A Quantum Algorithm for the Bottleneck Travelling Salesman Problem

by

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Abstract

We develop a quantum algorithm leveraging quantum phase estimation to address the decision problem variant of the Bottleneck Travelling Salesman Problem. This algorithm's efficacy is evaluated through diverse orders of phase estimation applied to both 4-city and 5-city graphs. While the algorithm preserves the original complexity of the problem, $O((N-1)!)$, we introduce a strategy for parallelization, enabling simultaneous execution across all Hamiltonian cycles.

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Chapter 1

Introduction

Continuous advancements in quantum computing have allowed for contemporary approaches to solve complex computational problems that were previously considered intractable using classical methods. Well known examples of these advancements include Shor's [1] and Grover's [2] algorithms for factoring and unstructured search respectively. The Bottleneck Traveling Salesman Problem (BTSP) serves as a challenging optimization problem in the field of logistics and operations research. Its practical applications range from optimizing vehicle routes, to circuit design. Consequently, the achievement of an efficient solution is highly sought after. However, the BTSP is classified as an NP-hard problem, indicating it is at least as difficult as the hardest problems in the NP class. For reference, an NP problem must satisfy two conditions: no known solution in polynomial time, and the verification of a solution in polynomial time. An NP-hard problem does not need to satisfy the verification condition. To address this problem, many heuristic approaches are explored [3][4]. However, inherent to such methods is a trade-off between precision and efficiency.

We embark on a journey at the intersection of quantum computing and optimization by introducing a quantum algorithm tailored to address the BTSP. It requires finding a closed tour through a set of cities while minimizing the largest cost, the "bottleneck", along any route. Its computational complexity grows exponentially with the number of cities, rendering classical solutions impractical for large-scale instances. Our approach is to capitalize on the inherent quantum parallelism, as well as the unique feature of phase encoding in quantum computing. By exploiting these phenomena, we aim to encode and manipulate the costs associated with various routes efficiently.

In the upcoming chapter, we delve into the complexities of the BTSP. We will then explore quantum computing fundamentals and progress to an in-depth discussion on quantum phase estimation. We follow this with a detailed explanation of our proposed algorithm as well as run various simulations. Finally, we will discuss the benefits and drawbacks of our algorithm in the context of the results from the simulations.

Chapter 2

Theory

2.1 The Bottleneck Travelling Salesman Problem

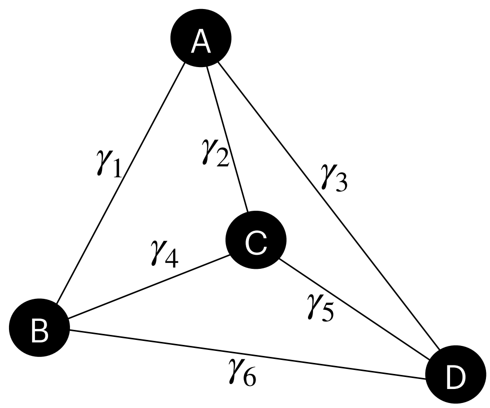


Figure 2.1: An undirected weighted graph represention of a symmetric 4-city system. The vertices represent cities and the edge weights represent the cost of travel.

We start with a graph, whose vertices are labelled A through D, representing a 4-city system. We define movement from one vertex to another as a walk, done through the edges connecting our vertices. We are interested in a particular walk known as a Hamiltonian cycle that contains every vertex exactly once before returning to the start. Our graph also includes edge weights, we define as γ_i. The BTSP is to find the Hamiltonian cycle in a graph, where the largest edge weight (bottleneck) is minimized. This is distinct from the Travelling Salesman Problem (TSP) where the combined edge weights in a given cycle is minimized. The total possible Hamiltonian cycles is given by $(N-1)!$, where N is the number of nodes. We present a symmetric case in FIG .2.1, $N_k \to N_{k+1} = N_{k+1} \to N_k = \gamma_i$. Thus the total possible cycles is $(N-1)!/2$. It is important to note that a solution to either BTSP or TSP is not unique. Moreover, BTSP solutions do not necessarily equate to the TSP solutions. We can illustrate an example below. Consider all the Hamiltonian cycles for a symmetric 4-city system:

$$A \to B \to C \to D \to A$$
$$A \to B \to D \to C \to A$$
$$A \to C \to B \to D \to A$$

Assigning some arbitrary weights, we can see the total costs of the cycles below. The first cycle is the solution to the BTSP as its largest edge weight at 5 is the smallest among all three. The last cycle is a solution to the TSP as its combined edge weight is the smallest.

$$\gamma_1 + \gamma_4 + \gamma_5 + \gamma_3 = 4 + 4 + 5 + 4 = 17$$
$$\gamma_1 + \gamma_6 + \gamma_5 + \gamma_2 = 4 + 6 + 5 + 2 = 17$$
$$\gamma_2 + \gamma_4 + \gamma_6 + \gamma_3 = 2 + 4 + 6 + 4 = 16$$

By simply changing the weight of γ_6 to 5, we can illustrate that all cycles are solutions to the BTSP.

$$\gamma_1 + \gamma_4 + \gamma_5 + \gamma_3 = 4 + 4 + 5 + 4 = 17$$
$$\gamma_1 + \gamma_6 + \gamma_5 + \gamma_2 = 4 + 5 + 5 + 2 = 16$$
$$\gamma_2 + \gamma_4 + \gamma_6 + \gamma_3 = 2 + 4 + 5 + 4 = 15$$

The computational complexity of the BTSP is known to be NP-hard, implying there is no algorithm for a solution in polynomial time. A brute-force approach would imply that we can run an algorithm in $\mathcal{O}((N-1)!)$ time.

