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

F. F. Seelig and G. A. Becker[a]

Institute for Physical and Theoretical Chemistry, University of Tübingen, Germany
[a] *Present address:* Radiological Clinic, University of Tübingen, Germany

Reprint requests to Prof. F. F. S.; Fax: +49 7071 295490,
E-mail: friedrich-franz.seelig@uni-tuebingen.de

Z. Naturforsch. **54 a,** 711–717 (1999); received October 29, 1999

Dedicated to Prof. Hans Kuhn, Switzerland, on the Occasion of his 80th Birthday

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.