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Geometry of fermion nodes and its impact on many-body effects in quantum Monte Carlo LUBOS MITAS, North Carolina State University — Fermion nodes, which are zero sets of stationary fermionic many-body wavefunctions, play an important role in quantum Monte Carlo calculations. In the diffusion Monte Carlo method the so-called fixed-node approximation allows us to avoid well-known inefficiencies of the fermion sign problem and to use the method for large systems. Besides this practical importance fermion nodes are also related to spectral properties of second order differential operators and to several physical effects and quantities. In order to understand these relationships we study fermion nodal hypersurfaces, both their topologies and shapes, as determined by wavefunctions built from different types of correlations such as pairing orbitals and backflow many-body coordinates. We analyze the impact of particle interactions on the changes of nodal topologies and the conditions under which such changes can occur. We investigate impact of nodal topologies on properties of wavefunctions with periodic boundary conditions as well as relationship of the nodal surfaces to kinetic energy and some other quantities. We further attempt to elucidate the nodal properties on examples of exactly solvable models.

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