2.2 An Introduction to Quantum Computing

Quantum computing represents a fundamentally different approach to computation compared to it's classical counterpart. At its core, quantum computing leverages principles of quantum physics to process information in ways that classical computers can't. Let us look at some key differences:

1. Information Representation: Classical bits are binary and can only be in one state at a time (0 or 1). Qubits, however, can be in a superposition of the basis states.

2. Determinism: Classical computing is deterministic, implying the output of a computation is predictable if you know the input and the algorithm. Quantum computing, however, is probabilistic. Only after measurement we achieve a deterministic reading. This means that quantum algorithms can give different outcomes with each run with respect to their probabilites.

3. Operations: Classical computers perform operations using logical gates (AND, OR, NOT). In quantum computers perform operations using unitary operators that define quantum logic gates. Unitary operators satisfy the condition $U^{\dagger}U = \mathbb{I}$. This implies all quantum operations are reversible, which is not generally the case in classical computation.

2.2.1 Frequently Used Notation

Let us start by looking at single qubit states, these are, by convention, in the computational basis:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

We can have a superposition of basis states:

$$|s\rangle = \alpha|0\rangle + \beta|1\rangle$$

Were: $|\alpha|^2$ represents the probability of measuring state $|0\rangle$, and $|\beta|^2$ represents the probability of measuring state $|1\rangle$. Thus our amplitudes should satisfy the condition:

$$|\alpha|^2 + |\beta|^2 = 1$$

Below we can see the Pauli-X gate, and we can see the result on the single qubit states is analogous to the NOT gate in classical computation.

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\begin{aligned} X|0\rangle &= |1\rangle \\ X|1\rangle &= |0\rangle \end{aligned}$$

Below we can see the Hadamard gate and the result of its application to single qubit states, frequently employed to establish a uniform superposition.

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$\begin{aligned} H|0\rangle &= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle \\ H|1\rangle &= \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle \end{aligned}$$

Multiple qubit states are achieved through tensor products of single states. An n-qubit system will span a Hilbert space $N = 2^n$. We can see with the 2-qubit system we have 4 states.

$$|00\rangle = |0\rangle \otimes |0\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, |01\rangle = |0\rangle \otimes |1\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

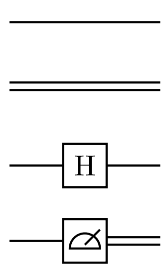
$$|00\rangle = |1\rangle \otimes |0\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, |01\rangle = |1\rangle \otimes |1\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

The Hadamard gate can also be extended to multiple qubit states. Let us see it applied to $|00\rangle$:

$$\begin{aligned} H^{\otimes 2}|00\rangle &= H|0\rangle H|0\rangle \\ &= |+\rangle|+\rangle \\ &= (\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle))(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)) \\ &= \frac{1}{2}(|0\rangle + |1\rangle)(|0\rangle + |1\rangle) \\ &= \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle) \end{aligned}$$

2.2.2 Quantum Circuit Components

We can represent unitary operations on qubits through quantum circuit diagrams similiar to classical circuits. Frequently used circuit components are listed below:



quantum wire

classical wire

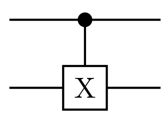
single qubit gate

qubit measurement

2.2.3 Controlled Gates

A controlled gate operates on two or more qubits, where one or more qubits act as the "control" qubits, and the others as the "target" qubit. For the context of this thesis, we will discuss controlled operations in the context of a single control qubit.

Let us start with the controlled-X gate. Below we can see the quantum circuit and matrix representation as well as its affect on all 2-qubit states:



control qubit

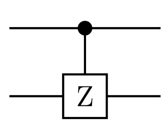
target qubit

$$CX = \begin{bmatrix} \mathbb{I}_2 & 0 \\ 0 & X \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$\begin{aligned} X|00\rangle &= |00\rangle \\ X|01\rangle &= |01\rangle \\ X|10\rangle &= |11\rangle \\ X|11\rangle &= |10\rangle \end{aligned}$$

In this operation, only the only the states $|10\rangle$ and $|11\rangle$ undergo any change. The first qubit, positioned on the left, serves as the control qubit, determining whether the operation is applied. The second qubit, on the right, is the target qubit that is only affected if the control qubit is in state $|1\rangle$.

Let us now look at the controlled-Z gate. Again, we can look at the quantum circuit and matrix representation as well as its affect on all 2-qubit states.



