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Application of Generalized Sturmians to the Bound States of Two-Electron Atoms and Molecules EDDIE RED, ALBERT WYNN III, CHARLES WEATHERFORD, Florida A&M University — A variation on the method of Generalized Sturmians [J. Avery, *Hyperspherical Harmonicsand GeneralizedSturmians*, Kluwer, 2000], is applied to the calculation of the ground and excited states of two-electron atoms and molecules (etc. He, H_2). In the present implementation of this method, each determinant formed from a set of primitive one-electron Sturmians, is required to separately solve the Schödinger equation. In the process, the screening constant of each one- electron Sturmian orbital is non-iteratively uniquely determined. The resultant generalized eigenvalue problem however has a non-positive- definite overlap matrix. The method of 'corresponding orbitals' [H.F. King et. al. J. Chem. Phys. 47, 1936 (1967)] is used to produce a positive-definite overlap matrix. A CI calculation is then performed whereby the Hartree-Fock calculation is avoided. Results will be presented and compared with Hartree-Fock based CI calculations.

Charles Weatherford
Florida A&M University

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