

Error Mitigating Quantum Computations of Molecular Ground States

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Abstract

Quantum Computers have the potential to solve chemistry problems of great industrial importance but near term devices are susceptible to errors. Thus, error mitigation techniques like Richardson Extrapolation are being explored to reduce the effect of errors. **In this project, we compare the Richardson method with a simpler polynomial-fitting method to determine the zero noise ground state energy of the hydrogen molecule.** Results and implications are discussed.

Background

- Quantum Computers use quantum mechanical properties such as superposition and entanglement to perform computations.
- Recently, a hybrid quantum-classical algorithm – Variational Quantum Eigensolver (VQE) – has been devised which optimizes electrons in molecular orbitals to minimize the energy of molecular systems.
- However quantum computers are plagued with errors due to hardware deficiencies like imperfect qubits and quantum gates.
- Constrained by the number of qubits, error mitigation techniques are being explored to reduce the effects of errors.

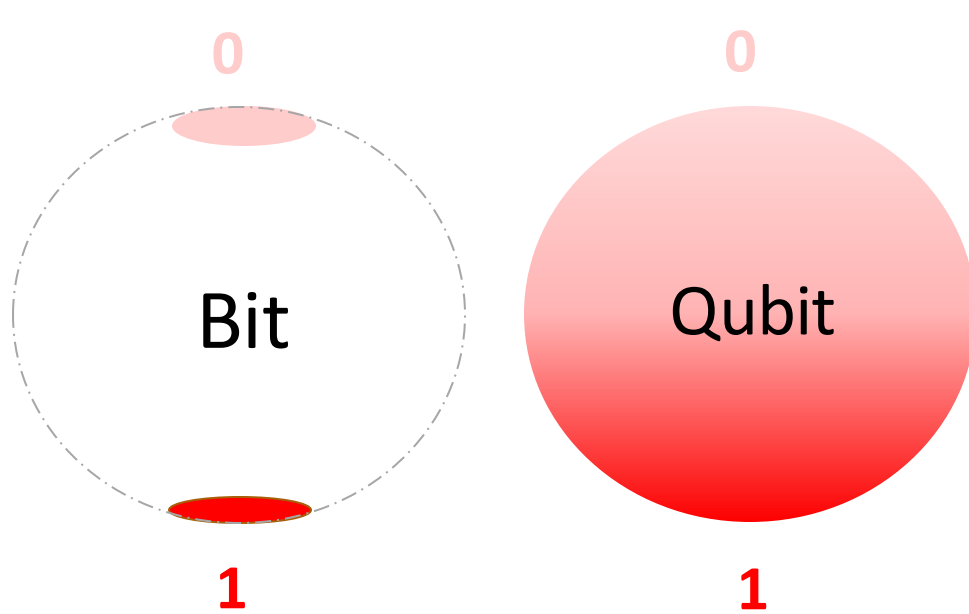


Fig 1: Comparing the space of states of classical bits with that of qubits.

