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Triplet pairings and fermion wave functions nodal topologies LUBOS MITAS, MICHAL BAJDICH, SHUMING HU, North Carolina State University — Fixed-node quantum Monte Carlo methods rely on accurate fermion nodes of trial wave functions. Recently, we have shown that BCS wave functions possess for generic singlet ground states possess the correct minimal number of two nodal cells. This contrasts with the Hartree-Fock wave functions which exhibit higher counts of four or more nodal domains resulting in incorrect nodal topologies. We prove that for fully spin-polarized systems one can show the same effect. As a simple example, we consider the HF wave function for the lowest quartet of S symmetry and even parity for three electrons in a Coulomb potential. The wave function of this state ${}^4S(1s2s3s)$ has six nodal cells corresponding to $3!$ reordering of the radii. We show that pfaffian with triplet pairings is the simplest wave function which has the correct topology with two nodal cells. We further expand the study to some exactly solvable models to study the exact nodal structures dependence on potentials.

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