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Density dependence of fixed-node errors in quantum Monte Carlo: spin-polarized systems and triplet correlations[1] ADEM KULAHLIOGLU, KEVIN RASCH, SHUMING HU, LUBOS MITAS, North Carolina State University — We present an analysis focused on the fixed-node bias of trial wave functions for fully spin-polarized atomic systems. We benchmark the case of three electrons in the lowest state for a given symmetry which exhibits near-degeneracy effects similar to the in Be-like systems. The trial wave functions examined have been constructed at the HF level and at the pairing level in the form of a pfaffian. We find very significant fixed-node errors at the HF level, of the order of tens of percent. On the other hand, we observe that the pfaffian wave function correlated in the triplet pair channel enables us to get essentially exact results. We demonstrate that the key reason behind the large fixed-node erorr of the HF wavefunction is its artificial nodal domain topology. In addition, the fixed-node error is studied as a function of electron density by varying the atomic charge Z. We find that it scales linearly with Z what is very similar to our previous study on Be-like systems with similar dependence on density but pairing in the singlet channel.

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