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Optimal Sturmian basis functions for atomic three-body systems
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We discuss the optimisation of the Configuration Interaction method for three-body atomic systems in which the configurations are defined as products of Sturmian functions (SF). Our study in the case of two-electron atoms [1] clearly shows that the use of basis functions which fulfil the electron-nucleus cusp conditions and with adequate asymptotic behavior considerably improves the energy convergence rate. Using the SF basis, we transform the two-electron Schrodinger equation into a matrix eigenvalue problem. The results of the diagonalization are better than those obtained with highly accurate calculations which use Coulomb Sturmians Functions (CSF) [2]. Our results can be considered as the most accurate results obtained with uncorrelated basis functions [1]. An extension to atomic three-body systems with general masses will be presented.

[1] J.M. Randazzo, L.U. Ancarani, G. Gasaneo, A..L. Frapiccini and F.D. Colavecchia, Phys. Rev. A 81, 042520 (2010).
[2] M.W.J. Bromley and J. Mitroy, Int. J. Quantum Chem. 107, 1150 (2007).

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