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Numerical solution of atomic systems and its response to external perturbation

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ABSTRACT

Electronic structure properties of Hydrogen atom kept inside fullerene (C_{60}) is studied using two model potentials; step and Jellium. Electronic properties such as radial wavefunction, radial probability distribution, energy spectrum etc. are studied for the two model cases of endohedral Hydrogen atom. A systematic study of variation of electronic properties with respect to strength of the model potential is carried out. In this analysis, well known 'band crossing' phenomenon is observed, leading to 'mirror collapse' of wavefunctions [1]. Furthermore, photoionization of these confined systems have also been studied in this work.