Abstract Submitted
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Study of adiabatic connection in ground-state density functional theory MANOJ HARBOLA, RABEET CHAUHAN, Indian Inst of Tech-Kanpur, RABEET S. CHAUHAN COLLABORATION — By employing modified [1] variational form of Le-Sech wavefunctions [2] for two-electron systems, accurate wavefunctions for He-like atoms corresponding to their ground-state density are obtained for varying strength, given by a parameter α ($0 \leq \alpha \leq 1$), of electron-electron interaction. Using these, it is shown explicitly that (i) the total energy varies almost linearly as a function of α, and (ii) the ionization potential remains unchanged [3] as α is varied. Furthermore, kinetic energy contribution to the density-functional exchange-correlation energy is calculated using the adiabatic connection formula [4] and shown to match that calculated on the basis of Kohn-Sham calculation. Finally, the exchange-correlation energy obtained for different values of α is employed to analyze several hybrid exchange-correlation energy functionals in use. [1] R.S. Chauhan and M.K. Harbola, Chem. Phys. Lett. **639C**, 248(2015) [2] C. Le Sech, J. Phys. B: Atom. Mol. Opt. Phys. **30**, L47(1997) [3] M. Levy, J. P. Perdew and V. Sahni, Phys. Rev. A **30**, 2745(1984) [4] R. Harris and R.O. Jones, J. Phys. F: Met. Phys. 4 1170 (1974); D.C. Langreth and J.P. Perdew, Phys. Rev. B **15**, 2884 (1977)

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