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Fixed-node errors in electronic structure quantum Monte Carlo: interplay of density and node nonlinearities[1] LUBOS MITAS, KEVIN RASCH, SHUMING HU, North Carolina State University — We analyze valence electronic structure quantum Monte Carlo (QMC) calculations of first- and second-row atom systems. It turns out that there are significant differences (twofold or more) between the valence fixed-node errors of the first- vs second-row atom systems for single-configuration trial wave functions. The differences are illustrated on a set of atoms, molecules and Si and C solids that are valence isoelectronic, have similar correlation energies, bond patterns, geometries, same ground states and symmetries. Our analysis shows that the root cause of these differences is the increase of electron density combined with the degree of the node nonlinearity. The findings have implications for QMC fixed-node biases in systems with many elements including transition metals and others, which fall under the same electronic structure pattern. The finding has implications for both for accuracy of fixed-node energies, efficiency in elimination of the fixed-node bias and also for pseudopotential construction for very heavy elements. It has potential implications also for other correlated wave function approaches.

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