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Full Configuration Interaction Quantum Monte Carlo: The Use of Spin-pure and Non-Orthogonal Spaces SIMON SMART, NICK BLUNT, University of Cambridge, GEORGE BOOTH, Princeton University, ALI ALAVI, University of Cambridge — Full configuration interaction quantum Monte Carlo[1] (FCIQMC) allows for exact results to be obtained for the ground state within a finite-basis approximation of the Schrödinger equation. Working within imposed symmetry constraints permits dramatic reductions in the size of the Hilbert space considered, reducing the computational cost, as well as permitting exclusion of the natural ground-state to extract a series of excited states of the system. All converged solutions are eigenfunctions of $\hat{S}^2$ as well as the Hamiltonion and projected spin. Working within a spin-pure basis allows this property to be used in the same manner as other imposed symmetries. FCIQMC requires frequent calculation of Hamiltonian matrix elements between random pairs of basis functions. In order to make use of an efficient scheme[2] for calculating these matrix elements between spin-projected basis functions, FCIQMC has had to be extended to work in non-orthogonal (and optionally non- normalised) bases. This has consequences for our understanding of the nature of spawning and death within FCIQMC.

[1] G. H. Booth, A. Thom, and A. Alavi, J. Chem. Phys. 131 054106 (2009)
[2] F. E. Harris, J. Chem. Phys. 46, 2769 (1967)

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