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Fixed-phase vs fixed-node quantum Monte Carlo with local and nonlocal interactions LUBOS MITAS, CODY MELTON, North Carolina State Univ — We study several systems that can be formulated in the fixed-phase and/or fixed-node framework in quantum Monte Carlo calculations. In particular, we try to understand the differences between the biases caused by these approximations that result from using complex vs real trial wave functions. One system is a model that enables us to construct systematically the same type of nodal errors in both real and complex formalism. The errors are comparably similar whenever trial functions are correspondingly accurate. Another aspect of the fixed-phase vs fixed-node approximations is studied for systems with nonlocal operators such as with pseudopotentials and/or spin-orbit effects. We specify how to obtain variational formulation for complex wave functions and nonlocal operators in a manner analogous to the fixed-node calculations with T-moves algorithm. In particular, we show that the fixed-phase/fixed-node is the primary condition for proving that the upper bound property holds.

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