

The Contracted Schrödinger Equation: Imposing Spin-representability Constraints upon the Correlation matrix

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Abstract: The iterative solution of the spin-adapted Contracted Schrödinger Equation (CSE) method can now be considered a competitive approach to the study of the electronic structure of atoms and molecules. This satisfactory status has been mainly achieved through the purification procedures applied to the approximated Reduced Density Matrices entering the equation and, in particular, to the second-order one. The well known N-representability conditions, jointly with the set of Spin-conditions that the Correlation matrix must satisfy, are imposed at each iteration. The results obtained in some applications to singlet states are reported. The spin relations linking the spin-components of the Correlation matrix corresponding to a pure doublet state and to a pure triplet state are also reported here.

Some open questions which are now being studied in our group concerning the connection between the CSE and the Spin-adapted Reduced Hamiltonian theory will also be presented.

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