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Simulating the energy landscape of dihydrogen via a superconducting quantum computer

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Introduction

Quantum computing has recently gained traction as a powerful means of simulating molecular phenomena. However, presently near-term devices are unable to implement fault-sensitive algorithms without significant loss in accuracy. Thus, this study aims to explore the variational quantum eigensolver (VQE) algorithm in simulating the energy landscape of dihydrogen, paving the way towards simulating more complex molecules.

Methodology

Starting from the fermionic Hamiltonian $\hat{H}_e$, the VQE algorithm aims to approximate the ground state energy E_0 (**Fig. 1**):

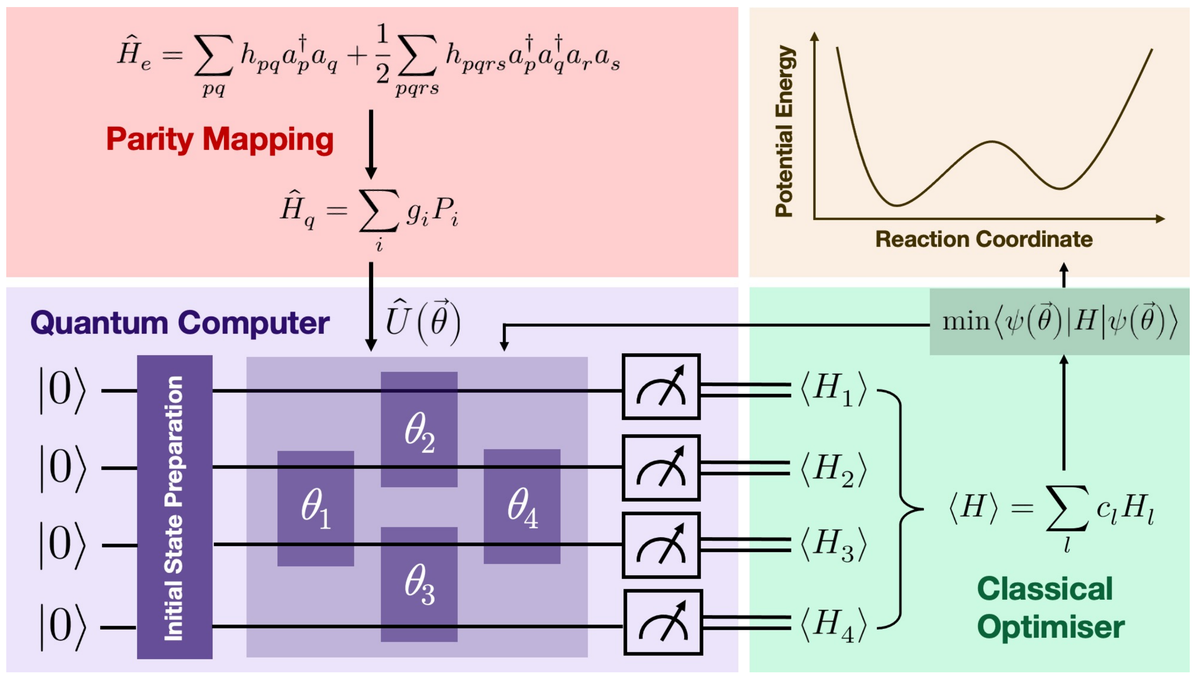


Fig. 1. Overview of the VQE algorithm implemented in this study.

A chemically inspired ansatz approximating $\hat{U}(\vec{\theta})$ is the unified coupled cluster (UCC) (**Fig. 2, 3**):