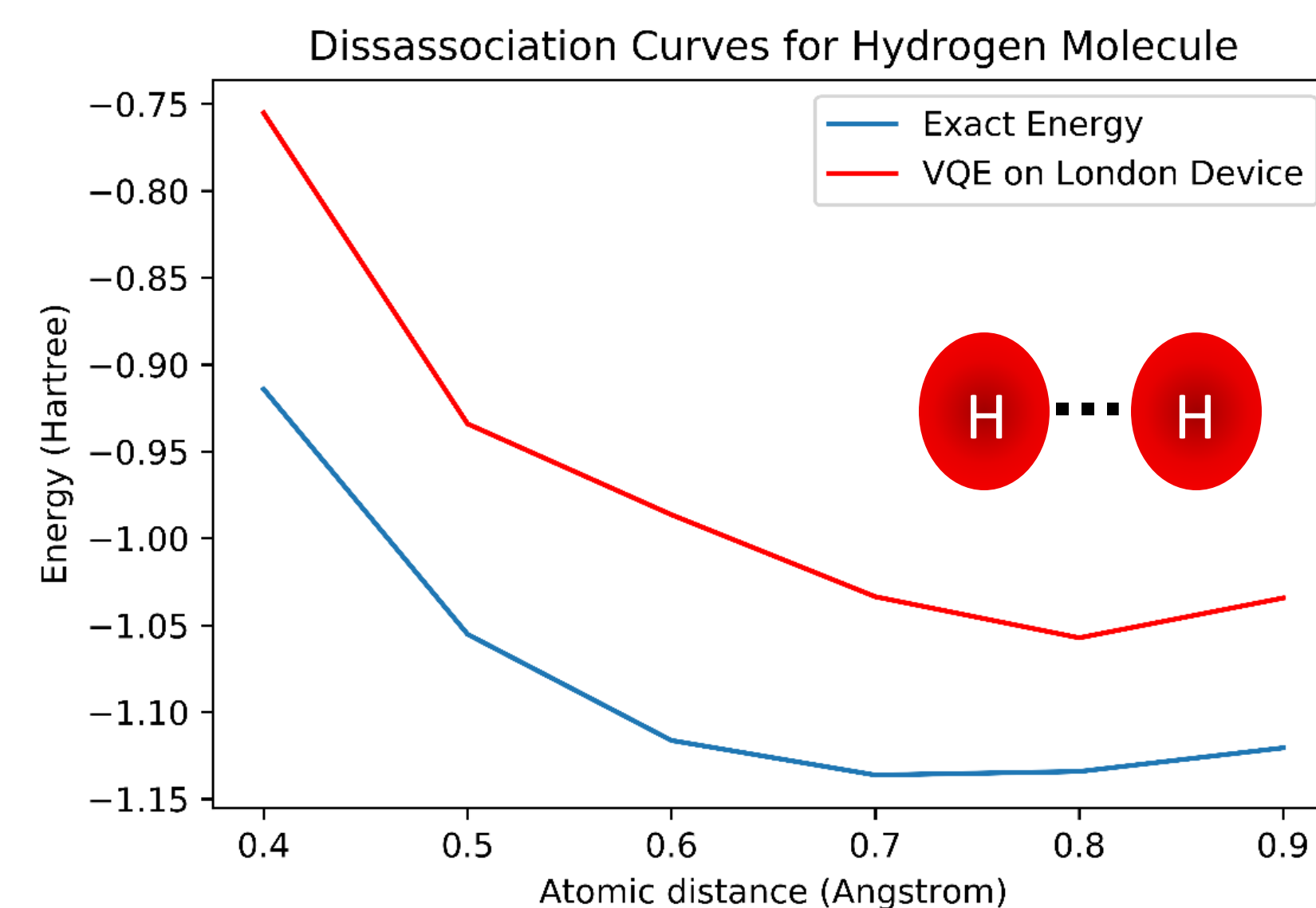


Fig 2: As we stretch 2 hydrogen atoms apart, we compute the minimum energy of the molecule using VQE on IBM's noisy quantum computer at London and compare it with the exact energy.

Error Mitigation Techniques

Richardson Extrapolation

- Noisy expectation value of any observable can be expressed as $E(\lambda) = E^* + a_1\lambda + a_2\lambda^2 + a_3\lambda^3 + \dots$ where λ is the noise rate and E^* is the noise free expectation value.
- By cancelling out terms from the expansion, we can better our approximation.
- For such cancellation, we need to obtain noise amplified energies as shown in Fig 4a.

Polynomial Extrapolation

- Given energies at various noise scaling factors, we can fit polynomial function using nonlinear least squares as shown in Fig 4b.
- Evaluating these functions at zero noise, we can extrapolate noise free energy.

Results

Fig 4: Using noise model simulation of IBM's quantum computer at London, we compare Richardson technique with polynomial fitting technique in improving the VQE-computed ground state energy of the Hydrogen molecule. Noise was amplified while optimizing in the VQE process.

