpha\alpha\beta - \alpha\beta\beta\alpha + \beta\beta\alpha\alpha) \times abcd$$

$$\mathbf{A}^{[1^N]}\psi = 4(|ab\overline{cd}| - |\overline{a}bc\overline{d}| - |a\overline{bc}d| + |\overline{abcd}|. \tag{II}$$

Method C (orbital Q–P):

$$\Psi = \{\alpha_1\alpha_2\beta_3\beta_4\}\{[E - (12) - (34) + (12)(34)][E + (13) + (24) + (13)(24)]a_1 b_2 c_3 d_4\}$$

$$= \{\alpha_1\alpha_2\beta_3\beta_4\} \times \{[E + (13) + (24) + (13)(24) - (12) - (132) - (124) - (1324)$$

$$- (34) - (143) - (234) - (1423) + (12)(34) + (1432) + (1234) + (14)(23)]$$

$$\times a_1 b_2 c_3 d_4\} = \alpha\alpha\beta\beta \times (abcd + cbad + adcb + cdab - bacd - bcad - dacb$$

$$- cdba - abdc - cbda - adbc - cdba + badc + bcda + dabc + dcba)$$

$$A^{[1^N]}\Psi = |ab\overline{cd}| + |cb\overline{ad}| + |ad\overline{cb}| + |cd\overline{ab}| - |ba\overline{cd}| - |bc\overline{ad}| - |da\overline{cb}| - |cd\overline{ba}|$$

$$- |ab\overline{dc}| - |cb\overline{da}| - |ad\overline{bc}| - |cd\overline{ba}| + |ba\overline{dc}| + |bc\overline{da}| + |da\overline{bc}|$$

$$+ |dc\overline{ba}|) = 4(|ab\overline{cd}| - |\overline{a}bc\overline{d}| - |a\overline{bc}d| + |\overline{abcd}|). \tag{III}$$

Method D (double P–P):

$$\Psi = \{[E + (12) + (34) + (12)(34)]\alpha_1\alpha_2\beta_3\beta_4\}\{[E + (13) + (24)$$

$$+ (13)(24)]a_1 b_2 c_3 d_4\} = (\alpha\alpha\beta\beta + \alpha\alpha\beta\beta + \alpha\alpha\beta\beta + \alpha\alpha\beta\beta)$$

$$\times (abcd + cbad + adcb + cdab) = 4(ab\overline{cd} + cb\overline{ad} + ad\overline{cb} + cd\overline{ab})$$

$$\mathbf{A}^{[1^N]}\Psi = 4(|ab\overline{cd}| + |cb\overline{ad}| + |ad\overline{cb}| + |cd\overline{ab}|)$$

$$= 4(|ab\overline{cd}| - |\overline{a}bc\overline{d}| - |a\overline{bc}d| + |\overline{abcd}|). \tag{IV}$$

Method E (double Q–Q):

$$\Psi = \{[E - (13) - (24) + (13)(24)]\alpha_1\alpha_2\beta_3\beta_4\}a_1b_2c_3d_4\}$$

$$= (\alpha\alpha\beta\beta - \beta\alpha\alpha\beta - \alpha\beta\beta\alpha + \beta\beta\alpha\alpha) \times abcd$$

$$= 4(ab\overline{cd} - \overline{a}bc\overline{d} - a\overline{bc}d + \overline{ab}cd)$$

$$A^{[1^N]}\Psi = 4(|ab\overline{cd}| - |\overline{a}bc\overline{d}| - |a\overline{bc}d| + |\overline{ab}cd|). \tag{V}$$

Method F (P'–P'):

$$\Psi = \{\alpha_1\alpha_2\beta_3\beta_4\}\{[E + (13) + (24) + (13)(24)]a_1b_2c_3d_4\}$$

$$= (\alpha\alpha\beta\beta) \times (abcd + cbad + adcb + cdab)$$

$$= ab\overline{cd} + cb\overline{ad} + ad\overline{cb} + cd\overline{ab}$$

$$A^{[1^N]}\Psi = |ab\overline{cd}| + |cb\overline{ad}| + |ad\overline{cb}| + |cd\overline{ab}|$$

$$= |ab\overline{cd}| - |\overline{a}bc\overline{d}| - |a\overline{bc}d| + |\overline{ab}cd|. \tag{VI}$$

