Excited states and spectral functions within full configuration interaction quantum Monte Carlo GEORGE BOOTH, GARNET CHAN, Princeton University — Here we consider a modified propagator in order to obtain stable convergence to excited states within the full configuration interaction quantum Monte Carlo framework.[1] By working with a Gaussian propagator, the dominant eigenstate is one which is closest to an initial guess energy for the state. Issues with the speed of convergence compared to the ground state propagator are discussed, with results presented for pilot applications, and potential improvements for the algorithm considered.

[1]G. H. Booth and G. K.-L. Chan, ArXiv:1210.6643 (2012)

George Booth
Princeton University

Date submitted: 28 Nov 2012   Electronic form version 1.4