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Density Dependence of Fixed-Node Errors KEVIN RASCH, LUBOS MITAS, Center for High Performance Simulation, Dept of Physics, North Carolina State University — With both variational and diffusion Monte Carlo (VMC and DMC) methods, we calculate the ground state energy of isoelectronic free ions in the first row of the periodic table for both Hartree-Fock and Configuration Interaction based trial wave functions. As it is well-known, the fixed-node DMC is exact in the limit that the fermion nodes of the trial wave function are also exact. This study is focused on understanding of the density dependence of the fixed-node error since one expects that with increasing density of electrons the errors would be more pronounced due to higher frequency of sampling of the nodal regions and/or areas with low potential energy. For this purpose we construct Hartree-Fock and multi-reference wave functions and quantify the fixed-node biases. We compare strongly bonded highly localized cations, neutral atoms and weakly bonded anions. We compare the absolute and relative sizes of fixed-node errors and their relationships to multi-reference wave functions.

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