Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Compact and Flexible Basis Functions for Quantum Monte Carlo Calculations[1] FRANK PETRUZIELO, Laboratory of Atomic and Solid State Physics, Cornell University, JULIEN TOULOUSE, Laboratoire de Chimie Theorique - UMR 7616, Universite Pierre et Marie Curie, CYRUS UMRIGAR, Laboratory of Atomic and Solid State Physics, Cornell University — Molecular calculations in quantum Monte Carlo frequently employ a mixed basis consisting of contracted and primitive Gaussian functions. While standard basis sets of varying size and accuracy are available in the literature, we demonstrate that reoptimizing the primitive function exponents within quantum Monte Carlo yields more compact basis sets for a given accuracy. Particularly large gains are achieved for highly excited states. For calculations requiring non-diverging pseudopotentials, we introduce Gauss-Slater basis functions that behave as Gaussians at short distances and Slaters at long distances. These basis functions further improve the energy and fluctuations of the local energy for a given basis size. Gains achieved by exponent optimization and Gauss-Slater basis use are exemplified by variational Monte Carlo calculations for the ground state of carbon, the lowest lying excited states of carbon with ${}^5S^o$, ${}^3P^o$, ${}^1D^o$, ${}^3F^o$ symmetries, and carbon dimer. Basis size reduction enables quantum Monte Carlo treatment of larger molecules at high accuracy.

[1]This work was supported by the NSF.

Frank Petruzielo
Laboratory of Atomic and Solid State Physics, Cornell University

Date submitted: 17 Nov 2009 Electronic form version 1.4