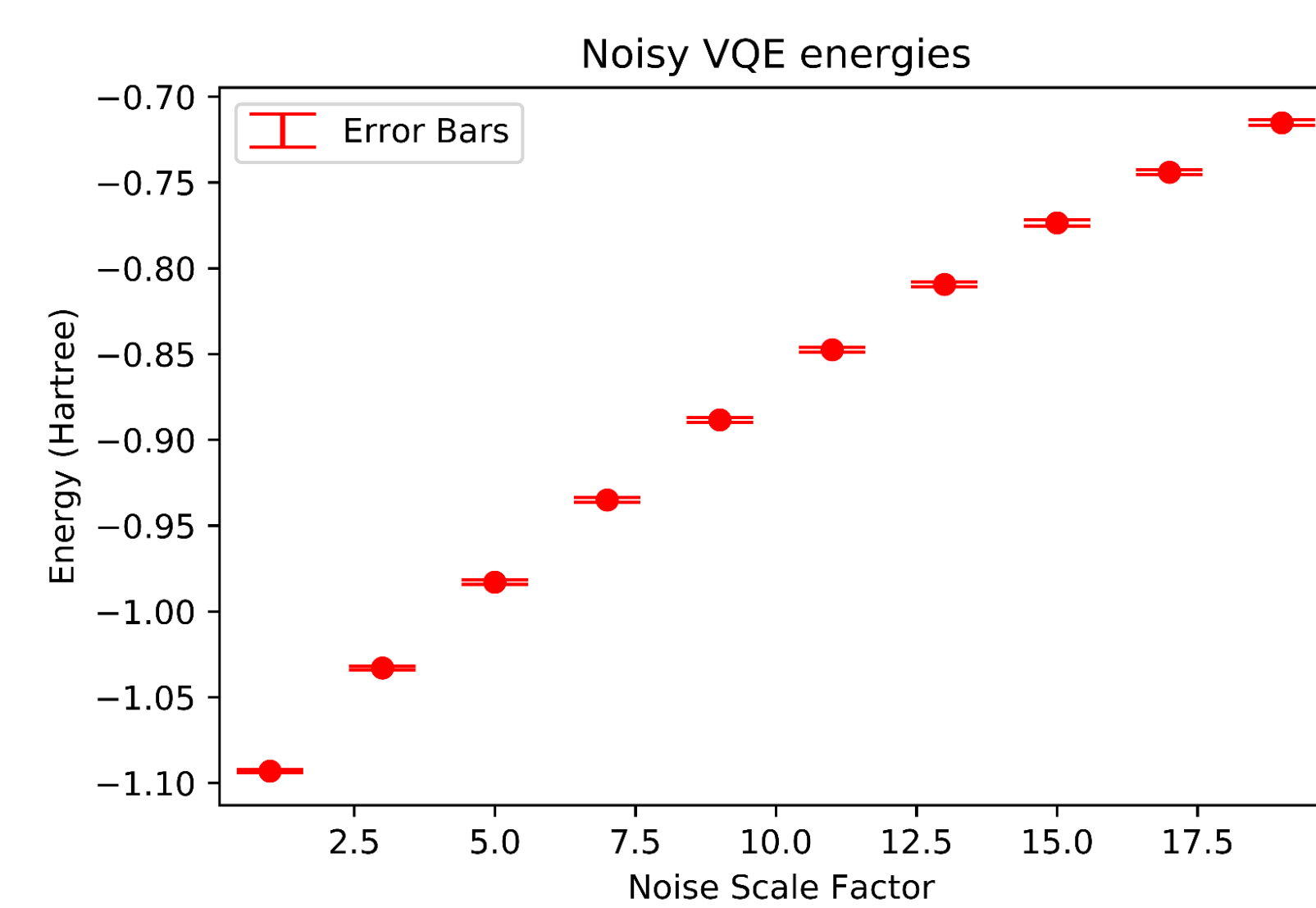


Fig 4a: As the noise is increased the deviation of the calculate ground state energy from the exact value (1.137 Hartree) increases.

