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Fixed-Node Correlation Function Diffusion Monte Carlo: an approach to Fermi excited states BRIAN AUSTIN, Department of Chemistry, University of California, Berkeley, California, WILLIAM LESTER, Department of Chemistry, University of California, Berkeley and Chemical Sciences Division, Lawrence Berkeley National Laboratory, LESTER GROUP TEAM — We have coupled the fixed-node (FN) approximation with the correlation function quantum Monte Carlo (CF-QMC) method to derive a more robust approach to computing properties of Fermi excited states. The FN constraint prevents the DMC simulation from converging to lower energy Bose states while the diagonalization step of the CF procedure orthogonalizes the FN-DMC solutions. Because the CF method wraps the FN-DMC wavefunctions with a linear variational procedure, the excitation energies will satisfy the Hylleras-Undeheim theorem. The FN-CF technique therefore improves upon FN-DMC energies for both ground- and excited-state energies. The new method is applied to nine low-energy states of the beryllium atom.

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