

Abstract Submitted  
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**Simple geometry optimization with Variational Quantum Monte Carlo method** DAN NISSENBAUM, B. BARBIELLINI, A. BANSIL, Northeastern U. — Stochastic optimization methods may be combined with Quantum Monte Carlo (QMC) integration to obtain a computational scheme for treating many body wavefunctions suitable for addressing modern problems in nanoscale physics. In this connection, we are investigating the range of applicability of the Stochastic Gradient Approximation (SGA) technique [1]. The SGA possesses the important advantage that the updating of the electronic variational parameters and the nuclear coordinates can be carried out simultaneously and without an explicit determination of the total energy for each geometry. We present illustrative results using simple variational functions for describing the hydrogen molecule, the lithium dimer, and the neutral and charged  $\text{Li}_4$  clusters. We computed highly accurate potential energy surfaces on a fine grid in order to test the efficacy of the SGA in locating the energy minima in the parameter space. Work supported in part by the USDOE.

[1] A. Harju, B. Barbiellini, S. Siljamäki, R.M. Nieminen, and G. Ortiz, Phys. Rev. Lett. **79**, 1173 (1997).

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