Introduction to the Unitary Group Approach

*Isaiah Shavitt*

Department of Chemistry
University of Illinois at Urbana–Champaign
This tutorial introduces the concepts and results underlying the unitary group approach to electronic structure calculations and its graphical representation.

These results are given without proofs. Detailed derivations can be found in:


and references therein.
Other references:


Spin is a symmetry property

Simple example: two-electron system

Antisymmetric spin function \((\alpha\beta - \beta\alpha)\) forces a symmetric spatial function \((a^2\text{ or } ab + ba)\) \(\rightarrow\) singlet states.

Symmetric spin functions \((\alpha\alpha, \alpha\beta + \beta\alpha, \beta\beta)\) force antisymmetric spatial function \((ab - ba)\) \(\rightarrow\) triplet states.

In many-electron cases the relationship is more complicated, and can be treated by the symmetric group.
The Symmetric Group

The symmetric group $S_N$ is the group of all permutations of $N$ objects.

Its irreps are identified by Young shapes (also called Young frames) with $N$ boxes, with the number of boxes in each row non-increasing downwards:
The individual **components** of each irrep are specified by populating the boxes with distinct **tokens**, representing the objects being permuted (e.g., orbitals, electrons, etc.). For the symmetric group these tokens usually are the numbers 1–$N$:

```
1  2  4  7  11
3  5  6
8 10 12
9 13
```

This is called a **Young tableau**.
A *standard* Young tableau is one in which the numbers increase from left to right in each row and from top to bottom in each column.

The set of all the distinct standard Young tableaux for a given Young shape describe all the components of the irrep represented by that Young shape. (The order requirement is needed to avoid duplication of equivalent tableaux.)
The tableau represents a linear combination of permutation operators over the tokens.

This linear combination operates on a function that depends on the tokens (e.g., orbital indices).
Two types of operators are of particular importance:

1. The row symmetrizer $S_i$, which is the sum of all permutations of the tokens in the $i$th row,

2. The column antisymmetrizer $A_i$, which is the sum of all even permutations of the tokens in the $i$th column, minus the sum of all their odd permutations.
Glossing over some important, but complicated details, the tableau essentially represents a product of row symmetrizers times column antisymmetrizers,

$$\prod_i S_i \prod_j A_j,$$

where the product over $i$ is over the rows of the tableau, and the product over $j$ is over the columns.

(The details involve exact adaptation to the unitary irreps of $S_N$.)
Special irreps

The antisymmetrizer $\mathcal{A}$ is represented by a one-column tableau (in which the tokens may represent spinorbitals)

The symmetrizer $\mathcal{S}$ is represented by a one-row tableau.

Each corresponds to a one-dimensional irrep.
An extension of this formalism deals with permutations of objects some of which may be indistinguishable.

This extension allows tokens to be repeated (but not in the same column), resulting in Weyl tableaux, and is particularly suitable for dealing with spatial orbitals that may be more than singly occupied and with spin functions.
A *standard* Weyl tableau is one in which the numbers are non-decreasing from left to right in each row and increasing from top to bottom in each column.

The Weyl tableau representation is used for spin functions (where the tokens are $\alpha$ and $\beta$), and for configuration-state functions (CSFs) in the spin-adapted unitary group approach (UGA).
To create configuration state functions (CSFs), we are interested in working with orbitals, not spinorbitals, and we separate the description of the space part and the spin part.

To obtain a totally antisymmetric function we combine a spatial tableau with a spin tableau of complementary shape.
Complementary shapes are such that the column layout of one is like the row layout of the other, and vice versa.

This combination of the two tableaux is not a simple product, but represents a linear combination of products (we shall not go into details).

The spin tableau for electrons can have at most two rows, because the electron has just two states, and tokens cannot repeat in the same column. Therefore the space tableau can have at most two columns.
Spin Tableau

\[
\begin{array}{cccc}
\alpha & \alpha & \alpha & \alpha \\
\beta & \beta & \beta \\
\end{array}
\]

\[a = \text{no. of two-box columns}\]

\[b = \text{no. of one-box columns}\]

\[N = 2a + b = \text{no. of electrons}\]
The *shape* determines the total spin quantum number,

\[ S = \frac{1}{2}b. \]

The *tableau* determine the spin component,

\[ M_S = \frac{1}{2}(n_\alpha - n_\beta). \]
Because of the lexical ordering requirement, all $\alpha$’s must go into the beginning of the first row.