Example 3. Spin functions

Using the above methods to construct spin functions is even simpler. To make this process easily understandable, let us begin with the Young tableau of the spin part. Due to the electron spin one-half quantum number, these tableaux have only one or two rows. They are of the form

A	B
C	

$$\equiv \begin{array}{|cccc|ccccc|} \hline \alpha_1 & \alpha_2 & \cdots & \alpha_m & \alpha_{m+1} & \cdots & \alpha_k\beta_{k+1} & \cdots & \beta_{N-2m} \\ \hline \beta_{N-2m+1}\beta_{N-2m+2} & \cdots & \beta_N & & & & & & \\ \hline \end{array}$$

where the areas A and C are occupied by different spin functions (one for spin up and one for spin down) while the objects in part B can be purely α or β or their mixture.

According to the general Young operator method, it is necessary to apply the operator which includes all of the permutations, such as

$$Y = Q_{A+C}(P_{A+B}P_C), \tag{24}$$

where Q_{A+C} is the column-antisymmetrizer for the part A + C, while P_{A+B} and P_C are the row-symmetrizers for the parts A + B and C, respectively, and they commute: $P_{A+B}P_C = P_C P_{A+B}$. But, since the basic idea in this work is that the items appearing in the basis function are correct for the independent pictures in the Young tableau, it is only necessary to find these independent pictures by our equivalent methods.

From the discussion in the second section, it is easy to find the correct formula for both spin function and its related spin–orbital function by the following formulas:

$$\text{spin–orbital} \iff \varphi_i = A^{[1^N]}(\Omega^0 N^{[\lambda]_r}\Phi^0)$$

$$= A^{[1^N]}(N^{[\lambda]_r}\Omega^0\Phi^0)$$

$$= A^{[1^N]}(N^{[\tilde{\lambda}]_r}\Psi^0); \tag{25}$$

$$\text{spin} \iff \theta_i = A^{[1^N]}(N^{[\tilde{\lambda}]_r}\Omega^0), \tag{26}$$

where $\Psi^0 \equiv \Omega^0 \Phi^0$. This one-to-one correlation for spin function (θ_i) and electronic wave function (φ_i) shows that once we have the basis functions for a partition $[\lambda]$, then we have the spin functions for the conjugate partition $[\tilde{\lambda}]$ because the operators in both Eqs. (25) and (26) are the same. Since the new methods are quite simple for the construction of electronic basis functions, so are the spin functions. The following is an example for a four-electron system with $M_s = S = 0$ by the Method D.

Let $\begin{array}{|c|c|}\hline \alpha & \alpha \\\hline \beta & \beta \\\hline\end{array}$ and $\begin{array}{|c|c|}\hline a & b \\\hline c & d \\\hline\end{array}$ stand for spin and space, respectively, and consider

the independent pictures of the YT of space part (there is only one picture for such spin when using the Method D; although all the methods are equivalent, the proper choice of methods will give the result most directly):

$$\begin{array}{|c|c|}\hline a & b \\\hline c & d \\\hline\end{array} \rightarrow \begin{vmatrix} a & b \\ c & d \end{vmatrix}; \begin{vmatrix} b & a \\ c & d \end{vmatrix}; \begin{vmatrix} a & b \\ d & c \end{vmatrix}; \begin{vmatrix} b & a \\ d & c \end{vmatrix} \qquad (27)$$

we have the following determinants directly from the four independent pictures

$$\varphi_\xi = |a\bar{b}cd| + |b\bar{a}cd| + |a\bar{b}d\bar{c}| + |b\bar{a}d\bar{c}|$$

$$= |a\bar{b}cd| - |\bar{a}bcd| - |a\bar{b}\bar{c}d| + |\bar{a}b\bar{c}d| \qquad (28)$$

and the corresponding form for spin:

$$\theta_\xi = \alpha\beta\alpha\beta - \beta\alpha\alpha\beta - \alpha\beta\beta\alpha + \beta\alpha\beta\alpha. \qquad (29)$$

Similarly, another basis function is

$$\varphi_\zeta = |ab\bar{c}d| + |cb\bar{a}d| + |ad\bar{c}b| + |cd\bar{a}b|$$

$$= |ab\bar{c}d| - |\bar{a}bcd| - |a\bar{b}\bar{c}d| + |\bar{a}\bar{b}cd|, \qquad (30)$$

its spin function is

$$\theta_\zeta = \alpha\alpha\beta\beta - \beta\alpha\alpha\beta - \alpha\beta\beta\alpha + \beta\beta\alpha\alpha. \qquad (31)$$

In all these procedures, the θ_ξ and θ_ζ are just simply "copied" from φ_ξ and φ_ζ, respectively.

