

The Graphical Unitary Group Approach in COLUMBUS

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Josef Paldus introduced the Unitary Group Approach (UGA) to the quantum chemistry community in a series of papers [1-7] starting in 1974. This approach allows configuration state functions (CSF) to be defined that satisfy the Fermion antisymmetry properties and that are eigenfunctions of the spin operators S^2 and S_z . This early work by Paldus focuses on the connections between the UGA and various symmetric group approaches based on Young tableau and in particular the two-column Weyl tableau. Paldus simplified the representation of Gel'fand tableau within the UGA by introducing what is now called the *Paldus ABC tableau*. Each row consists of three nonnegative integers, (a_n, b_n, c_n) at orbital level n , with *betweenness conditions* imposed on the values of adjacent rows. At each level, these integers correspond to the quantum numbers $S_n = \frac{1}{2}b_n$, $N_n = 2a_n + b_n$ and $n = a_n + b_n + c_n$ where N_n is the cumulative number of electrons for that row. The betweenness conditions correspond to the four possible occupations and spin couplings of a spatial orbital. Each row labels an irreducible representation (irrep) of $U(n)$, and each CSF is thereby characterized uniquely as a genealogical spin eigenfunction denoted by the sequence of irrep labels $U(n) \supset U(n-1) \dots U(2) \supset U(1)$.

Shavitt[8-10] recognized that there are only a very limited number of *distinct rows* of the Paldus tableau. These distinct rows correspond to the nodes of a hierarchical, directed, acyclic, *Shavitt graph*, the arcs connecting these nodes correspond to the betweenness conditions, and each CSF then corresponds to a path from the tail to the head of the graph. This representation of the CSF expansion space is called the Graphical Unitary Group Approach (GUGA), and it is used extensively within COLUMBUS to organize and characterize MCSCF, MRCI, and Graphically Contracted Function (GCF)[11-12] wave functions and reduced density matrices.

This talk will review the use of UGA and GUGA within COLUMBUS[13-14].

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