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**Fast evaluation of multideterminant wavefunctions in quantum Monte Carlo**[1] MIGUEL A. MORALES, LLNL, BRYAN K. CLARK, Princeton, JEREMY MCMINIS, JEONGNIM KIM, UIUC, GUSTAVO SCUSERIA, Rice Univ. — Quantum Monte Carlo (QMC) methods such as variational and diffusion Monte Carlo depend heavily on the quality of the trial wave function. Although Slater-Jastrow wave functions are the most commonly used variational ansatz, more sophisticated wave functions are critical to ascertaining new physics. One such wave function is the multislater- Jastrow wave function which consists of a Jastrow function multiplied by the sum of slater determinants. In this talk we describe a method for working with these wave functions in QMC codes that is easy to implement, efficient, and easily parallelized. The algorithm computes the multi determinant ratios of a series of particle hole excitations in time $O(n^2)+O(n_s n)+O(n_e)$ where n, $n_s$ and $n_e$ are the number of particles, single particle excitations, and total number of excitations, respectively. This is accomplished by producing a (relatively) compact table that contains all the information required to read off the excitation ratios. In addition we describe how to compute the gradients and laplacians of these multi determinant terms.

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