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Quantum correlations in hydrogen bonded dimers. Insights from extended VQE calculations via matrix product states powered quantum computer emulator.

Hydrogen-bonded systems play a crucial role in chemistry, biology, and material sciences, underpinning key processes such as protein folding, molecular recognition, and drug binding. Accurately modeling these non-covalent interactions remains a major challenge as they require a precise description of electron correlation effects. Quantum computing has the potential to improve the study of such interactions by providing more efficient and scalable solutions compared to classical approaches. However, the capabilities of the contemporary quantum hardware/algorithms leave these problems largely unexplored.

In fact, quantum computing is currently in the noisy intermediate-scale quantum (NISQ) era, where a significant effort is being devoted to identifying applications that can achieve "quantum utility" before fault tolerance. In this context, the Variational Quantum Eigensolver (VQE)[1] is one of the most widely explored algorithm classes for solving electronic structure problems in quantum chemistry and condensed matter, showing significant promise. However, challenges such as vanishing gradients, the scaling of variational parameters, and the optimization complexity of VQE circuits remain open questions, limiting for now the size of the systems that can be simulated with this algorithm and directly impacting its practical utility.

In this work, we will leverage a highly parallelizable, Matrix Product State (MPS)-based quantum computer emulator (Quantum Matcha Tea)[2] to conduct extended VQE simulations on molecular systems such as H_2O, and HF and their hydrogen-bonded dimers, systematically analyzing both algorithmic performances and the systems quantum correlations properties.

Specifically, we will explore the effects of different adaptive VQE approximations and approaches on convergence performances. These will include the standard ADAPT-VQE[3], Tetris-ADAPT-VQE[4] and mutual information-assisted ADAPT-VQE[5]. By assessing the scaling of gradient evaluations, variational parameters, circuit depth, and entanglement production under different conditions of system size, geometry, and electron correlation, we aim to characterize the computational viability, precision, cost and efficiency of these methods.

Beyond algorithmic optimization, our study will provide a quantum information-theoretic perspective on the entanglement/quantum correlation properties of these molecular systems, particularly in the context of hydrogen bonding. By tracking the entanglement evolution/production during the VQE optimizations, we will examine how quantum correlation between molecular fragments is encoded in quantum circuits and explore the entanglement requirements (i.e. MPS bond dimension) for accurately capturing hydrogen-bonded interactions. These results will be placed in a broader context by comparing them with the total, quantum and classical correlation calculated using "high-level"(i.e. CASSCF) classical algorithms for the same molecular systems

These simulations will represent one of the first investigations of non-covalent interactions using NISQ-era algorithms, generating valuable insights into the role of quantum correlation in hydrogen-bonded molecular interactions.

References:

[1]J. Tilly, H. Chen, S. Cao et al., Physics Reports 986, 1–128. (2022)
[2]Ballarin, M. "Quantum Computer Simulation via Tensor Networks." Mater Thesis. (2021)
[3]Grimsley, H. R., Economou, S. E., Barnes, E., & Mayhall, N. J. Nature communications, 10(1), 3007. (2019)
[4]P.G. Anastasiou, Y. Chen, N. J. Mayhall, E. Barnes, and S. E. Economou. Phys. Rev. Research 6, 013254 (2024)
[5]Z.J. Zhang , T. H. Kyaw, J. S. Kottmann, M. Degroote and A. Aspuru-Guzik, Quantum Sci. Technol. 6, 035001. (2021)

Theme

Theme 3. Theoretical and experimental methods for quantum effects in energy processes

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