Abstract Submitted
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Correlated Wavefunction for the Li Atom[1] FRANK HARRIS, QTP, U. of Florida and Dept. of Physics, U. of Utah — Accurate wavefunctions are extremely valuable as tools for gaining understanding of quantum systems. Here we use a wavefunction explicitly containing all the interparticle distances to obtain a highly precise description of the ground state of the Li atom. In contrast to the widely used Hylleraas approach (in which the interelectron distances enter the wavefunction only as integer powers), our wavefunction exhibits an exponential dependence on all the interparticle distances, with a spatial dependence (before imposing spin and symmetry restrictions) of the form $\sum_{n=1}^{N} c_n \exp(-w_1 r_1 - w_2 r_2 - w_3 r_3 - u_1 r_{23} - u_2 r_{13} - u_3 r_{12})$, where r_i are electron-nuclear distances, r_{ij} are electron-electron distances, and w_i and u_i are parameters. When the nonlinear parameters are carefully optimized (a nontrivial task), this type of basis causes a far more rapid convergence (with N) than the Hylleraas basis. We will survey the results we have obtained and compare with other studies of the Li atom.

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