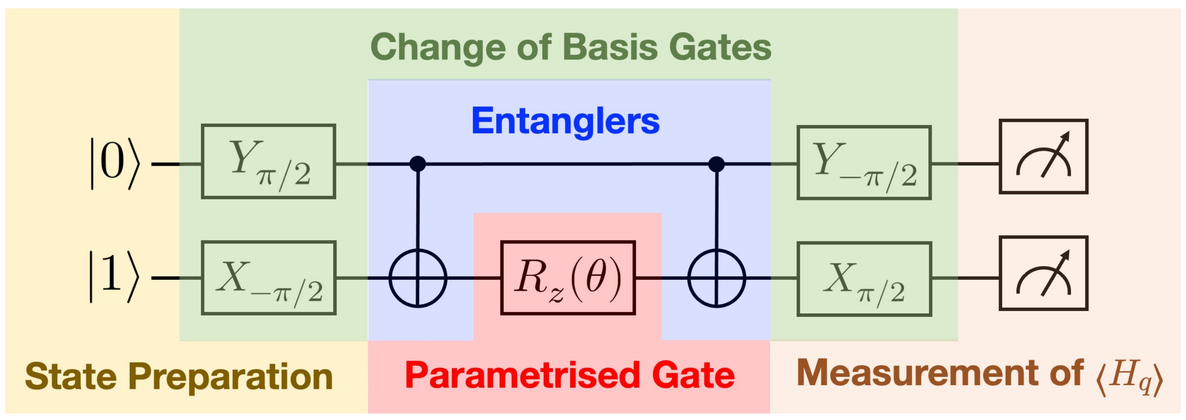


Fig. 2. Quantum circuit of the VQE algorithm using the UCC ansatz.

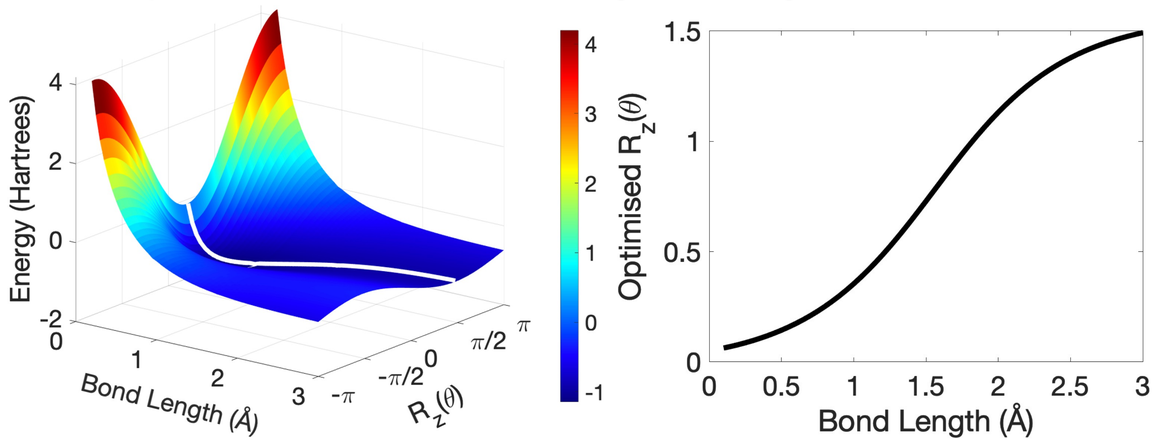
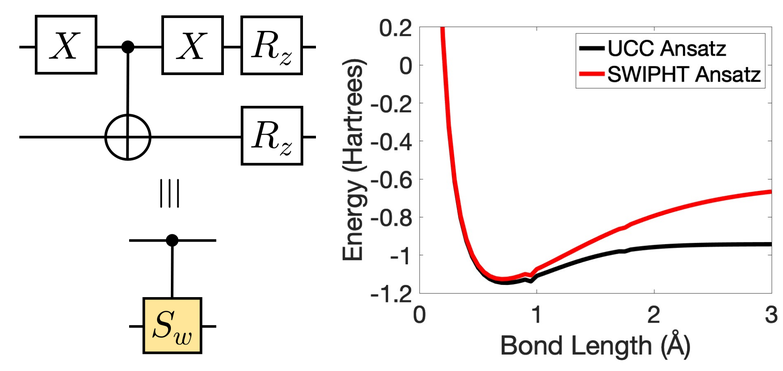


