

abstract

The individual optimization of quantum circuit parameters remains one of the main practical bottlenecks in variational quantum eigensolver (VQE) calculations for electronic structure problems. To address this challenge, several machine learning approaches have been proposed. However, most existing methods focus on learning parameters tailored to individual molecules, either for a single molecular structure or for different geometries of the same molecule.

In this work, we investigate machine learning strategies that enable the transfer of optimized quantum circuit parameters across different molecular systems. Using a well-established quantum circuit ansatz, we demonstrate systematic parameter transferability between chemically distinct molecules, including predictions for molecular systems significantly larger than those used during training. These results were published in [1].

Building on this work, we further exploit the predictable behavior of hydrogenic systems for Separable Pair ansätze. Specifically, we investigate the transfer of variational parameters learned from hydrogenic systems to chemically distinct, non-hydrogenic systems. Preliminary results indicate that this approach further improves

transferability, although these findings have not yet been published.

One example for this would be the projection of Methane C-H connections onto a sphere with hydrogens living on the surface, which can be seen in following Figure.

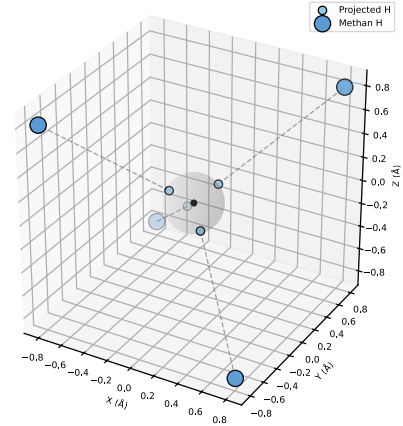


FIG. 5: Projecting Hydrogen Molecules on sphere with radius r at the Carbon position (black dot) mimicing Methane with H_8 .

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- [1] D. Bincoletto, K. Stein, J. Motyl, and J. S. Kottmann, transferable machine learning approach to predict quantum circuit parameters for electronic structure problems,

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