2020 Remote Summer Science Bi-Weekly Progress Report

Name of Student __Eesh Gupta___

Name of Faculty ___Stephen Schnetzer_____

Title of Project__Computing (Error Mitigated) Ground State Energies of Small Molecules__

Department ____Physics and Astronomy_____

1) Short introduction and objectives (Student to provide a brief statement about the objectives of the project)

In light of quantum computers being able to solve chemistry problems, our aim is to **benchmark recently proposed error mitigation techniques on the basis of types of noise they mitigate and their scalability with molecular systems.** We will then use those techniques (extrapolation, probabilistic error cancellation–if time permits) to study molecules such as H4 and water.

2) Accomplished work for specified period: From (June 29) To (July 10)

- **Experiment**:
    - **What**: Statistical Analysis of uncertainty of the various polynomial fits using Monte Carlo and covariance matrix methods
    - **Why:** Testing whether Richardson Extrapolation, a popular technique in literature, is the best way to extrapolate zero error energies
    - **Result**: Still encountering bugs in code but it seems there are other methods (lower degree polynomials like quadratic function) more accurate and precise than the Richardson scheme.
- **Experiment:**

- **What**: Amplifying noise in VQE circuits of H2 and LiH using Pauli conjugation (twirling+error simulation) and a twirled CNOT scheme.
- **Why:** These noise amplified results are needed for performing extrapolation and obtaining improved estimates of ground state energy
- **Result:** The schemes were not successful in amplifying noise in VQE results. We suspect bugs in the code and other errors in our implementation of the schemes.

- **Notes**:
  - Pauli Twirling and Error Simulation

3) Continued Plan of Work (State clearly what the continued plan is; State what assistance is needed)

- **Experiments**:
  - Fixing bugs in Monte Carlo uncertainty calculation scheme to get a consensus on whether polynomial fitting is better than Richardson technique.
  - Fixing bugs in implementation of Twirling to get noise amplified VQE curves for H2 and LiH
  - Extrapolating improved ground state energy estimates for H2 and LiH using Pauli conjugation or twirled-CNOT-pairs technique.

- **Notes:**
  - Refining Twirling Notes to include its mathematical derivation to understand its nuances on a deeper level.

4) Any other comments:

The professional development workshop with the grad school panel was really helpful, especially hearing experiences of Aidan and Morgan Taylor. Is it possible for you to share their contact information so I can ask them some more questions?

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Student Name __Eesh Gupta__

Signature ____  _____

Date _7/10/2020__

Comments by Supervisors:

1) Name: Steve Schnetzer Department; Physics & Astronomy

Comments: Eesh Gupta is doing excellent work and is making excellent progress

Signature  Date _July 10, 2020