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**Analysis of fixed-nodes errors in quantum Monte Carlo calculations of atoms and molecules** SHUMING HU, KEVIN RASCH, MINYI ZHU, MICHAL BAJDICH, LUBOS MITAS, Center for High Performance Simulation, Department of Physics, North Carolina State University — The accuracy of fixed-node QMC calculation is determined by the fermion nodes of the trial wavefunction. We analyze the fixed-node errors for a diverse set of atoms and molecules. In some cases, our simple wavefunctions have almost the exact nodes. But in other cases, it is very difficult to find the exact nodes even with wavefunctions of correlated many-body forms, such as extensive multi-reference expansions, pairing and backflow. We try to elucidate the impact of the size and extent of the basis sets as one of the factors influencing fixed-node biases. The testing systems also include transition metal atoms with all-electron and Ne-core pseudopotential calculations.

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