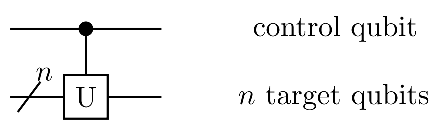
control qubit

target qubit

$$CZ = \begin{bmatrix} \mathbb{I}_2 & 0 \\ 0 & Z \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

$$\begin{aligned} Z|00\rangle &= |00\rangle \\ Z|01\rangle &= |01\rangle \\ Z|10\rangle &= |10\rangle \\ Z|11\rangle &= -|11\rangle \end{aligned}$$

We can see in this case, only the final state, $|11\rangle$ was affected and it specifically altered the state's phase. We can construct our own controlled gates with any unitary matrix U. A controlled-U designed to act on n target qubits, can be represented in block matrix notation. In this framework, $\mathbb{I}_n$ refers to the identity matrix with 2^n diagonal elements:



$$CU = \begin{bmatrix} \mathbb{I}_n & 0 \\ 0 & U \end{bmatrix} \tag{2.1}$$

2.3 Quantum Phase Estimation

The phase estimation algorithm initially proposed by Alexey Kitaev [5] plays an important role as a subroutine for the more widely known factoring algorithm by Peter Shor [1]. We first must briefly discuss the Quantum Fourier Transform (QFT) as it is key to understanding phase estimation [6]. Given a computational basis state $|x\rangle$, applying the QFT (F_N) results in:

$$F_N|x\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i x k N^{-1}} |k\rangle$$

Let us represent this in binary notation and decompose it into a tensor product. We can represent $|x\rangle$ as a string of bits, and the QFT as a tensor product of single qubit basis states:

$$|x\rangle = |x_1 x_2 ... x_n\rangle = |x_1\rangle \otimes |x_2\rangle \otimes ... \otimes |x_n\rangle$$

$$F_N|x\rangle = \frac{1}{\sqrt{2^n}} \bigotimes_{j=1}^{n} (|0\rangle + e^{2\pi i x 2^{-j}} |1\rangle) \tag{2.2}$$

$$= \frac{1}{\sqrt{2^n}} ((|0\rangle + \omega_1|1\rangle) \otimes (|0\rangle + \omega_2|1\rangle) \otimes ... \otimes (|0\rangle + \omega_n|1\rangle))$$

$$
\begin{aligned}
\omega_1 &= e^{2\pi i x 2^{-1}} = e^{2\pi i (0.x_n)} \\
\omega_2 &= e^{2\pi i x 2^{-2}} = e^{2\pi i (0.x_{n-1}x_n)} \\
&\dots \\
\omega_n &= e^{2\pi i x 2^{-n}} = e^{2\pi i (0.x_1 \dots x_n)}
\end{aligned}
$$

An important characteristic of the w_j is the bit shift occurring in the exponent. If we look at w_1, the exponent has a factor $x2^{-1}$, which is equivalent to one right bit shift: $x_1 ... x_{n-1}.x_n$. Integer multiples of the exponent would imply full rotations returning to the same point. Thus we can ignore all the values on the left of the decimal and what remains is $0.x_n$.

Let us discuss the phase estimation problem. Given an eigenstate $|\lambda\rangle$ of a unitary operator U, we want to calculate a good approximation for $\phi \in [0, 1)$ satisfying:

$$U|\lambda\rangle = e^{2\pi i\phi}|\lambda\rangle \tag{2.3}$$

The phase estimation algorithm uses two registers of qubits. The first one will be a set of n control qubits that determine the precision of our approximation. The second register will be a set of m qubits initialized to an eigenstate $|\lambda\rangle$.

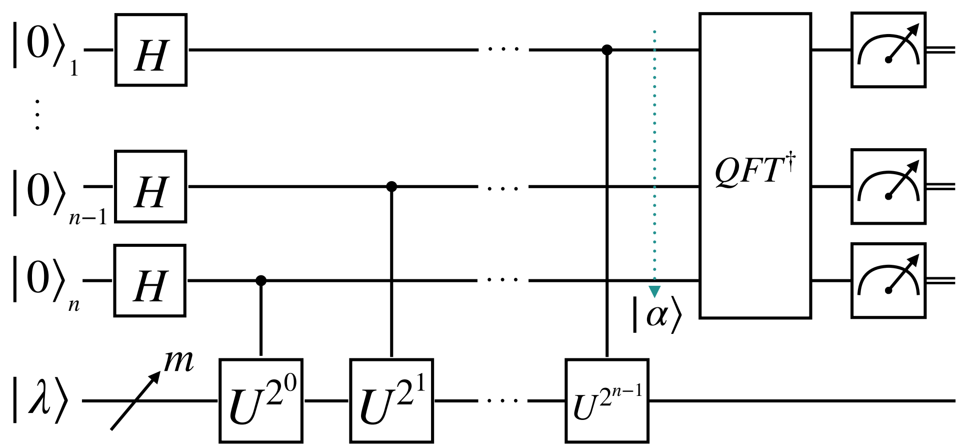


Figure 2.2: A quantum circuit representation of the phase estimation algorithm. Given $U|\lambda\rangle = e^{2\pi i\phi}|\lambda\rangle$, this algorithm allows us to generate an approximation for $\phi \in [0, 1)$. The circuit consists of two registers of qubits. The first n-qubits are initialized to $|0\rangle$ and contribute to the precision of the ϕ value obtained. The second register of m-qubits is initialized to the eigenstate of U. The Hadamard gates, H, are used to create a uniform superposition in the first register. The control gates based on U are responsible for encoding phase to the qubits in the first register. Finally, a $QFT^\dagger$ is performed on the first register to extract the encoded phase. Each subsequent qubit in the first register would require double the control gates. Thus, with a large n we obtain a more precise value for ϕ, but also exponentially increase our computation time.

