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Test 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 –Neon Atom ARCHANA DUBEY, H. PAUDEL, UCF Orlando, R.H. PINK, S.R. BADU, SUNY Albany, R.H. SCHEICHER, Uppsala University, Sweden, T.P. DAS, SUNY Albany — During the latter half of the last century, great advances were made, through the Bruckner Goldstone Diagrammatic Many Body Perturbation Theory (BGMBPT), in accurate quantitative understanding of atomic properties. These investigations have provided a wealth of data which can now be used to test the accuracy of variational procedures in use currently for investigations of electronic structures and properties of multicenter systems like molecules and solid state systems. In the present talk, we shall consider neon atom where an earlier BGMBPT investigation [1] has provided excellent agreement with experiment for the total energy including correlation contributions. We have focused for this comparison 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 neon. Results of our investigations will be presented and discussed.

[1] Taesul Lee, N.C. Dutta and T.P. Das, Phys. Rev. A4,1410(1971)

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