IBM Technical Challenge Report

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Abstract

This paper, which has been researched, coded, and written for the 2021 Quantum Coalition Hack IBM Quantum Technical Challenge, addresses IBM's hackathon prompt of using Qiskit Pulse to explore unique research opportunities for high energy states in quantum computing. These high energy states can be used to develop quantum computers with multi-level systems, namely qudits. Doing research in the application of qudits poses a unique opportunity to further develop quantum alorithms more efficiently. Specifically, we analyzed how to create the higher energy states and explored how to model ground state energies in chemical systems with a Variational Quantum Eigensolver (VQE) using qudrits. We found that there numerous advantages to using multi-level systems on a quantum computer to model molecules.

1 Introduction

The phenomena of high energy quantum computing states arises through the use of transmons, which allow for higher energy level representations and analysis. These systems, which are the basis for much of IBM's quantum hardware, contain superconducting circuits composed of a Josephson junction and a capacitor. [1] For the purposes of this paper, we plan on utilizing them to model multi-level energy states using the $\{|0\rangle, |1\rangle, |2\rangle\}$ subspace and will discuss how this representation relates to the field of research we'd like to propose further investigation in: ground state energy modeling of chemical systems using the Variational Quantum Eigensolver (VQE).

In §2 we'll discuss our process of discriminating the $\{|0\rangle, |1\rangle, |2\rangle\}$ subspace to excite higher energy states and how we would adapt this process for our VQE chemical and molecular simulation. §3 will then display and discuss our results from our higher state discriminator and how they'd relate to our proposed research topic. Next, §4 will delve into the specifics of our VQE molecular simulation model and the results we'd like to ascertain from the electron structure problem, which would improve the quantum computing community's understanding of energy levels in chemical systems. Finally, §5 will summarize our results and key findings, issues we faced in our hackathon process, and the potential future implications of our project.

2 Methods

This project utilizes the IBM Qiskit package to investigate levels beyond the qubit Hilbert subspace for transmon systems. The IBM Qiskit online textbook provides a methodology for expansion of the transmon Hilbert space into the $\{|0\rangle, |1\rangle, |2\rangle\}$ basis, and this procedure is generalized to incorporate the fourth-level $|3\rangle$ state into the discriminator basis.

The procedure for appending states to the transmon subspace consists of two separate measurements: a frequency sweep and a Rabi experiment. The combined results of these experiments yield the drive frequency and π-pulse amplitude for transitions between adjacent states in the transmon Hilbert space (e.g. $|1\rangle$ and $|2\rangle$). The results of these measurements are provided by the Qiskit textbook for the $|0\rangle \rightarrow |1\rangle$ and $|1\rangle \rightarrow |2\rangle$ transitions.

To generate inclusion of the $|3\rangle$ state, a frequency sweep is conducted over the 400MHz below the $|1\rangle \rightarrow |2\rangle$ frequency provided by Qiskit. Once the rough transition frequency is determined, a more detailed sweep is run on the range $\pm$ 20MHz from the rough peak location. This frequency sweep can be used to yield a precise driving frequency for the $|2\rangle \rightarrow |3\rangle$ transition. Using the $|2\rangle \rightarrow |3\rangle$ transition frequency, we next perform a Rabi experiment to determine the π-pulse amplitude of the $|2\rangle \rightarrow |3\rangle$ transition. To do this measurement, we apply a $|0\rangle \rightarrow |1\rangle$ π pulse and sweep amplitude at the $|2\rangle \rightarrow |3\rangle$ frequency using the sideband method. The resulting output signal oscillates periodically as a function of amplitude, and the π pulse amplitude for the $|2\rangle \rightarrow |3\rangle$ transition is half the period of this oscillation.