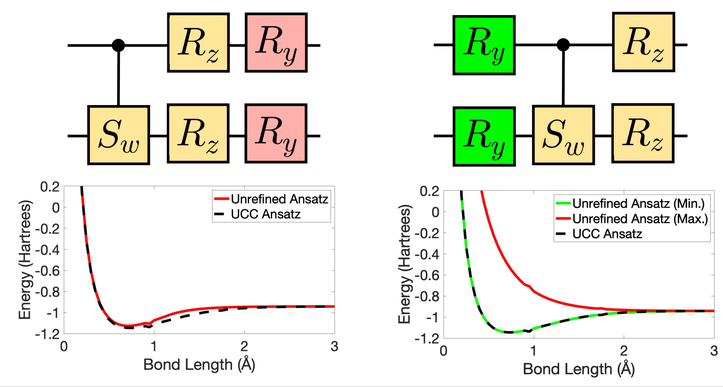
Fig. 3. (left) Contour plot of energy landscape of dihydrogen, with the white path depicting the minimum energy. **(right)** Plot of VQE-optimised θ against bond length.

Although the UCC ansatz preserves the chemical intuition and molecular symmetries from classical coupled cluster methods, it is computationally more expensive and hence more subject to various noise inputs. Hence, a hardware-efficient ansatz based on the entangling SWIPHT (S_w) gate was sought after (**Fig. 4**):

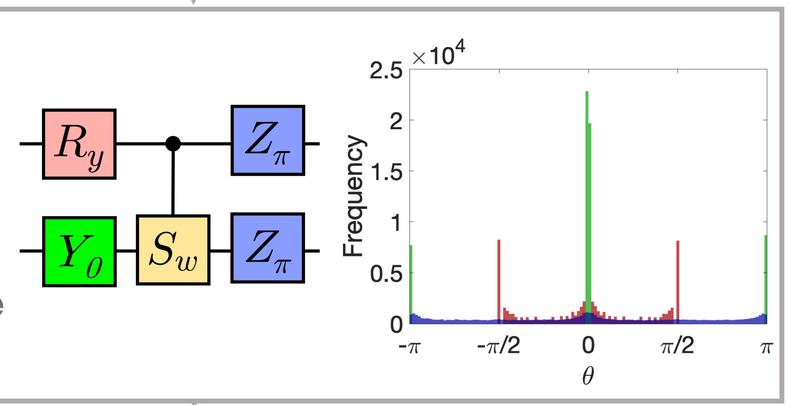
Initialise base entangling gates, compare with UCC ansatz
⇒ **Energy diverges from 0.45 Å onwards**



Grow circuit by adding adjacent rotation gates in order to access more states in the full Hilbert space



Parametrise all rotation gates, perform Monte Carlo-VQE and reduce parameters by considering gate correlations



Perform noisy simulations with Pauli channels and compare between ansätze

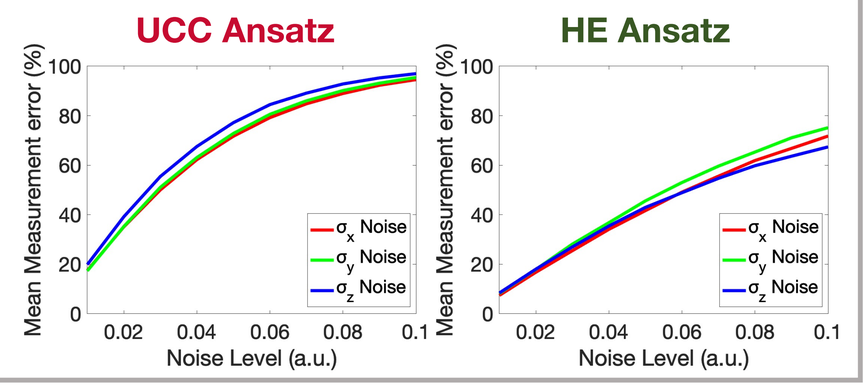


Fig. 4. Process in designing a hardware-efficient ansatz.

Conclusion

The hardware-efficient ansatz provides similar accuracy to the UCC ansatz whilst enjoying the advantage of lower computation time and gate complexity, thus it is predicted to be more resistant to noise inputs. Both of these ansätze will be simulated on a real-world quantum computer for future studies.