Generating Low-Depth, High Fidelity Quantum Variational Circuits for the Hydroxyl Cation

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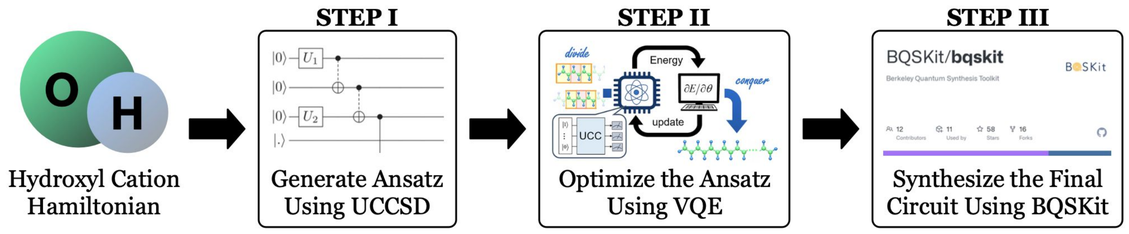
Introduction

Background
- Quantum simulations can dramatically accelerate drug discovery
- Simulations can be inaccurate due to noise

Problem
- Calculate the ground state energy of the hydroxyl cation (·OH)
  - Hydroxyl cation plays a significant role in physiological processes

Our Solution
- Generate low-depth, high-fidelity ansatz for ground state energy estimation

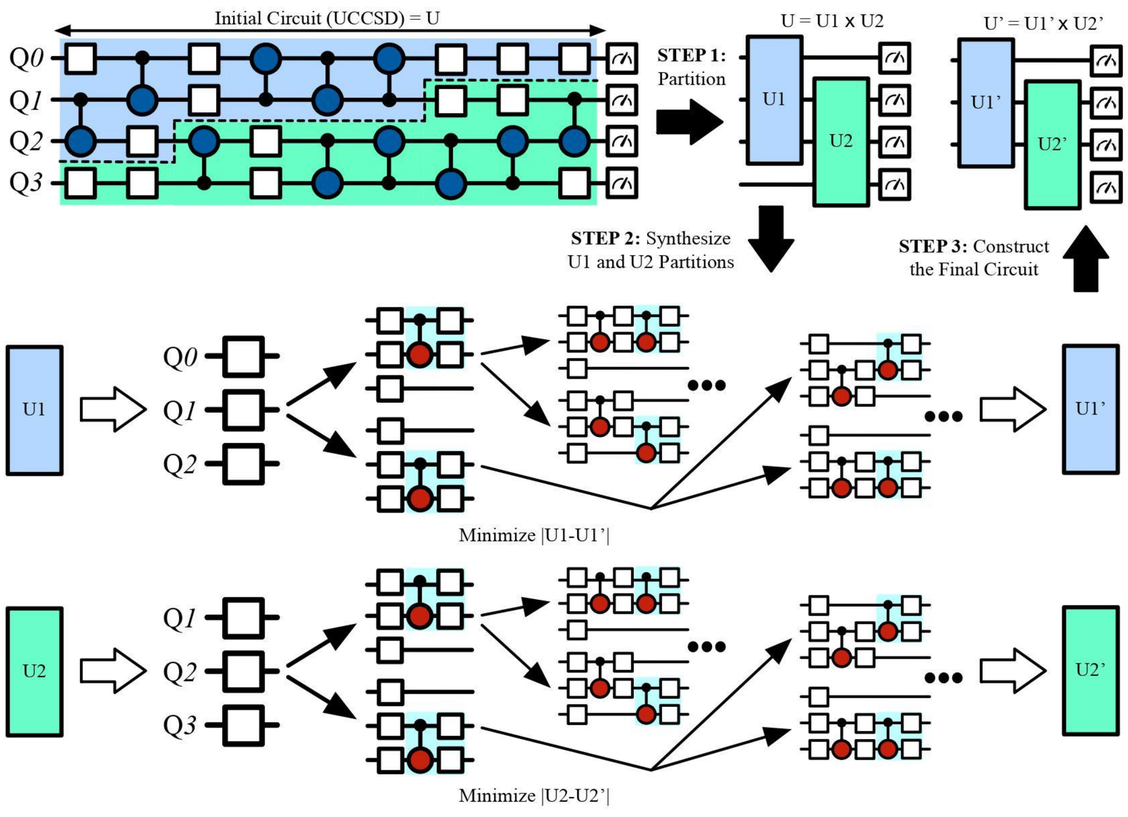


Approach. We take a three-step approach: (1) generate the ansatz using UCCSD, (2) train the ansatz using the VQE algorithm, and (3) minimize the depth of the ansatz using BQSKit approximation synthesis.