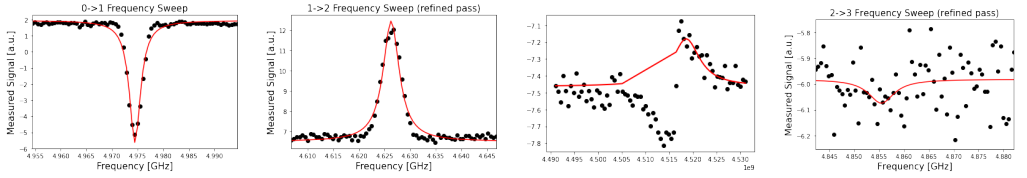
The above procedure allows us to prepare transmons in any state on the space spanned by $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$. The next logical step is to create a

discriminator so that we can reliably distinguish between these four states. To do this, we again follow the procedure outlined in the Qiskit textbook and make use of the previously defined π pulses. We first prepare a transmon in $|0\rangle$ and measure its centroid to characterize the $|0\rangle$ state. We then initialize in $|0\rangle$ again and then apply a $|0\rangle \rightarrow |1\rangle$ π pulse and re-measure to characterize the $|1\rangle$ state. This process of initialization in $|0\rangle$ and applying a ladder of π pulses to reach and characterize the appropriate state is repeated for the $|2\rangle$ and $|3\rangle$ states. With all states characterized, their centroids can be plotted in the I-Q plane, and used to delineate a separatrix which can be used to classify transmon states based on their IQ point.

This entire procedure was done twice on different machines to generate a maximally robust set of results for characterization of the $|3\rangle$ state and 4-dimensional Hilbert space $\{|0\rangle, |1\rangle, |2\rangle\, |3\rangle\}$ in the challenge time constraint.

3 Data Analysis

The first segment of data obtained from these measurements is the transitions frequencies associated with each pair of adjacent states in the Hilbert space. Results on the $|0\rangle \rightarrow |1\rangle$ and $|1\rangle \rightarrow |2\rangle$ transition frequencies are obtained from the IBM Qiskit textbook, and results for the $|2\rangle \rightarrow |3\rangle$ frequency are calculated using the algorithm specified above. The $|0\rangle \rightarrow |1\rangle$ and $|1\rangle \rightarrow |2\rangle$ are provided from IBM Qiskit as 4.974 GHz and 4.626 GHz, respectively. The $|2\rangle \rightarrow |3\rangle$ frequency was calculated twice, producing results of 4.518 GHz and 4.626 GHz.



(a) Frequency Sweep for $|0\rangle \rightarrow |1\rangle$ transition

(b) Frequency Sweep for $|1\rangle \rightarrow |2\rangle$ transition

(c) Frequency Sweep for $|2\rangle \rightarrow |3\rangle$ transition

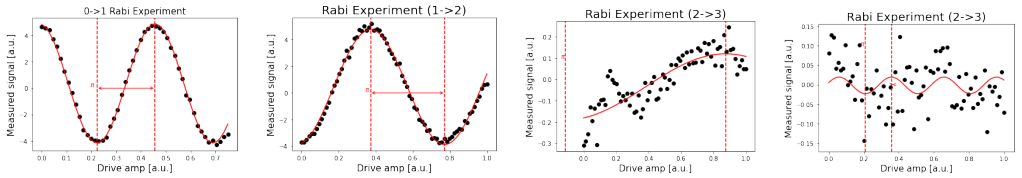
(d) Frequency Sweep for $|2\rangle \rightarrow |3\rangle$ transition

Figure 1: Frequency sweeps for transitions on the $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$ transmon Hilbert space.

It is clear from inspection of these plots that our results deviated significantly from those produced in the Qiskit textbook production. While we were able to model and utilize some Lorentzian peaks for further analysis,

our data for the $|2\rangle \rightarrow |3\rangle$ transition frequency were generally much noisier than the provided Qiskit runs. Furthermore, both runs show notable deviations from the expected Lorentzian peak shape, even in what appear to be lower-noise regions. These deviations from expected values can be potentially attributed to multiple error sources, including improper algorithm development and unaccounted-for quantum effects at the higher levels of the transmon.

Rabi experiments on the different transitions within $\{|0\rangle, |1\rangle, |2\rangle\, |3\rangle\}$ can also be compared, as can the associated π pulse amplitudes. The IBM Qiskit-provided amplitudes were 0.2232 a.u. for $|0\rangle \rightarrow |1\rangle$ pulses and 0.3725 for $|1\rangle \rightarrow |2\rangle$ pulses. For $|2\rangle \rightarrow |3\rangle$, the calculated π pulse amplitudes were 0.1123 and 0.2083.



