

Abstract Submitted
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Improved Energy Bounds and Basis Set Construction Strategies for Lithium¹ GORDON DRAKE, University of Windsor, LIMING WANG, ZONG-CHAO YAN, Univeristy of New Brunswick — Improved nonrelativistic energy bounds for the low-lying states of lithium are presented using the variational method in Hylleraas coordinates. For example, the nonrelativistic energies for the infinite nuclear mass case are $-7.478\,060\,323\,910\,147(1)$ a.u. for $1s^2 2s^2 S$, $-7.354\,098\,421\,444\,37(1)$ a.u. for $1s^2 3s^2 S$, $-7.318\,530\,845\,998\,91(1)$ a.u. for $1s^2 4s^2 S$, $-7.410\,156\,532\,652\,4(1)$ a.u. for $1s^2 2p^2 P$, and $-7.335\,523\,543\,524\,688(3)$ a.u. for $1s^2 3d^2 D$. The completeness of the angular momentum and spin configurations is investigated and examples presented for the $2P$ and $3D$ states to demonstrate the effect of different coupling schemes. In particular, the so-called second spin function (i.e. coupled to form an intermediate triplet state) is shown to have no effect on the final converged results, even for the expectation values of spin-dependent operators.

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