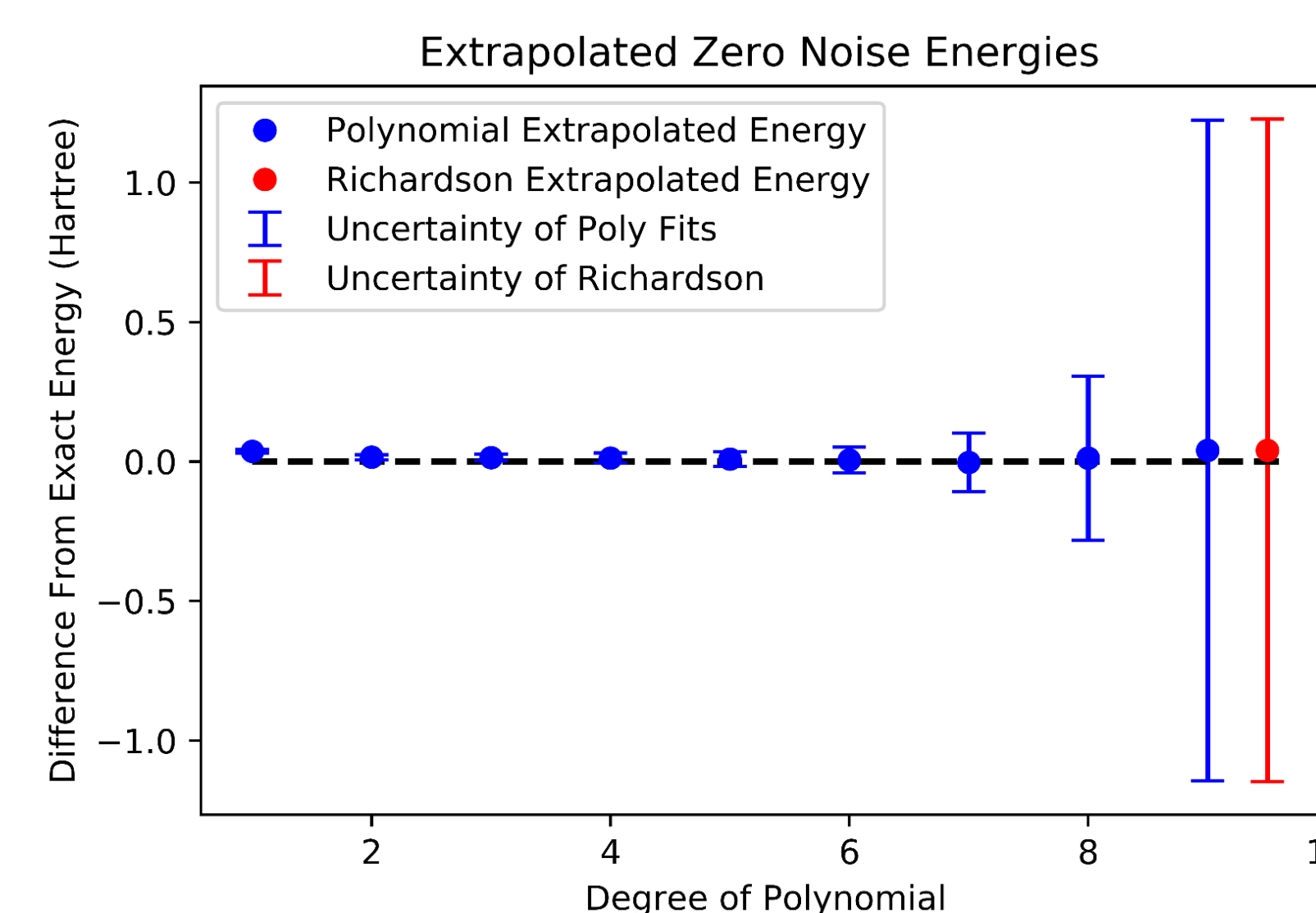


Fig 4c: Uncertainty of zero noise energy extrapolated by Richardson is worse than that by lower degree polynomials.

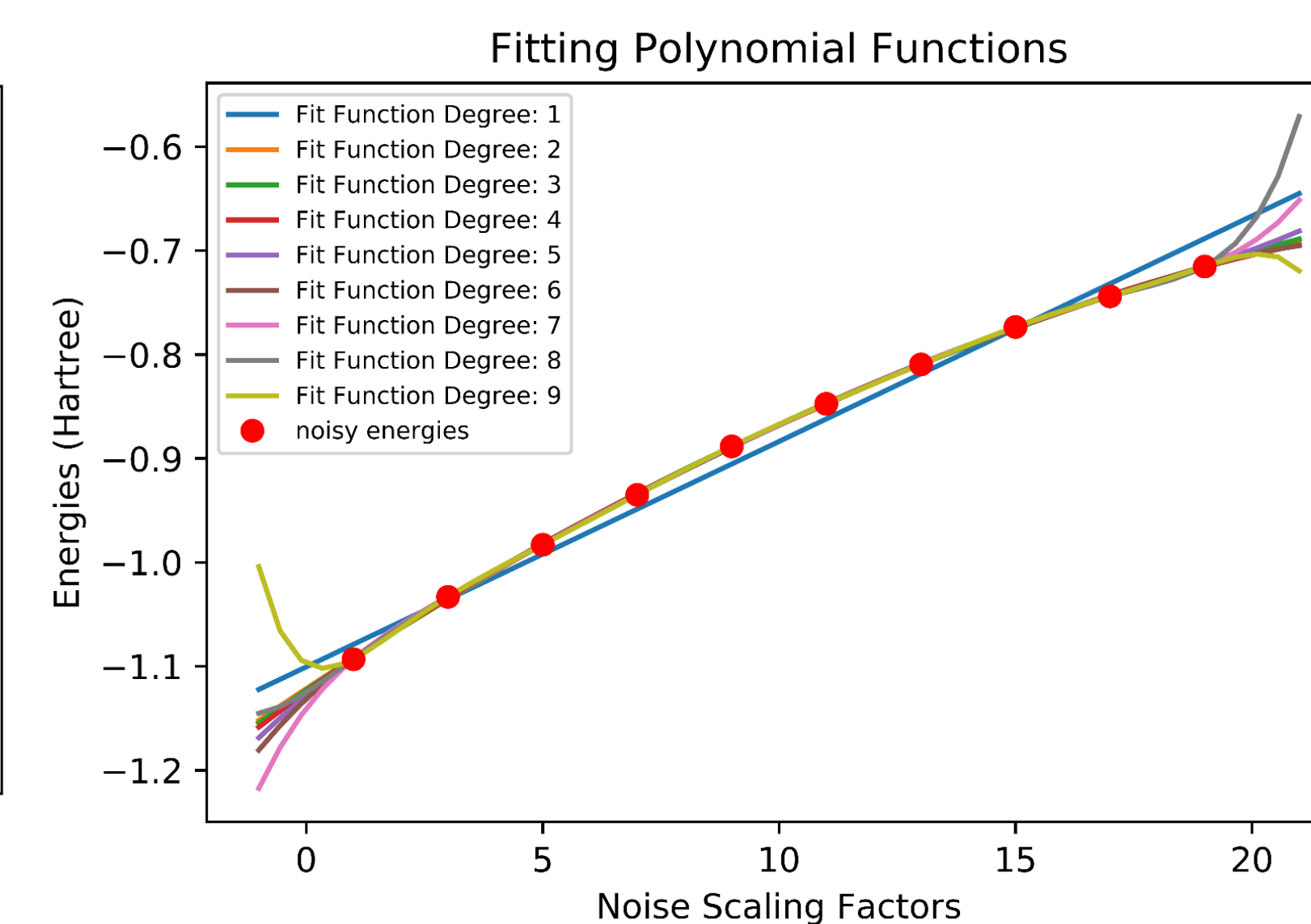


Fig 4b: Using Least Squares to fit polynomial functions through the noise energies.