Let us walk through the quantum circuit in FIG. 2.2, to understand the inner workings of this algorithm. Our initialized state is $|0^{\otimes n}\lambda\rangle$. From here we perform the same operation we find in (1), where all the qubits in the first register are set to a uniform superposition on all states 2^n. The next portion of the algorithm involves applying controlled gates based on the unitary operator U. The function of these CU gates is to apply the operator U on $|\lambda\rangle$ if the control qubit is in the state $|1\rangle$. We can have a look at the effect on the $\mathrm{n^{th}}$ qubit, after it has been prepared in a superposition by the Hadamard gate:

$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |\lambda\rangle = |0\lambda\rangle + |1\lambda\rangle$$

Applying CU and factoring out the eigenstate:

$$\begin{aligned} CU\frac{1}{\sqrt{2}}(|0\lambda\rangle + |1\lambda\rangle) &= \frac{1}{\sqrt{2}}(CU|0\lambda\rangle + CU|1\lambda\rangle) \\ &= \frac{1}{\sqrt{2}}(|0\lambda\rangle + e^{2\pi i\phi}|1\lambda\rangle) \\ &= \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i\phi}|1\rangle) \otimes |\lambda\rangle \end{aligned}$$

We can see that the eigenstate after the CU operation is left unchanged. The phase has been encoded into the control qubit instead, a result that is due to the phase kickback. Thus, we can reuse our eigenstate for the next qubit. Consecutive qubits have double the number of CU operators as the previous, thus squaring the eigenvalue each time:

$$\begin{aligned} \mathrm{qubit_{n\text{-}1}} &: |0\rangle + e^{2\pi i\phi 2}|1\rangle \\ &\dots \\ \mathrm{qubit_1} &: |0\rangle + e^{2\pi i\phi 2^n}|1\rangle \end{aligned}$$

We know that the value of $\phi < 1$. We can represent this in binary notation in the form $0.\phi_1\phi_2...\phi_n$:

$$\phi = \sum_{j=1}^{n} \phi_j 2^{-j}$$

If we have another look at the control qubits using binary notation for ϕ instead, we can see the result of the multiple CU operations simply results in right bit shifts:

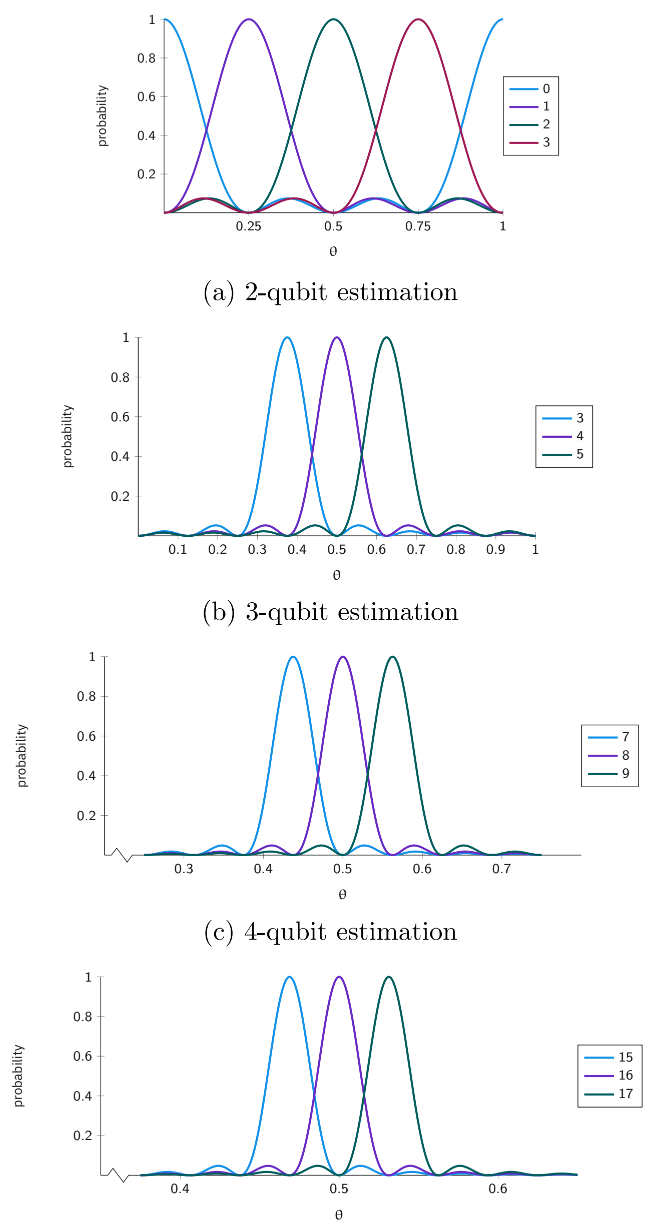
$$\begin{aligned} \mathrm{qubit_n} &: |0\rangle + e^{2\pi i(0.\phi_1\phi_2...\phi_n)}|1\rangle \\ \mathrm{qubit_{n\text{-}1}} &: |0\rangle + e^{2\pi i(0.\phi_2...\phi_n)}|1\rangle \\ &\dots \\ \mathrm{qubit_1} &: |0\rangle + e^{2\pi i(0.\phi_n)}|1\rangle \end{aligned}$$

