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.