Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Release-Node quantum Monte Carlo studies for molecules[1] NORM TUBMAN, Northwestern University, JONATHAN DUBOIS, RANDOLPH HOOD, BERNI ALDER, Lawrence Livermore National Lab — Release-Node quantum Monte Carlo (RN-QMC) is a method that calculates unbiased ground-state energies of fermionic systems. However, while RN-QMC has been successfully applied to the homogeneous electron gas with more than one hundred electrons, obtaining converged results for molecular systems has proven to be problematic for all but the smallest systems. A promising route to extending the method's success to a wider class of physically interesting Hamiltonians lies in the application of projection techniques such as Maximum Entropy (MaxEnt) which, in principle, allows for extrapolation to the converged ground-state energy. Direct application of MaxEnt to higher Z elements is, however, not entirely straightforward. We propose strategies for optimizing MaxEnt analysis of short time RN-QMC data and demonstrate their effectiveness in obtaining ground state energies for the first row dimers. Attention is given to the determination of statistical errors in the resulting extrapolations as well as an attempt to characterize the minimum decay time required for unbiased results.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344

Norm Tubman
Northwestern University

Date submitted: 19 Nov 2010 Electronic form version 1.4