The second row is filled with $\beta$’s, and any remaining $\beta$’s go into the remaining boxes in the first row.
## Examples

<table>
<thead>
<tr>
<th>$N$</th>
<th>$S$</th>
<th>$M_S$</th>
<th>tableau</th>
<th>Spin state</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{1}{2}$</td>
<td>$\alpha$</td>
<td>doublet</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$-\frac{1}{2}$</td>
<td>$\beta$</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>$\begin{array}{c} \alpha \ \beta \end{array}$</td>
<td>singlet</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>$\begin{array}{c} \alpha \ \alpha \end{array}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0</td>
<td>$\begin{array}{c} \alpha \ \beta \end{array}$</td>
<td>triplet</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$-1$</td>
<td>$\begin{array}{c} \beta \ \beta \end{array}$</td>
<td></td>
</tr>
</tbody>
</table>
### Examples

<table>
<thead>
<tr>
<th>$N$</th>
<th>$S$</th>
<th>$M_S$</th>
<th>tableau</th>
<th>Spin state</th>
</tr>
</thead>
</table>
| 3   | $1/2$ | $1/2$ | $\begin{array}{c}
\alpha \\
\beta 
\end{array}$ | doublet |
|     | $-1/2$ | $-1/2$ | $\begin{array}{c}
\alpha \\
\beta 
\end{array}$ |             |
| 3   | $3/2$ | $3/2$ | $\begin{array}{c}
\alpha \\
\alpha \\
\alpha 
\end{array}$ | quartet |
|     | $1/2$ | $1/2$ | $\begin{array}{c}
\alpha \\
\alpha \\
\beta 
\end{array}$ |             |
|     | $-1/2$ | $-1/2$ | $\begin{array}{c}
\alpha \\
\beta \\
\beta 
\end{array}$ |             |
|     | $-3/2$ | $-3/2$ | $\begin{array}{c}
\beta \\
\beta \\
\beta 
\end{array}$ |             |
Most spin-adapted electronic structure calculations are independent of $M_S$, thus we need not deal with the spin tableau in our treatment and may consider the space tableau only.

Therefore, the only effect of spin in these calculations is to determine the shape of the space tableau.
In the symmetric group approach (SGA) for constructing configuration-state functions (CSF’s) we use Young tableaux (no repetition of tokens) to spin-couple the singly occupied orbitals only (we know how to spin-couple the doubly occupied orbitals).

Therefore we use the group $S_N$ ($N =$ no. of electrons in singly occupied orbitals), and have different $N$’s for different sets of CSF’s.

In the unitary group approach (UGA) we use Weyl tableaux and include the doubly occupied orbitals, so $N$ is the same for all CSF’s.
In SGA we spin-couple the singly occupied orbitals one at a time, and the result is equivalent to the well-known genealogical construction.

The tableau determines the path we take in the branching diagram:
In the first step we had one box, with \( a = 0, b = 1 \), which results in a doublet state, \( S = \frac{1}{2} \), because \( S = \frac{1}{2}b \).

Adding the second singly occupied orbital, we get \( a = 0, b = 2 \), which results in a triplet state, \( S = 1 \).
Adding the third orbital in the tableau, in the second column, increases \( a \) and decreases \( b \) by 1 each, and we get

\[
a = 1, \ b = 1,
\]

which results in a doublet state again, \( S = \frac{1}{2} \).
Adding the fourth orbital, also in the second column, we get

\[ a = 2, \quad b = 0, \]

which results in a singlet state, \( S = 0 \).
Adding the fifth orbital, in the first column, we get

\[ a = 2, \ b = 1, \]

which results in a doublet state again, \( S = \frac{1}{2}. \)
Adding the sixth orbital, we get

\[ a = 2, \ b = 2, \]

which results in a triplet state again, \( S = 1 \).
Adding the seventh orbital, we get

\[ a = 3, \ b = 1, \]

which results in a doublet state again, \( S = \frac{1}{2} \).
Finally, adding the eighth singly occupied orbital, we get the final state,

\[ a = 3, \ b = 2, \]

which is a triplet state, \( S = 1 \).
A token (electron number) in the first column of the tableau corresponds to an up-going line (increased $S$) in the branching diagram, while a token placed in the second row corresponds to a down-going line (decreased $S$) in the branching diagram.

