Correlated Atomic Pair Functions by the $e^{-\varrho}$-Method.

I. Ground State $1^1S$ and Lowest Excited States $n^1S (n > 1)$ and $n^3S$ of Helium

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Some low $n^1S$ and $n^3S$ states of the helium atom are computed with the aid of the $e^{-\varrho}$ method which formulates the electronic wave function of the 2 electrons as $\Psi = e^{-\varrho} F$, where $\varrho = Z(r_1 + r_2) - \frac{1}{2} r_{12}$ and here $Z = 2$. Both the differential and the integral equation for $F$ contain a pseudopotential $\tilde{V}$ instead of the true potential $V$ that contrary to $V$ is finite. For the ground state, $F = 1$ yields nearly the Hartree-Fock SCF accuracy, whereas a multinomial expansion in $r_1, r_2, r_{12}$ yields a relative error of about $10^{-7}$. All integrals can be computed analytically and are derived from one single “parent” integral.

Key words: Electron Correlation; Pair Function; $S$-states of Helium.