Title: Optimizing quantum simulations and the DMRG method

Author: Jan Brandejs

Department: Department of Chemical Physics and Optics

Supervisor: doc. Dr. rer. nat. Jiří Pittner, DSc., J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences

Abstract: In this work, we explore the quantum information theoretical aspects of simulation of quantum systems on classical computers, in particular the many-electron strongly correlated wave functions. We describe a way how to reduce the amount of data required for storing the wavefunction by a lossy compression of quantum information. For this purpose, we describe the measures of quantum entanglement for the density matrix renormalization group method. We implement the computation of multi-site generalization of mutual information within the DMRG method and investigate entanglement patterns of strongly correlated chemical systems. We present several ways how to optimize the ground state calculation in the DMRG method. The theoretical conclusions are supported by numerical simulations of the diborane molecule, exhibiting chemically interesting electronic structure, like the 3-centered 2-electron bonds. In the theoretical part, we give a brief introduction to the principles of the DMRG method. Then we explain the quantum informational motivation behind our quantum chemical calculations and present the results of our computation.

Keywords: quantum simulation density matrix renormalization group quantum entanglement quantum information quantum chemistry