Abstract Submitted
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Compact and accurate quantum Monte Carlo wave functions for first-row atoms[1] F. R. PETRUZIELO, LASSP, Cornell University, JULIEN TOULOUSE, Universite Pierre et Marie Curie, Paris, France, W. A. AL-SAIDI, C. J. UMRIGAR, LASSP, Cornell University, R. G. HENNIG, Materials Science and Engineering, Cornell University — Many-body wave functions for the first row atoms (Li to Ne) are represented as expansions in eigenstates of $\hat{L}^2$, $\hat{L}_z$, $\hat{S}^2$, $\hat{S}_z$, multiplied by a Jastrow factor. This configuration state function (CSF) expansion provides a systematic means for improving a wave function by including CSFs corresponding to higher excitations. Optimization of all wave function parameters including Jastrow, CSF and orbital coefficients as well as basis exponents, starting from a simple initial guess, results in compact and accurate wave functions (low energy and variance of local energy). Further improvements by use of backflow transformations are explored. This work aims to develop insight into selecting the relevant CSFs particularly for large systems, where it is difficult to include all CSFs to a given order.

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Cyrus Umrigar
Cornell University

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