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Examination of Variational Procedures for Electronic Structure Studies by Comparison of Results for Energies of Atoms with Experiment and Results from Bruckner-Goldstone Many-Body Perturbation Theory –Lithium Atom H. PAUDEL, ARCHANA DUBEY, UCF Orlando, R.H. PINK, S.R. BADU, SUNY Albany, R.H. SCHEICHER, Uppsala University, Sweden, T.P. DAS, SUNY Albany — Through the use of the Bruckner-Goldstone Diagrammatic Many Body Perturbation Theory (BGMBPT) in the recent past, quantitative results in excellent agreement with experiment have been found for atomic properties which can be used to test the accuracy of the variational procedures in use currently for investigations of electronic structures and properties of multicenter systems like molecules and solid state systems by applying them to atomic systems. In the present talk, we shall consider lithium atom in its ground state where an earlier BGMBPT investigation [1] has provided very good agreement with experiment for the total energy including correlation effects. We have focused for the comparison in the present work on the Gaussian basis set based, first –principles Hartree-Fock procedure combined with Many-Body Perturbation Theory, and the B3LYP procedure using DFT based exchange and correlation potentials, for the total energy for lithium. Results of our investigation, and conclusions from our analysis, will be presented. [1]T.P. Das, Phys. Rev. 174, 1 (1968)

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