(a) Rabi experiment for $|0\rangle \rightarrow |1\rangle$ π pulse

(b) Rabi experiment for $|1\rangle \rightarrow |2\rangle$ π pulse

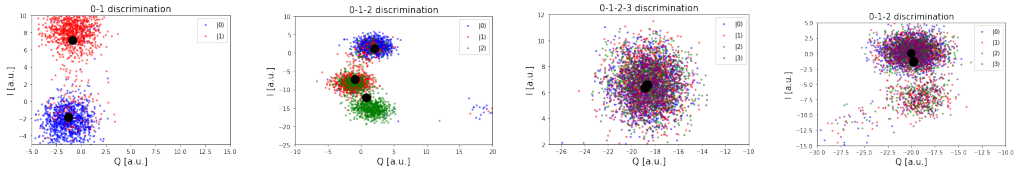
(c) Rabi experiment for $|2\rangle \rightarrow |3\rangle$ π pulse

(d) Rabi experiment for $|2\rangle \rightarrow |3\rangle$ π pulse

Figure 2: Rabi experiments for transitions on the $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$ transmon Hilbert space.

Again, we find that the lower-dimensional Qiskit plots are generally much less noisy and better fitted to their associated Rabi model than the measured $|2\rangle \rightarrow |3\rangle$ π pulse amplitudes. Again, algorithm implementation likely played a significant role in these deviations from the expected sinusoidal output.

The final data taken in this experiment were centroid IQ placements for the various states in $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$. The resulting placements are shown below:



(a) Rabi experiment for $|0\rangle \rightarrow |1\rangle$ π pulse

(b) Rabi experiment for $|1\rangle \rightarrow |2\rangle$ π pulse

(c) Rabi experiment for $|2\rangle \rightarrow |3\rangle$ π pulse

(d) Rabi experiment for $|2\rangle \rightarrow |3\rangle$ π pulse

Figure 3: Discriminator IQ plots for transitions on the $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$ transmon Hilbert space.

Noise and deviation from expected values played a significant role in the error on results at each step of this algorithm. Thus, it is unsurprising that we find the discriminator plots are subject to significant noise, and have extremely limited effectiveness in discerning between states. While the algorithm and pulse sequence development contributions to this error cannot be ignored, it is also relevant to note that, seen in succession, these discriminator plots clearly demonstrate the decrease in fidelity inherent to higher-dimensional qudit subspaces. This issue is one that cannot necessarily be remedied by improved pulse sequences alone, and is thus a highly relevant obstacle in the use of higher-dimensional subspaces for quantum computing.

4 Interpretation

Molecular simulation is one of the most useful known applications for quantum computation. Namely, we can use quantum computers to solve the electron structure problem, in which we are looking for the low lying energies of chemical systems.

For example, one commonly used method to simulate a given molecule is to map a molecular Hamiltonian to qubit operators using an established mapping method, such as Jordan Wigner or Bravyi-Kitaev. Then we can use the Variational Quantum Eigensolver (VQE) to solve for the ground state energy.

As a brief overview, VQE is a hybrid classical-quantum algorithm that attempts to find the lowest eigenvalue of a Hamiltonian. It is reliant on the Reayleigh-Ritz variational principle, which asserts that for a given paramatrized trial wave function expectation value $\langle\psi(\theta)|H|\psi(\theta)\rangle \geq E_0$, where $\psi(\theta)$ is the trial wave function, H is the Hamiltonian, and E_0 is the lowest energy

eigenvalue. The classical computer is used to update the paramaters and the quantum computer is used to prepare, store, and measure the wavefunctions[3]. In order to prepare the trial states, also known as the ansatz, we use paramaterized gates

$$U(\theta) = \sum_{i=1}^{N} = U_i(\theta_i), \tag{1}$$

which is a relation is given by

$$|\psi(\theta)\rangle = U(\theta)|\psi_{ref}\rangle. \tag{2}$$

The space of all states which can be created by the circuit consisting of the paramatrized gates is called the ansatz space [3].