In contrast to some other operators, the basis functions obtained from Young operators are not orthogonal, but they may be made so either by standard techniques (such as the Schmidt procedure of orthogonalization) or in terms of the connection between the Young operator and others (e.g., its connection to the Wigner projection operator [8, 12, 13]). For example, the singlet spin eigenfunctions are

$$\Omega_\xi = \alpha\beta\alpha\beta - \beta\alpha\alpha\beta - \alpha\beta\beta\alpha + \beta\alpha\beta\alpha = \theta_\xi,$$

$$\Omega_\zeta = 2\alpha\alpha\beta\beta + 2\beta\beta\alpha\alpha - \alpha\beta\alpha\beta - \beta\alpha\alpha\beta - \alpha\beta\beta\alpha - \beta\alpha\beta\alpha = 2\theta_\zeta - \theta_\xi. \quad (32)$$

4. Discussion

For any Fermion system the conjugate property of two quantities (say, electronic spin and orbital, nuclear spin and motion, etc) ensures that their total wave function satisfies the antisymmetrization principle: $[\lambda] \otimes [\tilde{\lambda}] = [1^N] \oplus \cdots$. This conjugacy produces the conjugate of the Young operators $N^{[\lambda]_k}$ and $N^{[\tilde{\lambda}]_k}$ (see the discussion above) and then, the antisymmetrizer projects out the required antisymmetric property for the total function. So, from the point of view of the Young operator, there are always a few equivalent operator sets which allow us to reach the same antisymmetric wave function for any Fermion system. Say for two conjugate quantities A and B, there are either

$$\Psi^{[\mu]} = A^{[1^N]}[(N^{[\mu]}\varphi_A^0) \otimes (N^{[\tilde{\mu}]}\varphi_B^0)]$$

or

$$\Psi^{[\mu]_\xi} = A^{[1^N]}[(N^{[\mu]_k}\varphi_A^0) \otimes \varphi_B^0] \ (B\text{-}free), \tag{33a}$$

$$\Psi^{[\mu]_k} = A^{[1^N]}[\varphi_A^0 \otimes (N^{[\tilde{\mu}]_{k'}}\varphi_B^0)] \ (A\text{-}free). \tag{33b}$$

Eqs. (33) give some insight into the rationale behind spin-free chemistry [15, 16] in a general sense.

It is necessary to emphasize that the permutations contained in the so-called equivalent operators are not the same. Take operators $N^{[\lambda]_k}$ and $N^{[\tilde{\lambda}]_k}$ as an example: their permutations are different in both permutation order and sign. If (123) occurs in the first operator $N^{[\lambda]_k}$, (132) will occur in the $N^{[\tilde{\lambda}]_k}$; if (1234) occurs in the first and $(-)(1432)$ will occur in the second, etc. Let n_i, p_i and q_i be any operator in the $N^{[\lambda]_k}$, $p^{[\lambda]_k}$ and $q^{[\lambda]_k}$, respectively, the forms for the related three "operator pairs" are:

$$\text{I.} \quad P^{[\lambda]_k} = \{p_i\} \quad Q^{[\tilde{\lambda}]_{k'}} = \{(-)^{p_i}p_i^{-1}\};$$

$$\text{II.} \quad Q^{[\lambda]_k} = \{q_i\} \quad P^{[\tilde{\lambda}]_{k'}} = \{(-)^{q_i}q_i^{-1}\};$$

$$\text{III.} \quad N^{[\lambda]_k} = \{n_i\} \quad Q^{[\tilde{\lambda}]_{k'}} = \{(-)^{n_i}n_i^{-1}\}. \tag{34}$$

Fortunately, all these differences will disappear under the action of the total antisymmetrizer and give the same final results. It is noteworthy to point out that the commutation of these Fermion operators with the antisymmetrizer is really what makes possible a spin-free quantum chemical approach to many-Fermion systems. The details of this statement will be discussed elsewhere.

