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Exploring quantum correlations in non-covalent bonded dimers: A mutual information approach using extended VQE simulations with MPS-emulator

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Non-covalent interactions (i.e. dispersions, hydrogen-bonding, polarization) are fundamental molecular interactions with key implications for the fields of chemistry, biology, and materials science. A precise understanding of these forces requires an accurate treatment of electron correlation effects, which remains a challenge for classical computational methods. Quantum computing offers a promising alternative, yet current noisy intermediate-scale quantum (NISQ) devices and algorithms face significant limitations.

In this study, we employ a highly parallelizable Matrix Product State (MPS)-based quantum computer emulator (QuantumMatchaTea[1]) to systematically investigate quantum correlations in Non-Covalent bonded dimers (e.g., He₂, (H₂)₂, (H₂O)₂ and (HF)₂). Our approach extends the capabilities of the Adaptive Variational Quantum Eigensolver 2 algorithm, enabling an on-the-run characterization of the quantum correlations in the simulated molecular systems. By computing the evolution of orbital entanglement and mutual information during the VQE optimization, we introduce a modified adaptive scheme. This strategy dynamically identifies the most relevant excitations and optimizes their parameters while accounting for the quantum correlations they generate. We then quantify how these correlations are encoded and distributed within the quantum circuit and relate them to the orbital representation of the Non-Covalent bonded molecules.

To contextualize our findings, we compare the Mutual Information extracted from our VQE simulations with similar results from high-level classical methods (e.g., CASSCF). This allows for a direct comparison between the two theoretical descriptions of the of Non-Covalent interactions and let us evaluate the different contributions that distinguish quantum from classical algorithms.

Our study provides one of the first systematic analyses of noncovalent interactions using NISQ-era quantum algorithms. By relating entanglement and mutual information to molecular interactions, we shed new light on the role of quantum correlations in noncovalent binding and extend the reach of quantum computing in electronic structure theory.

[1] Ballarin, Marco. "Quantum Computer Simulation via Tensor Networks." Mater Thesis. (2021).

[2] Grimsley, H. R., Economou, S. E., Barnes, E., & Mayhall, N. J. (2019). Nature communications, 10(1), 3007

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