Ultra-Compact accurate wave functions for He-like and Li-like iso-electronic sequences and variational calculus. III. Spin-quartet state of the Lithium sequence

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Abstract

As a continuation of Part I, dedicated to the ground state of He-like and Li-like isoelectronic sequences for nuclear charges $Z \leq 20$, and Part II, dedicated to two excited states of He-like sequence, two ultra-compact wave functions in the form of generalized Guevara-Harris-Turbiner functions are constructed for Li-like sequence. They describe accurately the domain of applicability of the Quantum Mechanics of Coulomb Charges (QMCC) for energies (2-3 significant digits (s.d.)) of the spin-quartet state 1^40^+ of Li-like ions (in static approximation with point-like, infinitely heavy nuclei). Variational parameters are fitted in Z by 2nd degree polynomials. The most accurate ultra-compact function leads to the absolute accuracy $\sim 10^{-3}$\,a.u. for energy, and $\sim 10^{-4}$ for the normalized electron-nuclear cusp parameter for $Z \leq 20$. Critical charge $Z=Z_B$, where the ultra-compact trial function for the 1^40^+ state looses its square-integrability, is estimated, $Z_B(1^4\,0^+) \sim 1.26 - 1.30$. As a complement to Part I, square integrability for the compact functions constructed for the {\it ground, spin-doublet state} $1^2\,0^+$ of the Li-like sequence is discussed. The critical charge, for which these functions stop to be normalizable, is estimated as $Z_B(1^2\,0^+) = 1.62 - 1.65$. It implies that at $Z=2$ - the negative helium ion He$^-$ - both states $1^2\,0^+$ and $1^4\,0^+$ exist as states embedded to continuum.

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