We have seen in the Eq. (2c) that parity conjugation produces another representation of the Young operator which switches the order of P and Q, viz.,

$$N^{[\tilde{\lambda}]_{k'}} = P^{[\tilde{\lambda}]_{k'}}Q^{[\tilde{\lambda}]_{k'}}.$$

These operators may also be obtained by the nonequivalent operation of Hermitian congugation, i.e.,

$$Y^{[\lambda]_k} = P^{[\lambda]_k}Q^{[\lambda]_k} = N^{[\lambda]_k^+} \tag{35}$$

since $P^{[\lambda]_k}$ and $Q^{[\lambda]_k}$ are Hermitian. Comparing its action on the spin part (it will be the same if applied to the spatial part)

$$Y^{[\lambda]_{k'}}\Omega^0\Phi^0$$

$$= (P^{[\tilde{\lambda}]_{k'}}Q^{[\tilde{\lambda}]_{k'}}\Omega^0)\Phi^0$$

$$= [(1 + p_{ij} + \cdots)(1 - q_{kl} + \cdots)\Omega^0]\Phi^0$$

$$= [(1 - q_{kl} + \cdots + p_{ij} + \cdots - p_{ij}q_{kl} + \cdots)\Omega^0]\Phi^0 \tag{36}$$

with that of the operator in the double Q method:

$$(\mathbf{Q}^{[\bar{\lambda}]_\kappa}\Omega^0)(\mathbf{Q}^{[\lambda]_\kappa}\Phi^0)$$

$$= (1 - q_{kl} + \cdots)\Omega^0(1 - q_{ij} + \cdots)\Phi^0$$

$$= \Omega^0\Phi^0 - q_{kl}\Omega^0\Phi^0 + \cdots + \Omega^0(-)q_{ij}\Phi^0 + \cdots - q_{kl}\Omega^0(-)q_{ij}\Phi^0 + \cdots,$$

$$(37)$$

it is easy to show that these two equations give rise to the exact same function when they are subsequently submitted to the total antisymmetrizer:

$$\mathbf{A}^{[1^N]}(\mathbf{Y}^{[\bar{\lambda}]_\kappa}\Omega^0)\Phi^0 = \mathbf{A}^{[1^N]}\Omega^0(\mathbf{Y}^{[\lambda]_\kappa}\Phi^0)$$

$$= \mathbf{A}^{[1^N]}(\mathbf{Q}^{[\bar{\lambda}]_\kappa}\Omega^0)\mathbf{Q}^{[\lambda]_\kappa}\Phi^0$$

$$= |\Omega^0\Phi^0| - |q_{kl}\Omega^0\Phi^0| + \cdots + |p_{ij}\Omega^0\Phi^0| + \cdots - |p_{ij}q_{kl}\Omega^0\Phi^0| + \cdots.$$

$$(38)$$

The equivalent methods for this alternative definition of the Young operator are shown in Table 2.

The main thrust of this work has been to use Young operators in order to determine and analyze efficient algorithms to obtain spin states from a given set of spin orbitals. All methods shown here lead to essentially the same linear combination of Slater determinants. Though the result of each method may have a different proportionality constant, the normalized result is unique and equal to that given by standard methods (within a phase factor), such as diagonalization or projection, i.e.,

$$\Psi_i^{[\lambda]_\kappa} = \mathbf{N}_i^{[\lambda]_\kappa} \sum_k \mathbf{C}_{ki}^{[\lambda]_\kappa}\mathbf{D}_k, \tag{39}$$
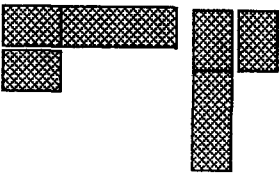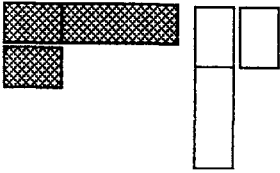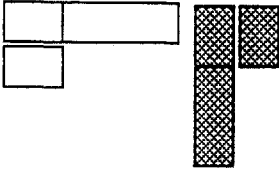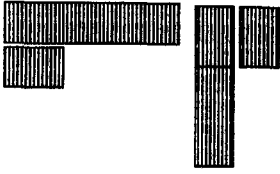
where $\mathbf{N}_i^{[\lambda]_\kappa}$ is a normalization constant, $\mathbf{C}_{ki}^{[\lambda]_\kappa}$ a scalar coefficient and $\mathbf{D}_k$ a Slater determinant of the spin-orbitals used. The matrix element of some operator H of interest in this basis of spin states, viz., $\langle\psi_i^{[\lambda]_\kappa}|H|\psi_j^{[\mu]_\kappa}\rangle$, are easily determined by using the expansion of Eq. (39) and subsequently applying the Slater rules for matrix elements in a determinantal basis, a well-known technique presented in many textbooks (cf. [17]).

