Quantum Monte Carlo: structure of many-body fermion nodes and spins as dynamical variables

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The node of a many-body stationary wave function is the set of particle configurations for which the wave function vanishes. More broadly, the node is a special case of the quantum phase. As such the node embodies the essence of "quantumness" such as antisymmetry, impact of correlations, nonlocalities and beyond. Knowledge of the node/phase allows to map calculations of quantum states onto equivalent statistical mechanical problems and solving it accordingly. In quantum Monte Carlo even approximate nodes enable us to carry out accurate calculations of many-body quantum states using fixed-node and fixed-phase methods. In this talk we first focus on fundamental properties on of the nodes such as nodal domain topologies and their properties. Second, we analyze the accuracy of the nodes of commonly used trial wave functions for a number of systems with main group elements. We find interesting trends in the fixed node errors which are related to the electronic occupations and bonding patterns with implications for practical calculations. We propose to explain these by the existence or nonexistence of homeomorphisms which map the nodes onto special cases of mean-field nodes. As the next step in the development of fixed-node approaches we will talk about our recent proogress in calculations of systems which require treating electronic spins as dynamical quantum variables. We will present results of calculations for heavy elements with Hamiltonians which explicitly include the spin-orbit operators.