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Title:	Complex Molecular Integral Evaluation using Long range Short range separation of nuclear-electron attraction integral
Authors:	Meena, Shivam Abhineet (/jspui/browse?type=author&value=Meena%2C+Shivam+Abhineet)
Keywords:	Chemistry Problem with molecules Nuclear Attraction Integral Gaussian Type Orbitals Wave Functions
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Abstract:	The main objective for this work was to calculate complex scaled nuclear attraction integral for atoms and molecules. By splitting the one electron Coulomb interaction into long-range and short-range components, the energy of a quantum electronic system is decomposed into long-range and short-range contributions using error function. We used Gaussian basis and the analytical form was solved using Gaussian product theorem and Fourier transformation. This form is then complex scaled using appropriate rotations in the complex plane for which Weierstrass transformation is performed to get a smooth function. Now, after getting the appropriate function Gaussian integral is modified to get all the analytical forms. Configuration interaction calculations are performed to get the correlation energies for He atom using the basis "coemd-ref" for s, p and d Cartesian Gaussian function is used because it gives us a good mix of high and low exponents of Gaussian function which is useful to capture the resonances. We constructed the plots for ground, first and doubly excited state for He atom.
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