If we look at the form of the first register after all the CU operations in the state $|\alpha\rangle$, it will resemble the result of performing the QFT we saw in equation 5. Here, our ω_j are:

$$\begin{aligned} \omega_1 &= e^{2\pi i x 2^{-1}} = e^{2\pi i(0.\phi_n)} \\ \omega_2 &= e^{2\pi i x 2^{-2}} = e^{2\pi i(0.\phi_{n-1}\phi_n)} \\ &\dots \\ \omega_n &= e^{2\pi i x 2^{-n}} = e^{2\pi i(0.\phi_1...\phi_n)} \end{aligned}$$

Simply performing the inverse QFT will give us $|\phi\rangle = |\phi_1\phi_2...\phi_n\rangle$. We can immediately see the approximation is limited by the number of qubits in the first register. A simple strategy would be to increase the number of qubits; however this would also increase the computational cost as we double our use of CU gates for each additional qubit.

It is possible our phase (ϕ) is not a discrete value that can be exactly decribed by n qubits, i.e. $|\phi\rangle \neq |\phi_1\phi_2...\phi_n\rangle$. Fortunately, this algorithm provides a good approximation regardless, where we can expect the best outcome to occur with a probability $\geq 4/\pi^2 \approx 40\%$. If we measure a worse outcome where the approximation is off by more than 2^{-n}, we can expect the probability to be at most 25% [7]. This is further illustrated in FIG. 2.3



(a) 2-qubit estimation

(b) 3-qubit estimation

(c) 4-qubit estimation

(d) 5-qubit estimation

Figure 2.3: Varying degree of precision by the phase estimation algorithm [7].

Chapter 3

Algorithm

The decision problem of the BTSP asks whether there exists a Hamiltonian cycle in which the weight of every edge is less than a specified threshold α. In such a cycle, if we denote the weight of any edge as γ_i, then it must satisfy the condition:

$$\gamma_i < \alpha \tag{3.1}$$

We will construct the algorithm in the following steps:

1. Normalize edge weights so no single hamiltonian cycle is greater than or equal to 1. This is to ensure we can appropriately use the phase estimation algorithm.

2. Construct a unitary operator that holds information regarding the hamiltonian cyles as phases in the diagonal. Our approach aligns with the findings presented by Ramakrishnan, Sharma, and Punnen: [8]

3. Set all edgeweights $\geq \alpha$ to zero and construct a secondary unitary operator similiar to step 2.

4. Create controlled gates using the unitary operators constructed in Step 2 and 3.

5. Identify all the eigenstates of the unitary operators that map to the phases associated with the hamiltonian cycles.

6. Perform phase estimation twice with an eigenstate using the control gates to evaluate the hamiltonian cycle before and after the edgeweights $\geq \alpha$ are set to zero.

7. Compare the two phases achieved. If they are equal, the corresponding hamiltonian cycle is a solution that satisfies the constraint.

3.1 Normalize Edge Weights

A hamiltonian cycle of a complete graph with N nodes requires N edge-weights to complete the cycle. A single graph consists a total of $N(N-1)$ edgeweights in a directed graph. we can choose the largest N and use these to normalize the edge weights. Let w describe our edge-weights and will be a list of $m = N(N-1)$ elements:

$$w = \{w_1, w_2, \ldots, w_m\}$$

Sort w in descending order to obtain:

$$w' = \{w'_1, w'_2, \ldots, w'_m\} \tag{3.2}$$

Where:

$w'_1 \geq w'_2 \geq \ldots \geq w'_m$

The sum S of the largest N items in w can be described as:

$$S = \sum_{i=1}^{N} w'_i \tag{3.3}$$

We can now perform the normalization. Let $\tilde{w}$ describe our normalized edge-weights:

$$\tilde{w} = (S + \epsilon)^{-1} w \tag{3.4}$$

Where: $\epsilon > 0$. The purpose of ϵ is to make sure if any normalized hamiltonian cycle is exactly equal to S then we do not have a zero phase.

3.2 Unitary Operator and Eigenstates associated with the Hamiltonian Cycles

We start by constructing diagonal matrices U_j, one for each node in a complete graph and describe the matrix elements:

$$[U_j]_{kk} = e^{2\pi i \gamma_{jk}(1-\delta_{jk})} \tag{3.5}$$

Where:

$1 \leq j, k \leq N$

N denotes the total number of nodes.

γ_{jk} represents the edgeweight connecting node $j \rightarrow k$.

Then we construct U, a tensor product of all the diagonal matrices:

$$U = \bigotimes_{j}^{N} U_j \tag{3.6}$$

U will be a $N^N \times N^N$ matrix with only the diagonal elements populated. Because the diagonal elements will entirely consist of phases $[U]_{kk} = e^{i\alpha_{kk}}$. We can confirm the unitary operator condition is satisfied: $U^\dagger U = \mathbb{1}$.

