Abstract Submitted
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Test of Variational Methods for Electronic Structures of Solid State and Molecular Systems by Application to Atomic Systems R.H. PINK, University at Albany, SUNY, S.R. BADU, University at Buffalo, SUNY, R.H. SCHEICHER, Uppsala University, T.P. DAS, University at Albany, SUNY — The Linked Cluster Many-Body Perturbation Theory [1,2] uses energies and wave-functions obtained from the one-electron Hartree-Fock equations for the ground state to determine the occupied states' contribution to properties such as magnetic hyperfine interaction. Both the occupied and unoccupied bound and continuum state energies and wave-functions are then used to include many-body effects through perturbation theory. This method has been found to provide excellent agreement between theoretical and experimental values for hyperfine constants for atomic systems [3,4]. Due to their multi-center nature, one cannot solve the Hartree-Fock differential equations by numerical integration methods for solid state and molecular systems, and must instead use variational methods [5,6,7]. We shall present our assessment of the accuracy of the variational procedure by determining the hyperfine constants for the Phosphorous [3] and Lithium [2] atoms. [1] Hugh P. Kelly, Phys. Rev. 144, 39 (1966) [2] E.S. Chang, R.T. Pu and T.P. Das, Phys. Rev. 174, 1 (1968) [3] N.C. Dutta, C. Matsubara, R. T. Pu, and T.P. Das, Phys. Rev. Lett. 21, 1139 (1968) [4] J. Andriessen, K. Raghunathan, S.N. Ray and T.P. Das, Phys Rev. B15, 2533 (1977) [5] C.C.J. Roothaan, Rev. Mod. Phys. 23, 69 (1951) [6] J.E. Rodgers and T.P. Das, Phys. Rev. A8, 2195 (1973) [7] W.J. Hehre, R.F. Stewart, and J.A. Pople, J. Chem. Phys. 51, 2657 (1969)

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