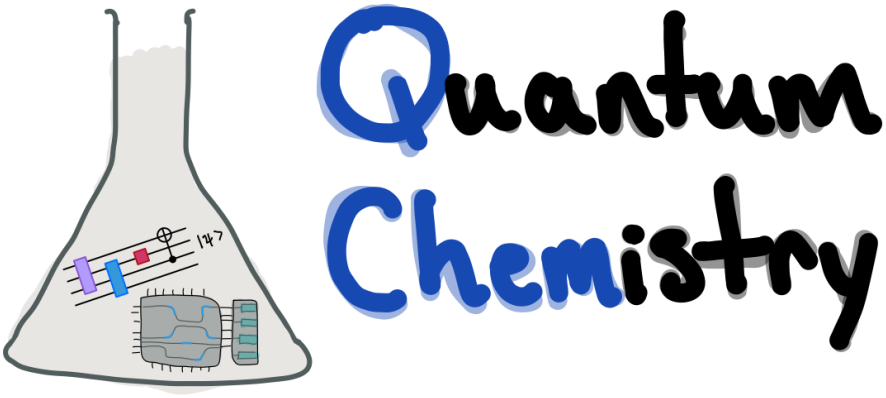

Quantum Chemistry: Universality of Givens Rotations [300 points]

Version: 1

Quantum Chemistry

Numerical techniques for determining the structure and chemical properties of molecules are a juggernaut area of research in the physical sciences. *Ab initio* methods like density functional theory have been a staple method in this field for decades, but have been limited in scalability and accuracy. As such, chemistry applications and problems are desirable candidates for demonstrating a quantum advantage.

It is therefore no surprise that quantum chemistry is one of the leading application areas of quantum computers. In the **Quantum Chemistry** category, you will be using PennyLane's core quantum chemistry functionalities to become familiarized with concepts and tools developed in this sub-field of quantum computing, like mapping molecular Hamiltonians to qubit Hamiltonians and quantum gates that preserve the electron number. Beyond these five questions in this category, there is a plethora of informative tutorials on the PennyLane website that will boost your understanding of topics that we will cover in this category. Let's get started!

Problem statement [300 points]

Givens rotations, as introduced in this PennyLane demo, are particle-conserving unitaries that are widely used in quantum chemistry. Arrazola et. al. have shown that it is possible to form generic particle-conserving gates using only Givens rotations. This property of Givens rotations is known as universality. To get

a flavour of how we can obtain any state with the same number of particles as some given initial state, let us form the six-qubit state

$$|\psi\rangle = a\,|110000\rangle + b\,|001100\rangle + c\,|000011\rangle + d\,|100100\rangle$$

starting from the ground state $|110000\rangle$. As stated in the paper, we can use the circuit in Figure 1.

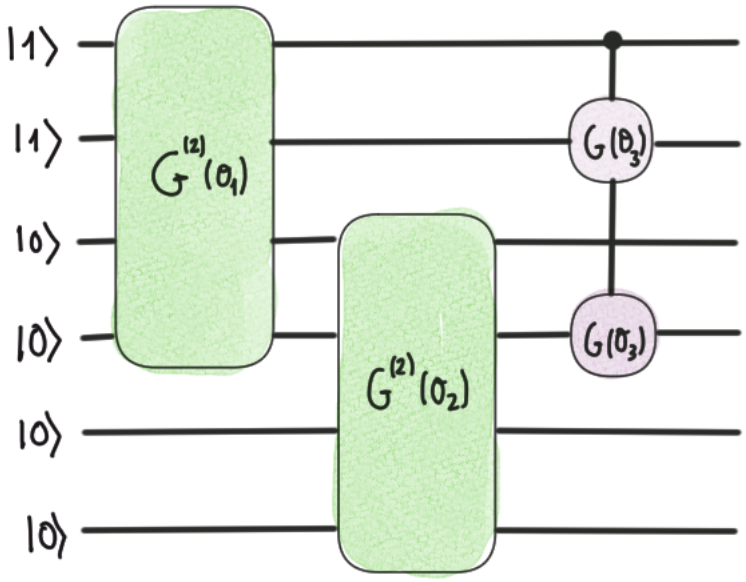

Figure 1: The circuit that produces the state $|\psi\rangle$

where G is the single-excitation gate, and $G^{(2)}$ is the double-excitation gate.

Given the real numbers a,b,c, and d, your task is to find the Givens rotations angles $\theta_1, \theta_2, \theta_3$ (see Figure 1) needed to prepare the state $|\psi\rangle$ as defined above. The angles θ_1, θ_2 and θ_3 range in the interval $[-\pi, \pi)$. For simplicity, assume $a > 0$.

In the provided template called `universality_givens_template.py`, there is a function called `givens_rotations` that you must complete. In this function, calculate the angles needed to prepare $|\psi\rangle$ with Givens rotations.

Input

- `list(float)`: The values `a`, `b`, `c`, and `d` (real numbers, already normalized) parametrizing the state $|\psi\rangle$.

Output

- `list(float)`: The three angles parametrizing the necessary Givens rotations to prepare the state $|\psi\rangle$, in the order that they appear in the circuit in Figure 1 from left to right. Recall that a must be positive.

Acceptance Criteria

In order for your submission to be judged as "correct":

- The outputs generated by your solution when run with a given `.in` file must match those in the corresponding `.ans` file to within the `1.0e-6` tolerance specified below. To clarify, your answer must satisfy

$$\text{tolerance} \geq \left| \frac{\text{your solution} - \text{correct answer}}{\text{correct answer}} \right|.$$

- Your solution must take no longer than the `60s` specified below to produce its outputs.

You can test your solution by passing the `#.in` input data to your program as stdin and comparing the output to the corresponding `#.ans` file:

```
python3 {name_of_file}.py < 1.in
```

WARNING: Don't modify the code outside of the `# QHACK #` markers in the template file, as this code is needed to test your solution. Do not add any print statements to your solution, as this will cause your submission to fail.

Specs
Tolerance: **1.0e-6**
Time limit: **60 s**

Version History

Version 1: Initial document.