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Test of Current Variational Procedures for Electronic Structures and Properties of Molecular and Solid State Systems by application to Atomic Systems-H^-Ion HARI PAUDEL, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, S.R. BADU, R.H. PINK, T.P. DAS, SUNY Albany — Electronic properties of atomic systems are obtainable using Linked Cluster Many-Body Perturbation Theory(LCMBPT) with high accuracy and excellent agreement with experiment, using complete sets of states obtained by differential equation procedures [1,2]. Unfortunately such procedures are not practicable for multi-center molecular and solid state problems and variational procedures have to be used for obtaining the occupied and excited one electron states to work on electronic properties of the latter systems. With the aim to assess the accuracies of the latter procedures with Gaussian basis states, like the first principles Hartree-Fock procedure together with many body perturbation theory, and density functional based procedures, we are testing them for both energy and wave function dependent properties of atoms. Results will be presented for H^- ion, where Hartree-Fock theory predicts instability with respect to auto ionization to H atom and electron correlation effects obtained by the LCMBPT procedure [3] restore stability, providing nearly exact experimental affinity for H^-.[1] Alfred Owusu et al., Phys. Rev. A56, 305(1997) [2] T.Lee et al., Phys. Rev. A4 1410(1971) [3]C.M. Dutta et al., Phys. Rev. A2, 2289(1970)

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