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Test of Variational Methods for Molecular and Solid State Properties by Application to Hyperfine Interaction in Phosphorous Atom T.P. DAS, R.H. PINK, S.R. BADU, Department of Physics, University at Albany, SUNY, ARCHANA DUBEY, Department of Physics, University of Central Florida, R.H. SCHEICHER, Department of Physics, Uppsala University, LEE CHOW, Department of Physics, University of Central Florida — As part of our program for testing the accuracy of variational methods for studying energy and wave-function dependent molecular and solid state properties, namely the Variational Hartree-Fock Many Body Perturbation Theory (VHFMBPT) and Variational Density Functional Theory (VDFT), we have studied the magnetic hyperfine interaction for ^{31}P nucleus in the ground state. Our investigations provide hyperfine constants of +35.2MHz by the VHFMBPT and -11.2 MHz by VDFT procedures as compared to +55.055 MHz from experiment [1]. The VHFMBPT procedure provides the same signs for one-electron and many-body contributions as obtained earlier [2] by the HFMBPT procedure which uses the needed one-electron atomic wave-functions for the occupied and unoccupied states obtained by solving the Hartree-Fock equations through numerical integration, and not variationally as in the VHFMBPT procedure. Possible avenues for improved agreement by both variational procedures will be suggested. [1] N.C. Dutta, C. Matsubara, R.T. Pu and T.P. Das, Phys. Rev. Lett. 21, 1139 (1963) and references therein, [2] T.P. Das Hyperfine Interactions 34, 149 (1987) and reference therein to the experimental result for phosphorous atom. [3] Alfred Owusu, R.W. Dougherty, G. Gowri, J. Andriessen, T.P. Das, Phys. Rev. A 56, 305 (1997) and references therein.

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