Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Generalized pairing wave functions in electronic structure quantum Monte Carlo MICHAL BAJDICH, LUBOS MITAS, Center for High Performance Simulation, Department of Physics, North Carolina State University, Raleigh, NC 27695, KEVIN E. SCHMIDT, Department of Physics, Arizona State University, Tempe, AZ 85287 — We investigate several types of trial wave functions with pairing orbitals in fixed-node quantum Monte Carlo. Following upon our previous study[1], we explore the possibilities of expanding the wave function in linear combinations of pfaffians. We observe that molecular systems require much larger expansions than atomic systems and linear combinations of a few pfaffians lead to rather small gains in correlation energy. Further, we test the wave function based on fully-antisymmetrized product of independent pair orbitals. Despite its seemingly large variational potential, we do not observe significant gains in correlation energy. Finally, we combine these developments with the recently proposed inhomogeneous backflow transformations[2]. The trade-offs between computational efficiency and amounts correlation energy recovered will be discussed.
[1] M. Bajdich et al. Phys. Rev. Lett. 96, 130201 (2006).
[2] N. D. Drummond et. al., J. Chem. Phys. 124, 224104 (2006).

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Date submitted: 22 Nov 2006 Electronic form version 1.4