The path through the branching diagram thus fully specifies the Young tableau, and vice versa.
This incremental process corresponds to using the sequence of symmetric groups \( S_1, S_2, \ldots, S_N \), in the group subduction chain

\[
S_N \supset \ldots \supset S_3 \supset S_2 \supset S_1,
\]

adapting the partial spin function to the corresponding irrep at each stage.
The Unitary Group

The unitary group $U(n)$ is the group of all unitary matrices of order $n$.

It is a continuous group, specifically a Lie group, all of whose elements can be generated by a finite set of operators, called the generators of the group.

The commutation properties of the generators of a Lie group fully define the group.
The generators of $U(n)$ are a set of operators $E_{ij} \ (i,j = 1, 2, \ldots, n)$ that satisfy the commutation relation

$[E_{ij}, E_{kl}] = \delta_{jk}E_{il} - \delta_{il}E_{kj}$.

This relation corresponds to

$E_{ij}E_{kl} - \delta_{jk}E_{il} = E_{kl}E_{ij} - \delta_{il}E_{kj}.$
This is the same commutation relation satisfied by the set of second-quantization spin-preserving substitution operators

\[ E_{ij} = X_{i\alpha}^\dagger X_{j\alpha} + X_{i\beta}^\dagger X_{j\beta}, \]

where \( X_{i\alpha}^\dagger \) and \( X_{i\alpha} \) are creation and annihilation operators, respectively, for spatial orbital \( i \) with spin \( \alpha \).

This is the most important connection between the unitary group and electronic structure theory.
The operator $E_{ij}$ moves an electron in orbital $j$ to orbital $i$ in CSFs on which it operates, without changing the spin state.

(If orbital $j$ was missing in the CSF, the result is 0. If it was doubly occupied it will become singly occupied. If orbital $i$ was singly occupied, it will become doubly occupied. If it was doubly occupied, the result is 0. In all cases, the spin state is unchanged.)

The number $n$ in $U(n)$ will be the number of (spatial) orbitals in our basis.
Like the irreps of the symmetric group $S_N$, the irreps of the unitary group $U(n)$ can be labeled (specified) by Young shapes, but instead of being restricted to $N$ boxes, the shapes can have any number of boxes (for application to electronic wave functions $N \leq 2n$).

The components of the irreps are identified by standard Weyl tableaux that may contain the tokens $1, 2, \ldots, n$, with repetitions and omissions allowed.
The tokens represent the orbitals in the orbital basis in their sequential order. Thus an orbital is always represented by the same token, unlike the case of the SGA, where the representation depends on which orbitals are occupied.
In the unitary group approach, unlike the SGA, we focus on the entire orbital basis, not the singly occupied orbitals, and spin-couple the orbitals in their original order, one at a time. For each orbital we have four possibilities:

• It may be left empty,

• It may be singly occupied so as to raise $S$ by $\frac{1}{2}$,

• It may be singly occupied so as to lower $S$ by $\frac{1}{2}$,

• Or it may be doubly occupied (no change in $S$).
Sequential orbital coupling in UGA

We begin with a null entry at the bottom of the table, and proceed upwards:

<table>
<thead>
<tr>
<th>Orbital $(i)$</th>
<th>$a_i$</th>
<th>$b_i$</th>
<th>$N_i$</th>
<th>$S_i$</th>
<th>$d_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>3</td>
<td>2</td>
<td>8</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>6</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>1</td>
<td>5</td>
<td>$\frac{1}{2}$</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Adding orbital 1:

\( d_i \) is the step number.

\( d_1 = 3 \) identifies a doubly occupied orbital.
Sequential orbital coupling in UGA

Adding orbital 2:

\[ d_2 = 1 \] identifies a singly occupied orbital coupled to raise \( S_i \) by \( \frac{1}{2} \).
Sequential orbital coupling in UGA

Adding orbital 3: $d_3 = 0$ identifies an empty orbital; no change in $S_i$.

<table>
<thead>
<tr>
<th>Orbital $(i)$</th>
<th>$a_i$</th>
<th>$b_i$</th>
<th>$N_i$</th>
<th>$S_i$</th>
<th>$d_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>3</td>
<td>2</td>
<td>8</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>6</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>1</td>
<td>5</td>
<td>$\frac{1}{2}$</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Adding orbital 4:

$d_4 = 1$ identifies a singly occupied orbital coupled to raise $S_i$ by $\frac{1}{2}$. 

```
<table>
<thead>
<tr>
<th>Orbital (i)</th>
<th>$a_i$</th>
<th>$b_i$</th>
<th>$N_i$</th>
<th>$S_i$</th>
<th>$d_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>3</td>
<td>2</td>
<td>8</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>6</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>1</td>
<td>5</td>
<td>$\frac{1}{2}$</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
```
Sequential orbital coupling in UGA

Adding orbital 5:

\[ d_5 = 2 \] identifies a singly occupied orbital coupled to lower \( S_i \) by \( \frac{1}{2} \).
Adding orbital 6: $d_6 = 1$ identifies a singly occupied orbital coupled to raise $S_i$ by $\frac{1}{2}$. 