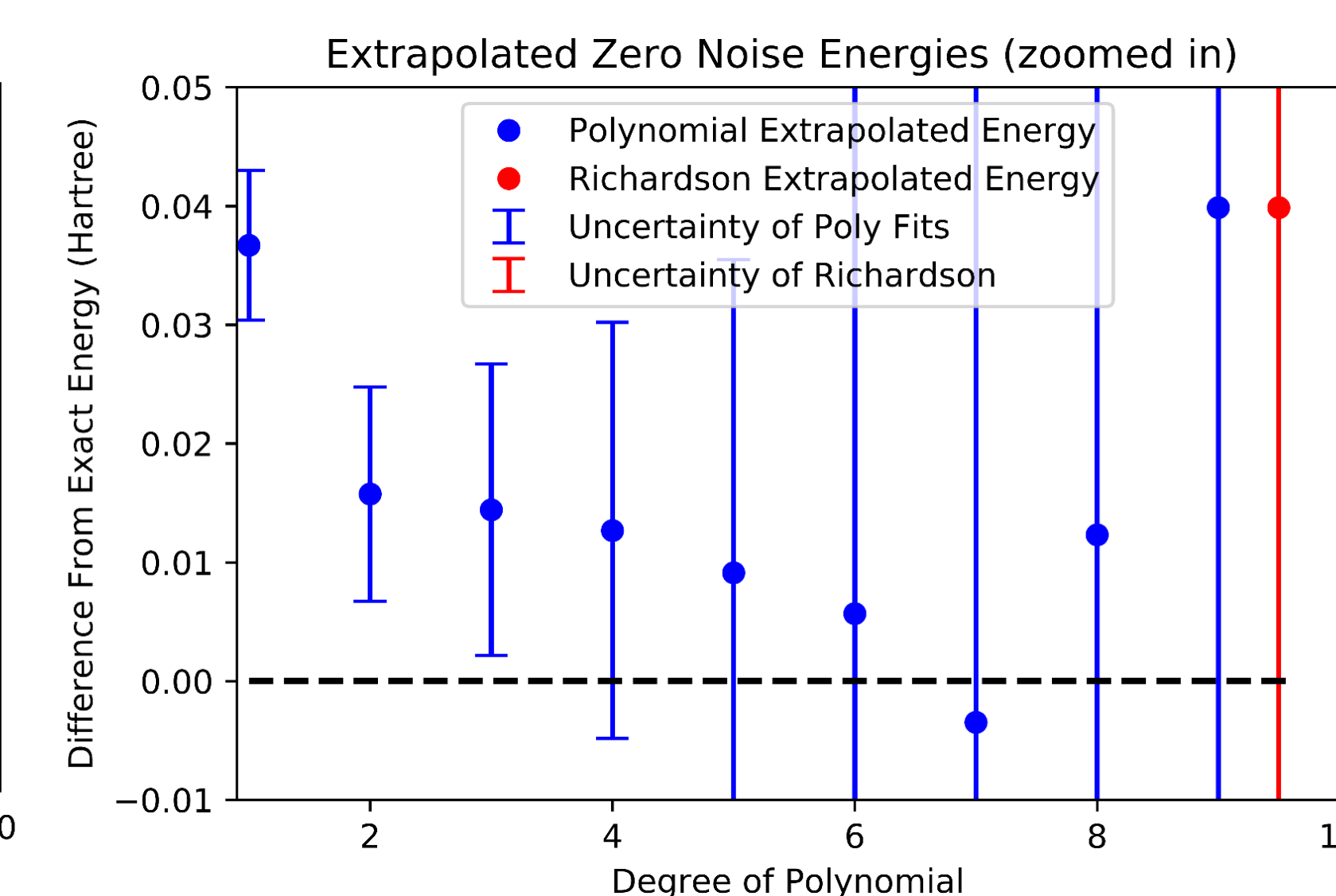


Fig 4d: Zero energy extrapolated by Richardson is worse than that of lower degree polynomials.

Fig 5: Using IBM's quantum computer at London, we compare Richardson technique with polynomial fitting technique in improving the VQE-computed ground state energy of the Hydrogen molecule. Noise was amplified after optimizing parameters in VQE.

