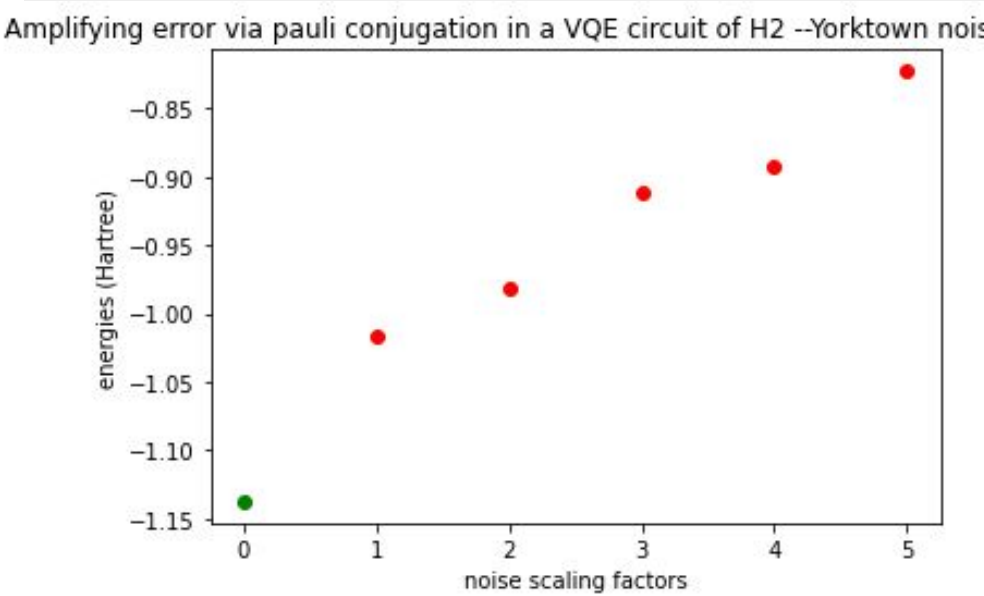
Update on Statistics and Twirling (3)