<table>
<thead>
<tr>
<th>Orbital $(i)$</th>
<th>$a_i$</th>
<th>$b_i$</th>
<th>$N_i$</th>
<th>$S_i$</th>
<th>$d_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>3</td>
<td>2</td>
<td>8</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>6</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>1</td>
<td>5</td>
<td>$\frac{1}{2}$</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Sequential orbital coupling in UGA

Adding orbital 7:

\[ d_7 = 3 \] identifies a doubly occupied orbital; \[ S_i \] is unchanged.
The two-column Paldus $ab$ tableau fully specifies the Weyl tableau, and is a compact and convenient way to represent the spin-coupled function (CSF).

<table>
<thead>
<tr>
<th>Orbital $(i)$</th>
<th>$a_i$</th>
<th>$b_i$</th>
<th>$N_i$</th>
<th>$S_i$</th>
<th>$d_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>3</td>
<td>2</td>
<td>8</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>6</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>1</td>
<td>5</td>
<td>$\frac{1}{2}$</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Paldus $abc$ tableau

The three-column Paldus $abc$ tableau is sometimes used instead, with

$$a_i + b_i + c_i = i.$$  

We define

$$\Delta a_i = a_i - a_{i-1},$$  

etc.

Then:

$$\Delta a_i + \Delta b_i + \Delta c_i = 1.$$
The four ways of coupling an orbital

$$\begin{array}{cccccc}
d_i & \Delta a_i & \Delta b_i & \Delta c_i & \Delta N_i = n_i & \Delta S_i \\
0 & 0 & 0 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 & 1 & \frac{1}{2} \\
2 & 1 & -1 & 1 & 1 & -\frac{1}{2} \\
3 & 1 & 0 & 0 & 2 & 0 \\
\end{array}$$

$$n_i = \text{occupation number of orbital } i.$$
The step vector

The step vector $d$ is the most compact representation of the CSF. It fully specifies the Paldus tableau and the Weyl tableau.

$$d_i = 3 \Delta a_i + \Delta b_i = 0, 1, 2, \text{ or } 3$$

<table>
<thead>
<tr>
<th>Orbital $(i)$</th>
<th>$a_i$</th>
<th>$b_i$</th>
<th>$N_i$</th>
<th>$S_i$</th>
<th>$d_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>3</td>
<td>2</td>
<td>8</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>6</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>1</td>
<td>5</td>
<td>$\frac{1}{2}$</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\frac{1}{2}$</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Because

\[ a = \sum_i \Delta a_i, \text{ etc.}, \]

and because

\[ d_i = 3 \Delta a_i + \Delta b_i, \]

the step vector must satisfy

\[ \sum_i d_i = 3a + b \]

\[ = (3/2)N - S. \]
The incremental orbital coupling process corresponds to using the sequence of Unitary groups $U(1), U(2), \ldots, U(n)$, in the group subduction chain

$$U(n) \supset \ldots \supset U(3) \supset U(2) \supset U(1),$$

adapting the partial CSF to the corresponding irrep at each stage.
The top \((a, b)\) row of the Paldus tableau identifies an irrep of \(U(n)\), as well as the corresponding electronic state,

\[
N = 2a + b, \quad S = \tfrac{1}{2}b.
\]

The dimension of the irrep,

\[
D_{abc} = \frac{b+1}{n+1} \binom{n+1}{a} \binom{n+1}{c}
\]

\((c = n - a - b)\), is equal to the dimension of the spin-adapted full-CI expansion for that state.
Each Paldus tableau with the top row \((a, b)\) specifies one of the CSF’s of the full-CI expansion according to the incremental coupling scheme described previously.

These tableaux specify an orthonormal set of CSF’s.

Thus we can specify the full-CI expansion set or any subset of it by the corresponding set of Paldus tableaux or the corresponding step vectors.
To allow systematic numbering of the Paldus tableaux, a lexical order is established for them.