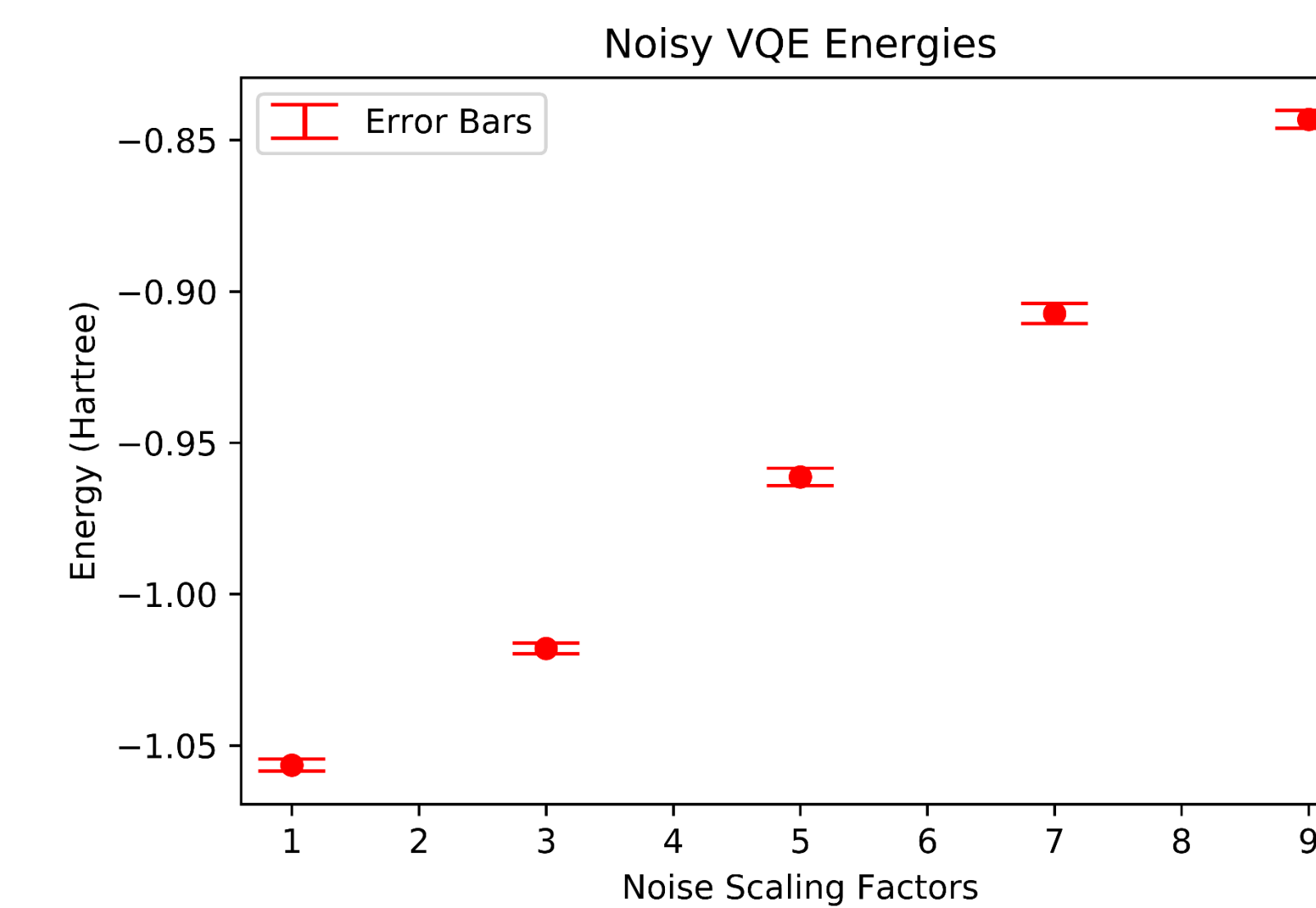


Fig 5a: As we amplify noise in the optimized circuit, the energies diverge more and more from the exact energy (1.137 Hartree).