July 13, 2020

1. Twirling Works

In amplifying noise in a sample VQE circuit of H2

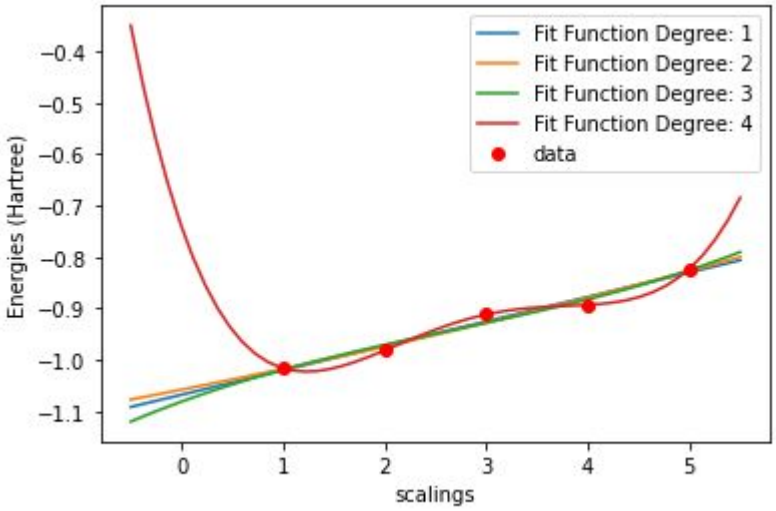


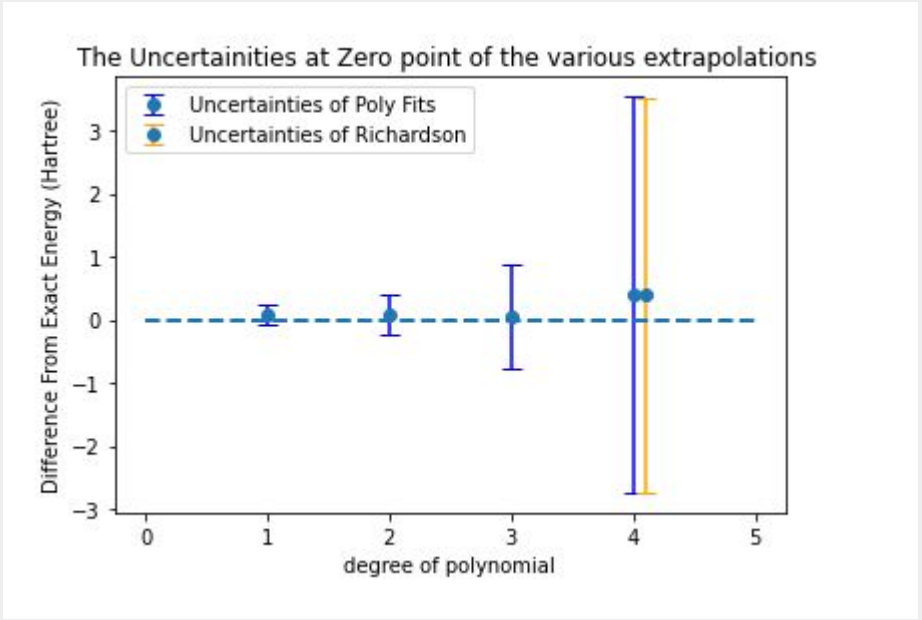
- Green point is the exact energy at 0.74 ang separation

How I did so

1. Do VQE for H2 atom at 0.74 ang separation on ideal simulator
2. Obtain the ‘optimal circuit’ i.e. circuit whose expectation values gives lowest energy at that distance.
3. Twirl that circuit at 5 noise scalings with barriers. Repeat this 512 times for each noise scaling.
4. Transpile these circuits using a set of basis gates.
5. Run these 5*512 circuits on a simulator with Yorktown noise model.
6. Compute mean of 512 results for each noise scaling and plot

Went on to do Extrapolation





Caveats

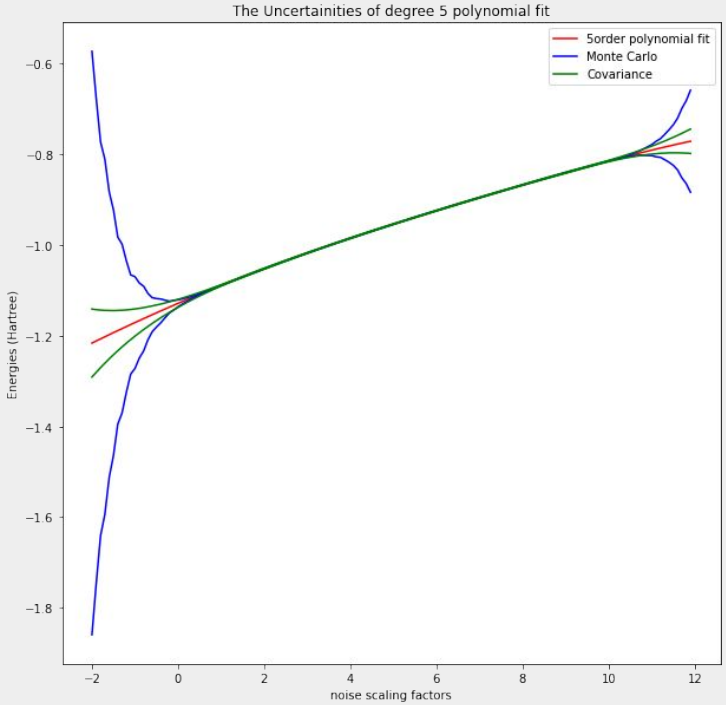
1. This was done for a particular circuit, not the entire VQE subroutine.
2. A better result would be to integrate twirling directly into VQE (Coding Job)

Future Tasks:

1. Repeat everything on a quantum computer (with much less samples)
2. Do twirling within VQE routine.

2. Monte Carlo vs Covariance

Neither square rooting nor squaring monte carlo brings it any closer to the covariance curves

