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Properties of wave functions/phases on nodal hypersurfaces in electronic structure quantum Monte Carlo LUBOS MITAS, CODY MELTON, M. CHANDLER BENNETT, North Carolina State University — Electronic structure quantum Monte Carlo (QMC) calculations often employ fixed-node/phase approximations to eliminate the well-known fermion sign problem(s). For real eigenstate the node is a zero locus of electron configurations in the position space, i.e., a codimension-1 hypersurface. We show several new properties of fermionic wave functions, in particular, for real eigenstates and for phases of stationary complex eigenstates on their corresponding nodal surfaces, as they apply for each eigenstate in the spectrum. In particular, for local potentials: a) generically, any spatial derivative of the eigenstate is itself an eigenstate on the node with the same eigenvalue; b) trace of the eigenstate gradient is itself an exact fermionic eigenstate on the node with the same eigenvalue. After some rearrangements related properties apply also to the eigenstate phases for inherently complex wave functions. Assuming continuity of eigenstates low-order derivatives almost everywhere, the node accuracy significantly impacts the wave function in general, supporting recent results on origins of fixed-node errors in QMC calculations. We further analyze the implications of these properties for accuracy of quantum Monte Carlo calculations and fixed-node/phase approximations.

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