Now that we have established how we would go about simulating a molecule and finding the ground state energy, we will talk about how we could implement the higher energy states described in the methods section. We propose that we use qutrits and qudits, where a qutrit is a three level system and a qudit is a 4 level quantum system, rather than using qubits to solve this problem.

Since qudits are multi-level systems they offer a larger state space for process information and to do multiple contol operations at once. To utilize the qudits that we developed with VQE we would need to understand how each of the paramatrized gates acts on the multilevel system and choose the gates accordingly. The advantage utilizing three level and four level systems is that we reduce the circuit complexity and simplify the experimental set up. [2]

In our modified VQE algorithm using qudits we would need to use gates that correspond to a d level system. Firstly, note that a qudit lives in a d dimensional Hilbert Space with a basis spanned by $\{|0\rangle, |1\rangle, ..., |d\rangle\}$. Similar to when we are dealing with qubits, universality also applies to qudit gates. With more time to do the research we would further explore how to use and implement the qudit gates. Another notable advantage of using qudits is that they only require $log_d N$ qudits to represent an N dimensional system whereas a qubit requres $log_2 N$ qubits [2]. Thus implementing the higher level states that we designed today would be greatly useful in VQE. However, the main issue, which was exemplified in our data, is that the fidelity decreases as we increase to higher energy states.

Finally, this research in chemical system ground state energies may also help answer unresolved questions about phenomena like high temperature superconductivity, solid-state physics, transition metal catalysis, and biochemical reactions like nitrogen fixation. This increased understanding may also help us to refine, and perhaps even one day design, new compounds and technologies of scientific and industrial importance, such as new metal ion battery designs [2].

5 Conclusion

The issues that we faced throughout this project were in large part due to the limit on time and the fact that running each of the jobs took over an hour. As a result we were only able to run each job once and had to use the data from the first run. As a result, the plots that we got were slightly different from what we expected. With a longer time scale we would fix the problems with our data and utilize the higher states to implement VQE with qudits.

Beyond the time constraints of our hackathon, it would be interesting for our project to ascertain a more robust analysis of multi-level energy models and a deeper understanding of how transmons technology could be physically employed. Further analysis should be done on our algorithms and results to bring them into better accordance with expected behavior for transmon systems, most importantly in the development of an accurate discriminator. Proper delineation between quantum states would allow for the creation of quantum logic gates on the full qudit Hilbert space, which could be the building blocks of more robust qudit systems which could perform quantum computations with greater efficiency and accuracy than current systems allow.

As far as future implications go for chemical system simulation at large, there's already a significant amount of impact that can be made in the near to medium term. It's been speculated that VQE may enable small quantum computers with 100 to 200 physical qubits to surpass classical methods [2]. Substantial additional work is required to verify if this would be possible, but if it is this quantum supremacy, along with our multi-level energy states, would greatly improve models of chemical systems.

The ground state wavefunction in particular can also be better modeled with longer circuits, but the length of a circuit that doesn't require error

correction is highly dependent on the amount of noise in the system. Error mitigation resulting in an optimistic two qubit gate error rate of 0.01 %, which is 10x better than our current error rates, would still limit us to 10,000 gates, and even these would likely only contribute a small multiplicative increase in depth [2]. Although it remains to be seen if methods to increase quantum circuit length are viable, the Fermi-Hubbard model, which employs Trotter steps on a Hamiltonian variational ansatz, has already demonstrated good convergence with 20 Trotter steps, and further work has already shown promising results for ground state modeling [4]. VQE error corrected simulations could also be used to suppress the error rate to a value low enough to obtain chemically accurate energies from the simulation [2]. These additional improvements, paired with advancements in high energy quantum computing, could potentially revolutionize the modeling and deeper understanding of chemical systems.

6 References

[1] https://qiskit.org/textbook/ch-quantum-hardware/accessinghigherenergystates.html2.-Disriminating-the-|0⟩,-|1⟩-and-|2⟩-states-

[2] https://arxiv.org/pdf/2008.00959.pdf

[3] https://arxiv.org/abs/1808.10402

[4] https://arxiv.org/abs/1811.04476