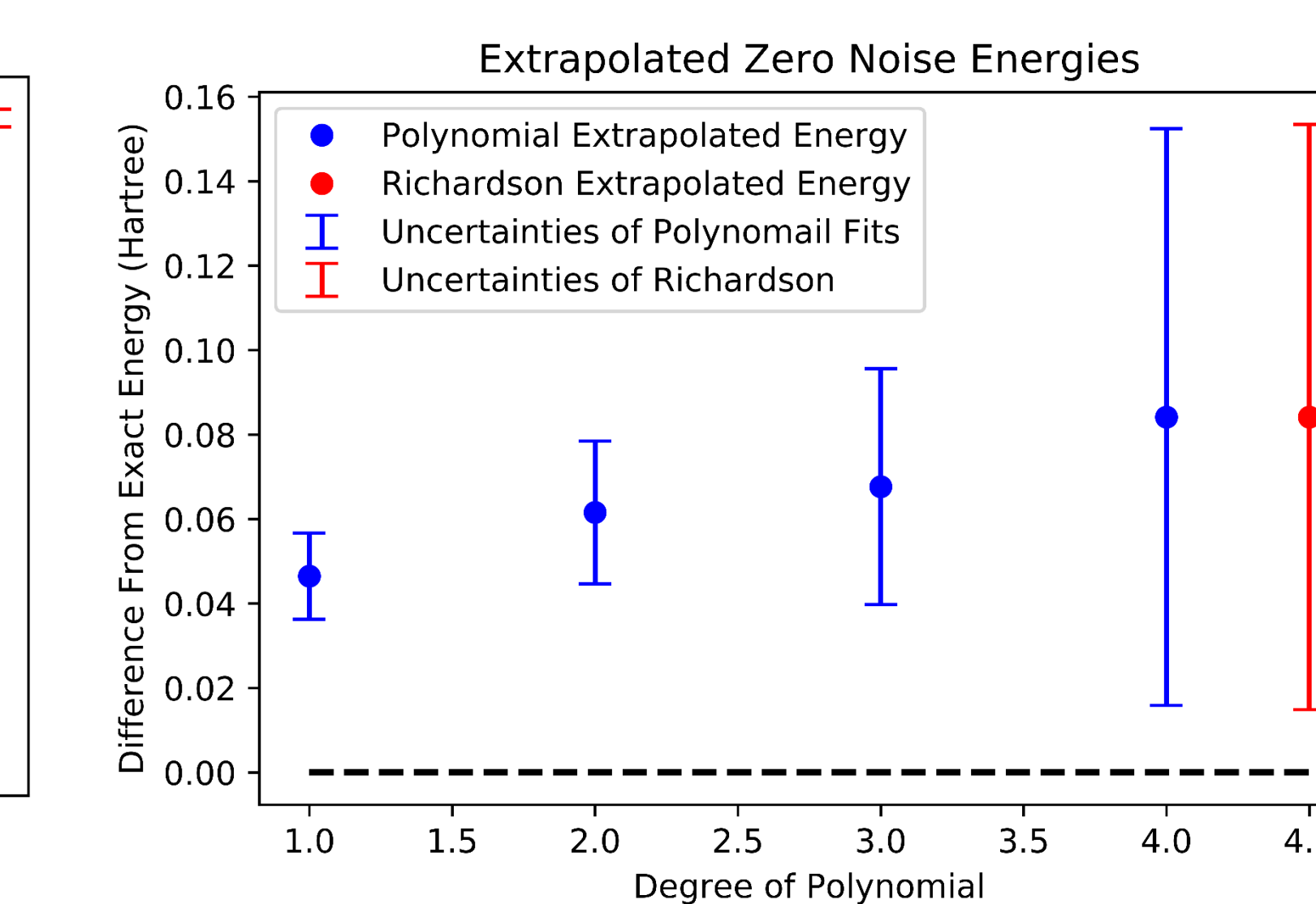


Fig 5b: Zero Noise energy extrapolated by Richardson is both worse in precision and accuracy than that extrapolated by lower degree polynomial fits.

Noise Amplification

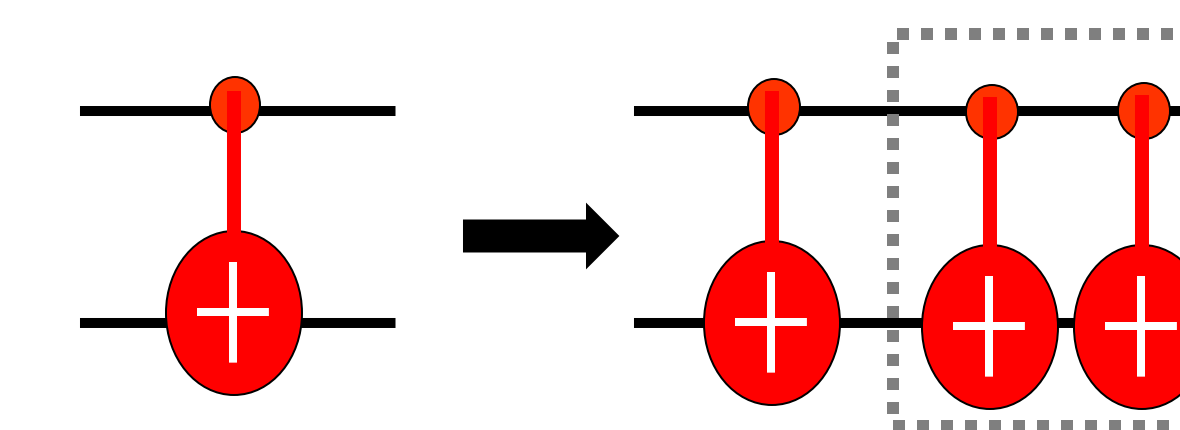


Fig 3: Since the dominant source of noise on IBM's quantum computers are 2 qubit gates, we can add redundant CNOT gates to amplify noise.