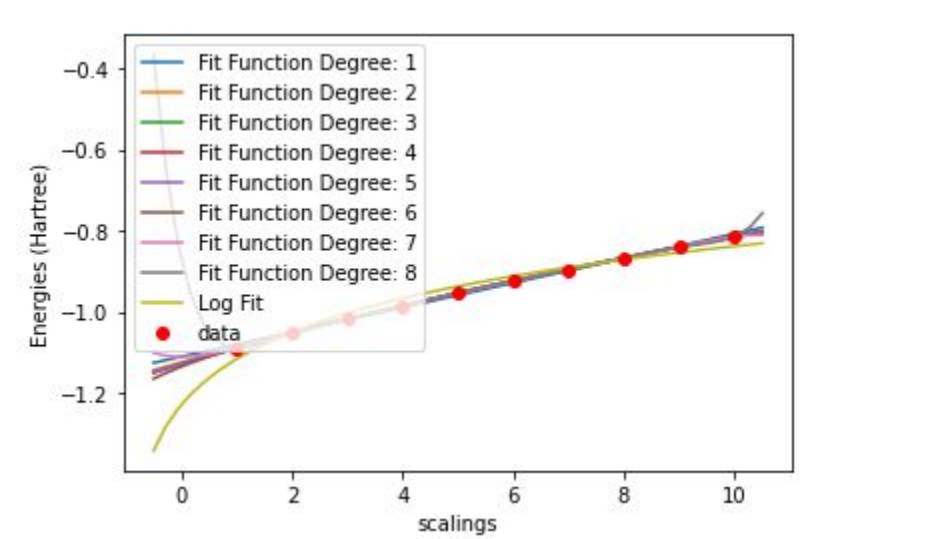


Squaring Monte Carlo works to some extent but as you go away from actual points (1-10), differences between the 2 uncertainties magnify

3. Log Fitting

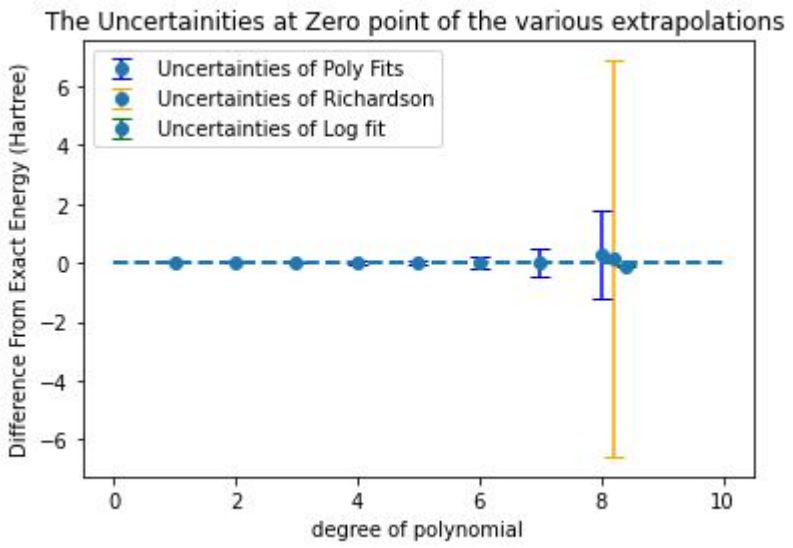
$f(x) = a*\ln(x+1) + b$

Had to add 1 so I don't get -infinity when I extrapolate zero noise result .



Log Fitting

Zero noise result was .1 Hartree below exact energy with uncertainty of 0.015 Hartree (comparable to first and second degree polynomial fits)



Very last dot on the right is the log fit point.

Log Fitting

$f(x) = a*\ln(x+b) + c$

This gave a much more accurate zero noise result (0.01 Hartree off) but when calculating uncertainties, it kept crashing because scipy couldn't find optimal parameters.

```
RuntimeError: Optimal parameters not found: Number of calls to function has reached maxfev = 800.
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