We assign a single **lexical index** $m$ to each tableau (and identify the corresponding CSF by $|m\rangle$), such that tableau $m'$ precedes tableau $m$, (i.e., $m' < m$) if, at the highest level $j$ at which the tableaux differ, 

\[
\begin{align*}
  a_j(m') &> a_j(m), \\
  \text{or} &\\
  a_j(m') &> a_j(m'), \\
  b_j(m') &> b_j(m').
\end{align*}
\]
The CSF represented by any of the tableaux can be expressed as a linear combination of Slater determinants (once we have chosen $M_S$) using an algorithm given, e.g., on p. 55 of: I. Shavitt, in *The Unitary Group* (Lecture Notes in Chemistry, No. 22), J. Hinze, ed. (Springer, Berlin, 1981), pp. 51–99.

\[
\begin{pmatrix}
1 & 1 \\
2 & 5 \\
4 & 7 \\
6 & \\
7 &
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
3 & 2 \\
2 & 2 \\
2 & 1 \\
1 & 2 \\
1 & 1 \\
1 & 1 \\
1 & 0 \\
0 & 0 \\
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
3 \\
1 \\
2 \\
1 \\
0 \\
1 \\
3
\end{pmatrix}
\Rightarrow
(1/\sqrt{6}) \times \left\{ | \begin{array}{ccccccc} 1 & 1 & 2 & 4 & 5 & 6 & 7 \end{array} | \right. \\
\left. + | \begin{array}{ccccccc} 1 & 1 & 2 & 4 & 5 & 6 & 7 \end{array} | \right. \\
\left. - 2 | \begin{array}{ccccccc} 1 & 1 & 2 & 4 & 5 & 6 & 7 \end{array} | \right. \\
\right\} \\
(\text{for } M_S = 1).
But we need not be concerned with the determinantal expansions of the CSFs, because the calculation of matrix elements and all other needed operations can be done entirely in terms of the corresponding Weyl or Paldus tableaux or step vectors, without reference to such expansions.
The second-quantized Hamiltonian is

\[ H = \sum_{ij} \sum_{\sigma} h_{ij} X_i^{\dagger} X_j^{\sigma} + \frac{1}{2} \sum_{ijkl} \sum_{\sigma\tau} [ij;kl] X_i^{\sigma} X_k^{\tau} X_l^{\tau} X_j^{\sigma} \]

where

\[ h_{ij} = \langle i|h|j \rangle, \quad [ij;kl] = \langle i(1)k(2)|1/r_{12}|j(1)l(2) \rangle \]

and \( \sigma, \tau \) are summed over the spins \( \alpha, \beta \).
Noting that

\[ X_{i\sigma}^\dagger X_{k\tau}^\dagger X_{l\tau} X_{j\sigma} = X_{i\sigma}^\dagger X_{j\sigma} X_{k\tau}^\dagger X_{l\tau} - \delta_{jk} \delta_{\sigma\tau} X_{i\sigma}^\dagger X_{l\sigma} \]

we have

\[ \sum_{\sigma} X_{i\sigma}^\dagger X_{j\sigma} = E_{ij}, \]

\[ \sum_{\sigma\tau} X_{i\sigma}^\dagger X_{k\tau}^\dagger X_{l\tau} X_{j\sigma} = E_{ij} E_{kl} - \delta_{jk} E_{il}, \]

and define

\[ E_{ij} E_{kl} - \delta_{jk} E_{il} \equiv e_{ij,kl} = e_{kl,ij}. \]
The Hamiltonian then takes the simple form:

\[ H = \sum_{ij} h_{ij} E_{ij} + \frac{1}{2} \sum_{ijkl} [ij;kl] e_{ij,kl} \]

A matrix element of \( H \) between two CSF’s can now be obtained as

\[ \langle m'|H|m \rangle = \sum_{ij} h_{ij} \langle m'|E_{ij}|m \rangle + \frac{1}{2} \sum_{ijkl} [ij;kl] \langle m'|e_{ij,kl}|m \rangle \]

Thus the matrix elements of the generators \( E_{ij} \) and \( e_{ij,kl} \) are the “coupling coefficients” needed for calculating the matrix elements of \( H \).
These matrix elements are fully determined by the Weyl tableaux (or any of the other tableau notations) for $\langle m'|$ and $|m\rangle$, and can be calculated by purely group-theoretical methods (Gel’fand and Tsetlin) or by the graphical techniques of spin algebras (Kent and Schlesinger, Paldus), but in the graphical unitary group approach (GUGA) we shall use a different graphical technique.