Given U's diagonal nature, its eigenstates align with the basis vectors. Our focus is on specific eigenstates corresponding to the Hamiltonian cycles, determined by the phases. To comprehend how the diagonal elements of U derive from the individual U_j matrices, we visualize the tensor product construction. Notably, the product populates the diagonal elements of U allowing a simplification where we consider these elements directly:

$$
\begin{aligned}
[U]_0 &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_0 \cdot [U_{N-1}]_0 \cdot [U_N]_0 \\
[U]_1 &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_0 \cdot [U_{N-1}]_0 \cdot [U_N]_1 \\
&\vdots \\
[U]_{N-1} &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_0 \cdot [U_{N-1}]_0 \cdot [U_N]_{N-1} \\
[U]_N &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_0 \cdot [U_{N-1}]_1 \cdot [U_N]_0 \\
&\vdots \\
[U]_{2N-1} &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_0 \cdot [U_{N-1}]_1 \cdot [U_N]_{N-1} \\
[U]_{2N} &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_0 \cdot [U_{N-1}]_2 \cdot [U_N]_0 \\
&\vdots \\
[U]_{N^2-1} &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_0 \cdot [U_0]_{N-1} \cdot [U_N]_{N-1} \\
[U]_{N^2} &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_1 \cdot [U_{N-1}]_0 \cdot [U_N]_0 \\
&\vdots \\
[U]_{N^2+N-1} &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_1 \cdot [U_{N-1}]_0 \cdot [U_N]_{N-1} \\
[U]_{N^2+N} &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_1 \cdot [U_{N-1}]_1 \cdot [U_N]_0 \\
&\vdots \\
[U]_{N^3-1} &= [U_1]_0 \cdot [U_2]_0 \cdot \ldots \cdot [U_{N-2}]_{N-1} \cdot [U_{N-1}]_{N-1} \cdot [U_N]_{N-1}
\end{aligned}
$$

This pattern indicates:

$$[U]_k = [U_1]_{\alpha_{N-1}} \cdot [U_2]_{\alpha_{N-2}} \cdot \ldots \cdot [U_{N-2}]_{\alpha_2} \cdot [U_2]_{\alpha_1} \cdot [U_N]_{\alpha_0} \tag{3.7}$$

Where:

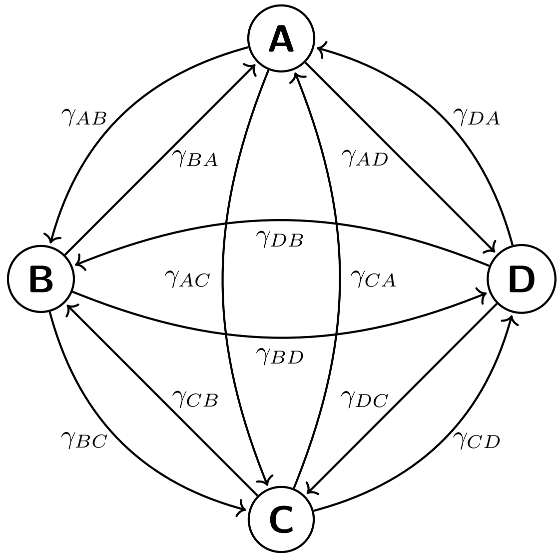
$$\alpha_i = \left(k // \left(N^i\right)\right) \% N$$

// denotes integer division

% is the modulus operation

We can see the pattern follows base-N counting where N is the total number of nodes. Simply converting k into base-N, will give us the indices of our original diagonal matrices. To locate the relevent eigenstates, we start by identifying the elements in U_j associated with a hamiltonian cycle, retrieve their respective indices, convert this string of indices from Base-N to k. and we would have identified our eigenstate $|k\rangle$.

3.2.1 The Four City Graph



For the 4 city problem we will start with four matrices to represent the 12 edgeweights from each node. Using 3.5, Where: $j, k \in \{A, B, C, D\}$. we can construct matrix A:

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{i2\pi\gamma_{AB}} & 0 & 0 \\ 0 & 0 & e^{i2\pi\gamma_{AC}} & 0 \\ 0 & 0 & 0 & e^{i2\pi\gamma_{AD}} \end{bmatrix}$$

Since we only populate the diagonal elements, we can ignore the other elements of the matrix. Let $a = \text{diag}(A)$, and lets construct the other diagonals:

$$a = \begin{bmatrix} 1 \\ e^{i2\pi\gamma_{AB}} \\ e^{i2\pi\gamma_{AC}} \\ e^{i2\pi\gamma_{AD}} \end{bmatrix} b = \begin{bmatrix} e^{i2\pi\gamma_{BA}} \\ 1 \\ e^{i2\pi\gamma_{BC}} \\ e^{i2\pi\gamma_{BD}} \end{bmatrix} c = \begin{bmatrix} e^{i2\pi\gamma_{CA}} \\ e^{i2\pi\gamma_{CB}} \\ 1 \\ e^{i2\pi\gamma_{CD}} \end{bmatrix} d = \begin{bmatrix} e^{i2\pi\gamma_{DA}} \\ e^{i2\pi\gamma_{DB}} \\ e^{i2\pi\gamma_{DC}} \\ 1 \end{bmatrix}$$

