UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

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New Density Matrix Renormalization Group-based Methods for Molecular Simulations

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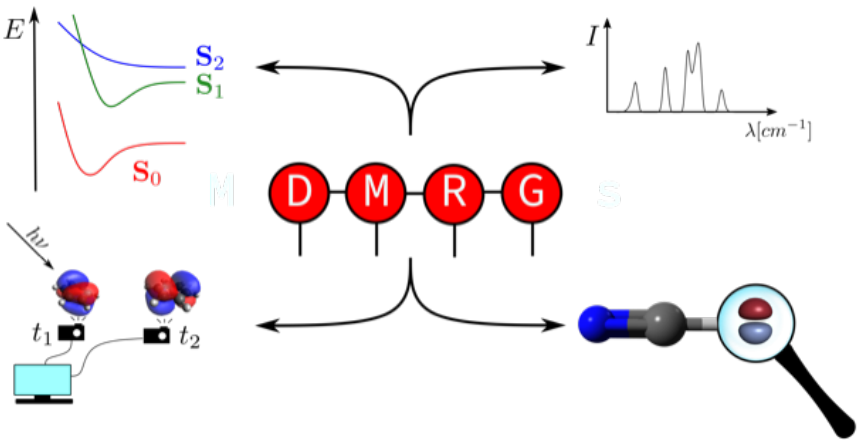

The full configuration interaction (full CI) is the primary method for simulating exactly molecular processes. However, its high computational cost, which grows exponentially with the system size, renders molecular simulations extremely impractical, if not for very small molecules. This prohibitive scaling can be tamed with tensor-based compression schemes, such as the density matrix renormalization group (DMRG).[1] Although DMRG has been mostly applied to electronic problems, in this talk we will describe how it can be applied to three new classes of molecular simulations.[1] We will first introduce DMRG-based algorithms for simulating vibrations spectra both within[2–5] and beyond[6,7] the Born-Oppenheimer approximation. Then, we will exploit the DMRG to solve exactly the time-dependent Schrödinger equation and simulate non-equilibrium phenomena in complex molecular systems.[8,9] Finally, we will introduce an explicitly-correlated DMRG variant that relies on the transcorrelated approach.[10,11]
In the last part of the talk, we will introduce a quantum computing method to solve the vibrational full CI problem on noisy intermediate-scale quantum computers[12] and identify the hardware requirement to observe a quantum advantage over DMRG-based methods.

[1] Baiardi, A.; Reiher, M. The density matrix renormalization group in chemistry and molecular physics: Recent developments and new challenges. *J. Chem. Phys.* **2020**, 152, 040903.
[2] Baiardi, A.; Stein, C. J.; Barone, V.; Reiher, M. Vibrational Density Matrix Renormalization Group. *J. Chem. Theory Comput.* **2017**, 13, 3764–3777.
[3] Baiardi, A.; Stein, C. J.; Barone, V.; Reiher, M. Optimization of highly excited matrix product states with an application to vibrational spectroscopy. *J. Chem. Phys.* **2019**, 150, 094113.
[4] Glaser, N.; Baiardi, A.; Reiher, M. Tensor Network States for Vibrational Spectroscopy. *ArXiv e-prints* **2021**, 2109.08961.
[5] Baiardi, A.; Kelemen, A. K.; Reiher, M. Excited-state DMRG made simple with FEAST. *J. Chem. Theory Comput.* **2021**, 18, 430.
[6] Muolo, A.; Baiardi, A.; Feldmann, R.; Reiher, M. Nuclear-electronic all-particle density matrix renormalization group. *J. Chem. Phys.* **2020**, 152, 204103.
[7] Feldmann, R.; Muolo, A.; Baiardi, A.; Reiher, M. Quantum Proton Effects from Density Matrix Renormalization Group Calculations. *J. Chem. Theory Comput.* **2022**, 18, 250.
[8] Baiardi, A.; Reiher, M. Large-scale quantum-dynamics with matrix product states. *J. Chem. Theory Comput.* **2019**, 15, 3481–3498.
[9] Baiardi, A. Electron Dynamics with the Time-Dependent Density Matrix Renormalization Group. *J. Chem. Theory Comput.* **2021**, 17, 3320–3334.
[10] Baiardi, A.; Reiher, M. Transcorrelated density matrix renormalization group. *J. Chem. Phys.* **2020**, 153, 164115.
[11] Baiardi, A.; Lesiuk, M.; Reiher, M. Explicitly correlated electronic structure calculations
with transcorrelated matrix product operators. *ArXiv e-prints* **2022**, 2202.08709
[12] Ollitrault, P. J.; Baiardi, A.; Reiher, M.; Tavernelli, I. Hardware efficient quantum algorithms for vibrational structure calculations. *Chem. Sci.* **2020**, 11, 6842–6855.