

# Graded orthogonality for Fermionic states

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## Abstract

The concept of  $p$ -orthogonality ( $1 \leq p \leq n$ ) between  $n$ -fermion states is introduced. It generalizes common orthogonality, which is equivalent to  $n$ -orthogonality, and strong orthogonality, which is equivalent to 1-orthogonality. Within the class of non  $p$ -orthogonal states a finer measure of non  $p$ -orthogonality is provided by Araki's angles between  $p$ -internal spaces. The  $p$ -orthogonality concept induces a new hierarchy of approximations for group function methods in quantum chemistry. This is illustrated with a constrained version of the EMFCI method [1]. The simplifications that occur in the calculation of matrix elements between 2-orthogonal group functions are presented and taken advantage of in non-strongly orthogonal geminal SCF calculations.

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## References

- [1] P. Cassam-Chenai, J. Chem. Phys **124**, 194109-194123 (2006).