Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Systematic improvement of trial wavefunctions for Constrained Path Quantum Monte Carlo[1] R. TORSTEN CLAY, Mississippi State University — Constrained Path Monte Carlo (CPMC) provides an approximate solution to the Fermion sign problem for lattice models such as the Hubbard model. In the zero-temperature CPMC algorithm, a trial wavefunction is used to eliminate random walkers when their overlap with the trial function becomes zero. CPMC often produces surprisingly good results for ground state energy and correlation functions, even when a simple trial function is used. However, there is no reason to expect that simple wavefunctions (free electron or Hartree Fock) will have any overlap with complex correlated ground states. We therefore describe a method to improve CPMC results by optimizing the trial wavefunction. The trial function we use is a sum of Slater determinants that is optimized by the Path Integral Renormalization Group (PIRG) procedure. The wavefunction produced by PIRG is a sum of L determinants, with an energy that is variational. We show CPMC+PIRG data for a system where CPMC with a free electron trial function fails, the Hubbard model on an anisotropic triangular lattice.

[1]Supported by the American Chemical Society (Petroleum Research Fund) and DOE

R. Torsten Clay
Mississippi State University

Date submitted: 17 Nov 2006 Electronic form version 1.4