Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

A diffusion Monte Carlo study of sign problems from non-local pseudopotentials NORM TUBMAN, University of Illinois at Urbana-Champaign, MIGUEL MORALES-SILVA, JONATHAN DUBOIS, RANDOLPH HOOD, Lawrence Livermore National Lab — Difficulties can arise in simulating various Hamiltonian operators efficiently in diffusion Monte Carlo (DMC) such as those associated with non-local pseudopotentials which require the introduction of an approximate form. The locality approximation and T-moves are two widely used techniques in fixed-node diffusion Monte Carlo (FN-DMC) that provide a tractable approach for treating non-local pseudopotentials, however their use introduces an uncontrolled approximation. Exact treatment of the non-local pseudopotentials in FN-DMC introduces a sign problem with the associated Green's function matrix elements which take on both positive and negative values. Here we present an analysis of the nature of the sign problem that non-local operators introduce into the Green's function. We then consider the feasibility of running DMC simulations in which the non-local pseudopotentials are treated exactly and demonstrate the algorithm on a few molecular systems.

Norm Tubman
University of Illinois at Urbana-Champaign

Date submitted: 13 Dec 2011 Electronic form version 1.4