Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Geometry optimization using Quantum Monte Carlo[1] LUCAS WAGNER, JEFFREY GROSSMAN, Massachusetts Institute of Technology — One of the long-lasting challenges in Quantum Monte Carlo (QMC) has been to find minimum energy structures efficiently, particularly for the projector Monte Carlo methods. The primary obstacles to this goal are the difficulty of calculating efficient and accurate gradients of the energy and the inherent stochastic nature of the algorithm, which is shared with many other interesting solution methods. We are particularly interested in the case of electronic structures of realistic systems, where for many interesting systems such as excited states, weak-binding, and transition metal oxides, the traditional methods based on DFT are not acceptably accurate. We present an algorithm that is well behaved in the presence of known noise and finds the minimum energy structure quickly. The Hessian matrix at the minimum is calculated simultaneously, and gradient information, if available, is easily and consistently included.

[1]Supported by DOE Grant #DE-SC0002623.

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Date submitted: 27 Nov 2009 Electronic form version 1.4