Methods

Why UCCSD?
- High accuracy ansatz, stemming from coupled-cluster theory
- However, UCCSD ansatz tends to be deep and scales unfavorably.

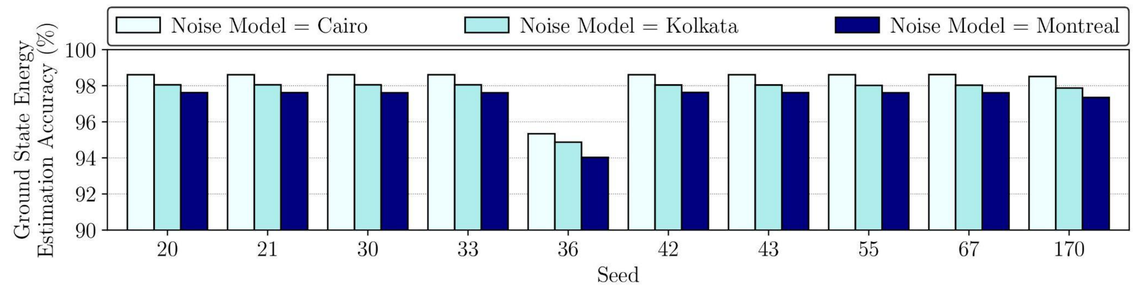
Leveraging Fine-Grained Approximation Synthesis



Circuit Synthesis. First, the deep circuit (U) is partitioned into manageable-sized circuits. Then, each partition is synthesized into shallow circuits using layer-by-layer construction until the distance between the original and the constructed partitions' unitaries becomes sufficiently small. Finally, the new shallow circuit (U') is constructed by combining the synthesized partitions.

Results and Analysis

Our approach helps us achieve an average ground state energy estimation accuracy of 98.07%, reducing the circuit to a depth of 1 in the best case.



Accuracy Plot. We plot the ground state energy estimation accuracy results to demonstrate the trend across the three noise models: Cairo consistently produces the highest accuracies and Montreal produces the lowest accuracies, with Kolkata always falling in between. Note the y-axis starts at 90%.

Circuit ID	Seed	Noise Model	Energy Estimation Accuracy (%)	Circuit Duration (dt)	Number of Shots (#)
1	20	Cairo	98.61	320	1,799,612
2	20	Kolkata	98.05		
3	20	Montreal	97.62		
4	21	Cairo	98.61	320	
5	21	Kolkata	98.05		
6	21	Montreal	97.62		
7	30	Cairo	98.61	320	
8	30	Kolkata	98.05		
9	30	Montreal	97.61		
10	33	Cairo	98.61	320	
11	33	Kolkata	98.05		
12	33	Montreal	97.61		
13	36	Cairo	95.34	67,776	
14	36	Kolkata	94.87		
15	36	Montreal	94.03		
16	42	Cairo	98.61	320	
17	42	Kolkata	98.04		
18	42	Montreal	97.63		
19	43	Cairo	98.61	320	
20	43	Kolkata	98.04		
21	43	Montreal	97.62		
22	55	Cairo	98.61	320	
23	55	Kolkata	98.02		
24	55	Montreal	97.61		
25	67	Cairo	98.62	320	
26	67	Kolkata	98.03		
27	67	Montreal	97.61		
28	170	Cairo	98.51	320	
29	170	Kolkata	97.87		
30	170	Montreal	97.35		
		Average	97.74	7,065.6	1,799,612

Key Results*
1. Average energy estimation accuracy of **98.07%***
2. Ranked **6th** for resource consumption, with average circuit duration of **7,095 dt**
3. Average number of **20 SX gates** and **5 CX gates**

Discussion
1. BQSKit optimization level of 3 has high iterations for circuit parameters, so shallow depth circuits are found
2. Methods can be extended to other molecules with same quantum resource cost

* These results were on the provided set of 10 seeds. The score of 98.07% is from the set of hidden seeds used for evaluation.