Since the Young operator, $\mathbf{N}^{[\lambda]_\kappa}$ or $\mathbf{Y}^{[\lambda]_\kappa}$, is essentially a projection operator, it is proper to compare these methods with standard projection operator techniques. Matsen's matric projector for S_N [1, 8, 18] requires the use of all $N!$ permutations of the symmetric group S_N, a much more laborious procedure than any of the approaches presented here. Salmon gave another algorithm for constructing matrix units [19]. Like Matsen's method, it is based on the chain of subgroups $S_1 \subset S_2 \subset \cdots \subset S_N$. For each Young tableau of S_N one can define a chain of tableaux (and hence a chain of Young operators) determined by successively omitting the numbers $N, N-1, N-2, \ldots$ etc. For the subgroup S_j, there will be $2^{p_j}p_j!(j-p_j)!$ permutations in the Young operator $\mathbf{N}_j^{[\lambda]_\kappa}$ and the projection operator has the recursive form,

$$\mathbf{e}^{[\lambda]_\kappa} = \prod_j (\mathbf{N}_j^{[\lambda]_\kappa}\mathbf{e}_{j+1}^{[\lambda]_\kappa})(\mathbf{N}_j^{[\lambda]_\kappa}\mathbf{e}_{j+1}^{[\lambda]_\kappa})/k_j^{[\lambda]_\kappa}, \tag{40}$$

where $k_j^{[\lambda]_\kappa}$ is a constant. Thus, it is seen that this product form contains many more permutations than those of either method presented here, for just the Young

Table 2. The four equivalent methods based on the young operator $\mathbf{Y}^{[\lambda]_r}$

Method	Basis function	Young tableau

G(double P–Q):

$$\mathbf{A}^{[1^N]}\left[(\mathbf{Y}^{[\bar{\lambda}]_r}\Omega^0)(\mathbf{Y}^{[\lambda]_r}\Phi^0)\right] \equiv$$

H(spin P–Q):

$$\mathbf{A}^{[1^N]}\left\{(\mathbf{P}^{[\bar{\lambda}]_r}\mathbf{Q}^{[\bar{\lambda}]_r}\Omega^0)\otimes\Phi^0\right\} \equiv$$

I(orbital P–Q):

$$\mathbf{A}^{[1^N]}\left\{\Omega^0\otimes(\mathbf{P}^{[\lambda]_r}\mathbf{Q}^{[\lambda]_r}\Phi^0)\right\} \equiv$$

J(double Q–Q):

$$\mathbf{A}^{[1^N]}\left\{(\mathbf{Q}^{[\bar{\lambda}]_r}\Omega^0)\otimes(\mathbf{Q}^{[\lambda]_r}\Phi^0)\right\} \equiv$$

operators alone appearing in the factor for the Young tableau of S_N are required for our most laborious approach, method A.

In more recent years Poshusta and Kinghorn [11] have employed the elimination theorem of algebrants to reduce the number of permutations in the Young operator to $[(p+1)!]^2(p+1)^{N-2p-1}$ and applied it to a set of atomic orbitals to obtain a valence-bond wave function. Their algorithm is based upon a spin-free formalism, whereas our methods are based upon Slater determinants, thereby requiring permutations to be carried out on both the spin and spatial parts. Nevertheless, it is still possible to make some comparison between their approach and our most efficient procedures (methods E and F of Table 1). Recalling that $2^p(N-p)!$ permutations are required to carry out methods E and F, we see that, for low values of p, the factorial predominates and thus the algebrant approach is more efficient than E and F. However, for

$$p \geqslant [(N-p)/2], \tag{41}$$

where the braces indicate the next lowest integer for an odd value of $N-p$, methods E and F require fewer permutations than those of the spin-free algebrant approach. This difference becomes more pronounced as N increases.

The blank areas indicate where no labor is involved. The vertical bars indicate those areas where column-antisymmetrization is required, and the pointed areas show where both of these operations are to be performed.

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