Abstract Submitted
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Influence of Angular and Spin-dependent Terms on Variational Energies of Lithium[1] GORDON DRAKE, University of Windsor, ZONG-CHAO YAN, LIMING WANG, University of New Brunswick — Improved nonrelativistic energy bounds for the low-lying states of lithium are presented using the variational method in Hylleraas coordinates [1]. 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. These results represent the most accurate nonrelativistic energies in the literature. 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. This resolves a long-standing controversy concerning the completeness of the spin-coupling terms.

[1] L.M. Wang, Z.-C. Yan, H.X. Qiao, and G.W.F. Drake, Phys. Rev. A **85**, 052513 (2012).

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