

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Comparison of energy minimization and variance minimization methods for optimizing variational parameters in many body wave functions¹ C.J. UMRIGAR, Theory Center and LASSP, Cornell University, CLAUDIA FILIPPI, Instituut Lorentz, Universiteit Leiden — The variance minimization method has become the standard method for optimizing many body wave functions for quantum Monte Carlo because it is far more efficient than performing a straightforward energy minimization. We have modified two recent energy minimization methods to make energy minimization highly efficient. First, we have modified the straightforward Newton method used by Lin, Zhang and Rappe, *J. Chem. Phys.* **112**, 2659 (2000) to reduce the statistical fluctuations by more than two orders of magnitude. Tests on a flexible Jastrow that includes 3-body electron-electron-nucleus correlation terms show that it is very efficient. Second, we have extended the generalized eigenvalue method of Nightingale and Melik-Alaverdian *Phys. Rev. Lett.* **87**, 043401 (2001), for linear parameters, to nonlinear parameters, and are currently testing this method.

¹CJU gratefully acknowledges valuable discussions with Peter Nightingale. Supported by NSF, Sandia, NASA and FOM, Netherlands

Cyrus Umrigar
Cornell University

Date submitted: 22 Dec 2004

Electronic form version 1.4