Methods

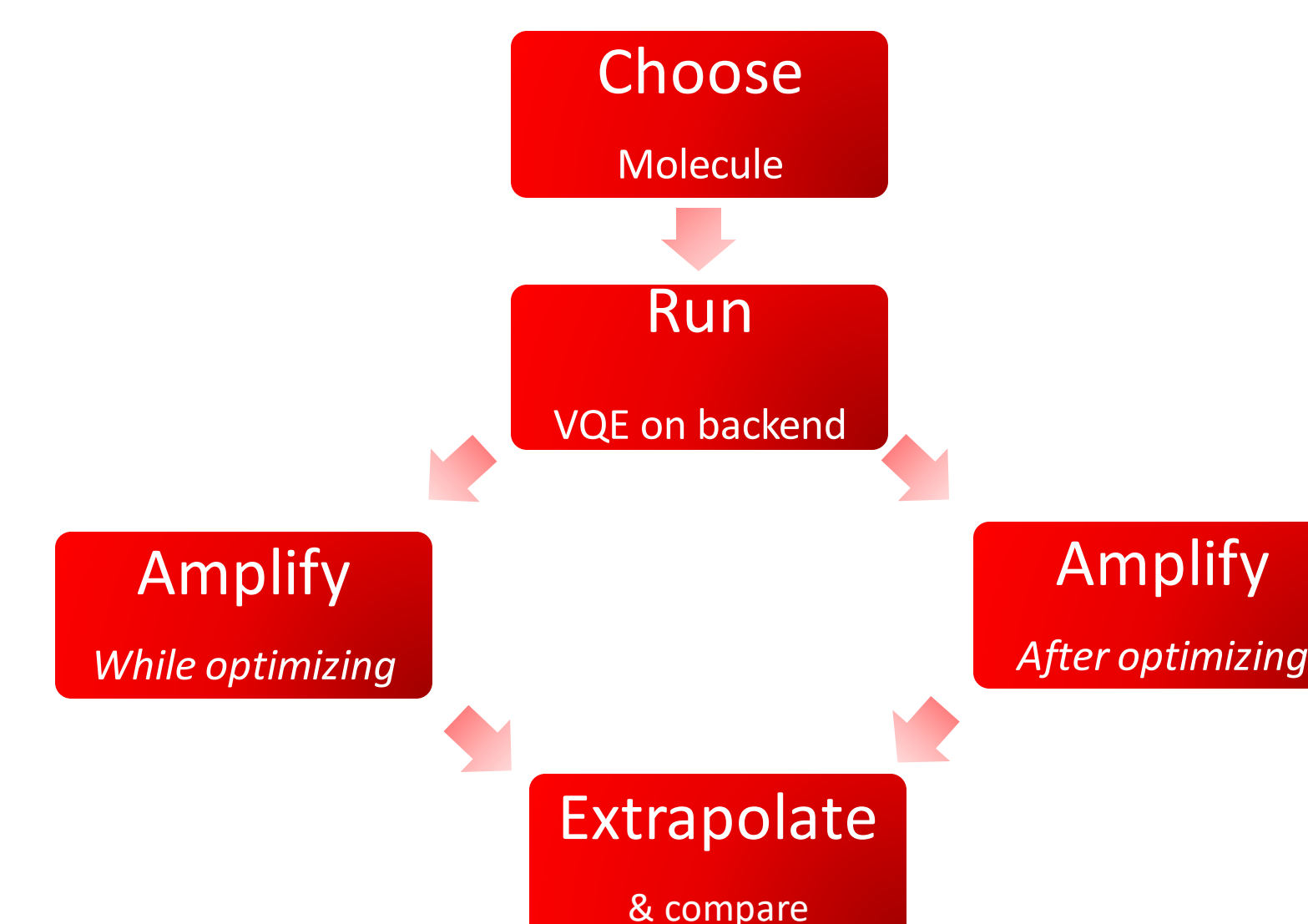


Fig 6: Procedure for comparing the two extrapolation techniques

Conclusion & Future Work

- Zero noise extrapolated energy obtained via polynomial fitting is more precise than that obtained via Richardson technique.
- We plan to improve the technique by amplifying the noise in finer steps in order to obtain an improved fit.
- Also, zero noise extrapolated energies we obtained are not within chemical accuracy.
- We plan to investigate other error mitigation strategies such as probabilistic error cancellation and quantum subspace expansion to obtain improved accuracy of the ground state energy
- We plan to extend these techniques to more complex molecules like LiH_3 and H_2O .

Acknowledgements

I would like to thank Professor Stephen Schnetzer foremost for his continued guidance and patience throughout this adventure. Special thanks to Rikab Gambhir and Professor Mark Hillery for insightful discussions. Lastly, I want to thank Aresty Research Center for this opportunity.

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