We then construct the tensor product with equation 3.6:

$$U = A \otimes B \otimes C \otimes D \tag{3.8}$$

The convience of dealing with only the diagonals we can similiarly state $u = \text{diag}(U)$, thus:

$$u = a \otimes b \otimes c \otimes d$$

Refering to equation 3.7 regarding the matrix elements for U, the diagonal elements for the 4-city problem will reduce to:

$$u_k = a_{\alpha_3} \cdot b_{\alpha_2} \cdot c_{\alpha_1} \cdot d_{\alpha_0} \tag{3.9}$$

With:

$$\alpha_i = \left(k // \left(4^i\right)\right) \%4$$

lets walk through identifying the eigenstate of one hamiltonian cycle. Lets say the cycle we choose is the following:

$$A \to D \to B \to C \to A \tag{3.10}$$

from here we can identify the edgeweights we care about are:

$$\gamma_{AD} + \gamma_{DB} + \gamma_{BC} + \gamma_{CA}$$

Thus the phase we would like to estimate would be given by the following element product:

$$a_3 \cdot d_1 \cdot b_2 \cdot c_0 = e^{i2\pi(\gamma_{AD}+\gamma_{DB}+\gamma_{BC}+\gamma_{CA})}$$

To correctly identify the eigenstate, we need to rearrange the product to match the form of equation 3.9:

$$a_3 \cdot d_1 \cdot b_2 \cdot c_0 = a_3 \cdot b_2 \cdot c_0 \cdot d_1$$

From here we simply read out the indices and based on our discussion under equation 3.7 , we can infer we are working in base 4. Thus we simply need to convert to base 10 to understand the exact column number and to base 2 to be used as the initialized eigenstate.

$$\text{base } 4 = 3201 \leftrightarrow \text{base } 10 = 225 \leftrightarrow \text{base } 2 = 11100001$$

Thus our eigenstate for 3.13 will be $|225\rangle$ or $|11100001\rangle$. We can perform an identical process for all the hamiltonian cycles to find their corresponding eigenstates. These are all listed in table 3.1 and and 3.2

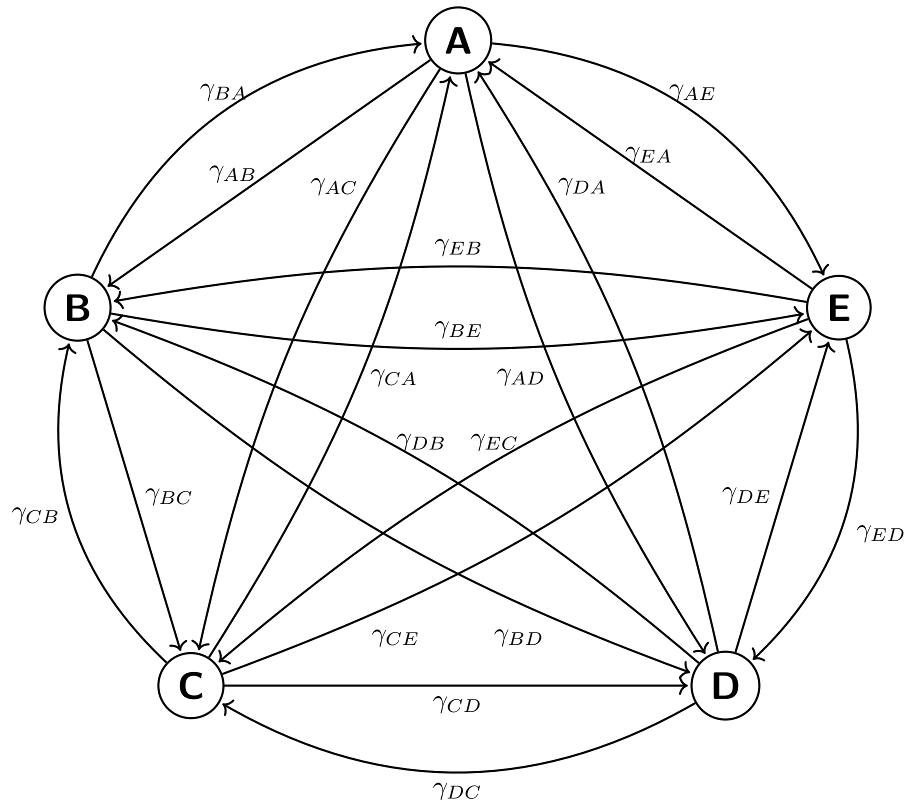
Hamiltonian Cycle	**Edge Weights Sum**	**Diagonal Elements Product**
$A \to B \to C \to D \to A$	$\gamma_{AB} + \gamma_{BC} + \gamma_{CD} + \gamma_{DA}$	$a_1 \cdot b_2 \cdot c_3 \cdot d_0$
$A \to B \to D \to C \to A$	$\gamma_{AB} + \gamma_{BD} + \gamma_{DC} + \gamma_{CA}$	$a_1 \cdot b_3 \cdot d_2 \cdot c_0$
$A \to C \to B \to D \to A$	$\gamma_{AC} + \gamma_{CB} + \gamma_{BD} + \gamma_{DA}$	$a_2 \cdot c_1 \cdot b_3 \cdot d_0$
$A \to C \to D \to B \to A$	$\gamma_{AC} + \gamma_{CD} + \gamma_{DB} + \gamma_{BA}$	$a_2 \cdot c_3 \cdot d_1 \cdot b_0$
$A \to D \to B \to C \to A$	$\gamma_{AD} + \gamma_{DB} + \gamma_{BC} + \gamma_{CA}$	$a_3 \cdot d_1 \cdot b_2 \cdot c_0$
$A \to D \to C \to B \to A$	$\gamma_{AD} + \gamma_{DC} + \gamma_{CB} + \gamma_{BA}$	$a_3 \cdot d_2 \cdot c_1 \cdot b_0$

Table 3.1: Hamiltonian cycles of the directed 4-city graph with their edgeweight summation and expected diagonal element products (3.9).

