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Very accurate quantum mechanical calculations on small atom with explicitly correlated Gaussian functions KEEPER SHARKEY, University of Arizona — Techniques and algorithms for very accurate calculations of ground and excited states of atoms with three and four electrons will be presented. The approach has been used to determine state energies and the corresponding wave functions. The effect of the finite mass of the nucleus is expicitly include in the calculations, which are done with the variational method and employ the analitical energy gradient in the optimization of the Gaussian nonlinear parameters. Some recenly obtained results for D states of the Li and Be atom will be shown.

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