

Strategies for computing electronic structure of molecules on quantum computers

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In this talk, I will review work recently completed on how to use the factorized form of the unitary coupled cluster ansatz as an efficient way to perform electronic structure calculations via the variational quantum eigensolver and its variants. I will describe the universal nature of the factorized form and how the variational principle improves accuracies more than expected from simple error bounds. I will discuss how this quantum computer ansatz compares with the conventional coupled cluster ansatz and I will discuss how one can trade off measurements for circuit depth to perform calculations on molecules that use very low-depth circuits. I will also describe how one can improve the circuit depth for higher-rank factors by incorporating additional ancilla. I will end with some prospects for the near term in how quantum chemistry calculations are likely to perform.