Variational Quantum Monte Carlo Methods for Accurate Energetics

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Abstract:

Quantum Monte Carlo (QMC) is a recent alternative for accurately computing the properties of highly correlated molecular systems. QMcBeaver, a new software package, performs Variational QMC (VMC) calculations on molecular systems. VMC improves a standard QM wavefunction by incorporating explicit two-body interactions. Current work is aimed at developing robust methods to variationally optimize the parameters describing these two-body interactions.
Figure: A Variational Quantum Monte Carlo (VMC) energy calculation of helium performed with and without a Jastrow function. With no Jastrow function, the VMC calculation reproduces the energy of the STO-3G, Hartree-Fock trial-wavefunction used in the calculation. With a two-parameter Jastrow function, a large portion of the correlation energy is obtained.

Acknowledgments: Acknowledgment is made to the ASCI program for support of this research. D. R. K. and M. T. F. are grateful for support of this research by graduate fellowships from the Fannie and John Hertz Foundation and Department of Energy Computational Science Graduate Fellowship Program respectively.