

Abstract Submitted
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Structure of fermion nodes and nodal cells for QMC wave functions¹ LUBOS MITAS, North Carolina State University — We study nodes of fermionic ground state wave functions. For $2D$ and higher we analytically prove that spin-polarized, noninteracting fermions in a harmonic well have two nodal cells for arbitrary system size. The result extends to other noninteracting/mean-field models such as fermions on a sphere, in a periodic box or in Hartree-Fock atomic states. Spin-unpolarized noninteracting states have multiple nodal cells, however, interactions and many-body correlations generally relax the multiple cells to the minimal number of two. This is again analytically proved, with some restrictions, for general interactions in $2D$ and higher-dimensional harmonic fermions of arbitrary size using the Bardeen-Cooper-Schrieffer variational wave function. We discuss implications and limits of the proofs for more complicated systems. The results offer an elegant and unifying framework for several previously conjectured or numerically investigated ideas and open exciting perspectives for studies of many-body effects which are beyond the usual fixed-node quantum Monte Carlo limits.

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