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Nodes of fermionic wavefunctions: coordinate transformations and topologies LUBOS MITAS, MICHAL BAJDICH, GABRIEL DROBNY, LUCAS K. WAGNER, Center for High Performance Simulation and Department of Physics, North Carolina State University — We study fermion nodes for both spin-polarized and spin-unpolarized states of a few-electron ions and molecules with s, p, d one-particle orbitals. We find exact nodes for some cases of two electron atomic and molecular states and also the first exact node for the three-electron atomic system in ${}^4S(p^3)$ state using appropriate coordinate maps and wavefunction symmetries. We analyze the cases of nodes for larger number of electrons in the Hartree-Fock approximation and for some cases we find transformations for projecting the high-dimensional node manifolds into 3D space. The node topologies and other properties are studied using these projections. We also propose a general coordinate transformation as an extension of Feynman-Cohen backflow coordinates to both simplify the nodal description and as a new variational freedom for quantum Monte Carlo trial wavefunctions.

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