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Convergence of the variational parameter without convergence of the energy in Quantum Monte Carlo (QMC) calculations using the Stochastic Gradient Approximation DANIEL NISSENBAUM, HSIN LIN, BERNARDO BARBIELLINI, ARUN BANSIL, Northeastern U. — To study the performance of the Stochastic Gradient Approximation (SGA) for variational Quantum Monte Carlo methods, we have considered lithium nano-clusters [1] described by Hartree-Fock wavefunctions multiplied by two-body Jastrow factors with a single variational parameter b. Even when the system size increases, we have shown the feasibility of obtaining an accurate value of b that minimizes the energy without an explicit calculation of the energy itself. The present SGA algorithm is so efficient because an analytic gradient formula is used and because the statistical noise in the gradient is smaller than in the energy [2]. Interestingly, in this scheme the absolute value of the gradient is less important than the sign of the gradient. Work supported in part by U.S. DOE.
[1] D. Nissenbaum *et al.*, Phys. Rev. B **76**, 033412 (2007).
[2] A. Harju, J. Low. Temp. Phys. **140**, 181 (2005).

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