Rearranged Indices (Base 4)	**Base 10**	**Base 2**
1230	108	01101100
1302	114	01110010
2310	180	10110100
2031	141	10001101
3201	225	11100001
3012	198	11000110

Table 3.2: Eigenstates of matrix U (3.8), containing the normalized hamiltonian cycle edge weight sum of the directed 4-city graph.

3.2.2 The Five City Graph



We construct our matrix U with the tensor product as in equation 3.6.

$$U = A \otimes B \otimes C \otimes D \otimes E \tag{3.11}$$

Similiar to the four-city graph we only populate the diagonal elements, Let $a = \text{diag}(A)$, and let us construct the other diagonals:

$$a = \begin{bmatrix} 1 \\ e^{i2\pi\gamma_{AB}} \\ e^{i2\pi\gamma_{AC}} \\ e^{i2\pi\gamma_{AD}} \\ e^{i2\pi\gamma_{AE}} \end{bmatrix} b = \begin{bmatrix} e^{i2\pi\gamma_{BA}} \\ 1 \\ e^{i2\pi\gamma_{BC}} \\ e^{i2\pi\gamma_{BD}} \\ e^{i2\pi\gamma_{BE}} \end{bmatrix} c = \begin{bmatrix} e^{i2\pi\gamma_{CA}} \\ e^{i2\pi\gamma_{CB}} \\ 1 \\ e^{i2\pi\gamma_{CD}} \\ e^{i2\pi\gamma_{CE}} \end{bmatrix} d = \begin{bmatrix} e^{i2\pi\gamma_{DA}} \\ e^{i2\pi\gamma_{DB}} \\ e^{i2\pi\gamma_{DC}} \\ 1 \\ e^{i2\pi\gamma_{DE}} \end{bmatrix} e = \begin{bmatrix} e^{i2\pi\gamma_{EA}} \\ e^{i2\pi\gamma_{EB}} \\ e^{i2\pi\gamma_{EC}} \\ e^{i2\pi\gamma_{ED}} \\ 1 \end{bmatrix}$$

We can state $u = \text{diag}(U)$, thus:

$$u = a \otimes b \otimes c \otimes d \otimes e$$

Refering to equation 3.7 regarding the matrix elements for U, the diagonal elements for the 5-city problem will reduce to:

$$u_k = a_{\alpha_4} \cdot b_{\alpha_3} \cdot c_{\alpha_2} \cdot d_{\alpha_1} \cdot e_{\alpha_0} \tag{3.12}$$

With:

$$\alpha_i = \left(k // \left(5^i\right)\right) \% 5$$

Let us walk through identifying the eigenstate of one hamiltonian cycle:

$$A \rightarrow E \rightarrow D \rightarrow C \rightarrow B \rightarrow A \tag{3.13}$$

from here we can identify the edgeweights we care about are:

$$\gamma_{AE} + \gamma_{ED} + \gamma_{DC} + \gamma_{CB} + \gamma_{BA}$$

Thus the phase we would like to estimate would be given by the following element product:

$$a_4 \cdot e_3 \cdot d_2 \cdot c_1 \cdot b_0 = e^{i2\pi(\gamma_{AE}+\gamma_{ED}+\gamma_{DC}+\gamma_{CB}+\gamma_{BA})}$$

To correctly identify the eigenstate, we need to rearrange the product to match the form of equation 3.12:

$$a_4 \cdot e_3 \cdot d_2 \cdot c_1 \cdot b_0 = a_4 \cdot b_0 \cdot c_1 \cdot d_2 \cdot e_3$$

From here we simply read out the indices and based on our discussion under equation 3.7 , we can infer we are working in base 4. Thus we simply need to convert to base 10 to understand the exact column number and to base 2 to be used as the initialized eigenstate.

$$\text{base } 5 = 40123 \leftrightarrow \text{base } 10 = 2538 \leftrightarrow \text{base } 2 = 100111101010$$

Thus our eigenstate for 3.13 will be $|2538\rangle$ or $|100111101010\rangle$. We can perform an identical process for all the hamiltonian cycles to find their corresponding eigenstates. These are all listed in table 3.3 and 3.4

Hamiltonian Cycle	Edge Weights Sum	Matrix Elements Product
$A \to B \to C \to D \to E \to A$	$\gamma_{AB} + \gamma_{BC} + \gamma_{CD} + \gamma_{DE} + \gamma_{EA}$	$a_1 \cdot b_2 \cdot c_3 \cdot d_4 \cdot e_0$
$A \to B \to C \to E \to D \to A$	$\gamma_{AB} + \gamma_{BC} + \gamma_{CE} + \gamma_{ED} + \gamma_{DA}$	$a_1 \cdot b_2 \cdot c_4 \cdot e_3 \cdot d_0$
$A \to B \to D \to C \to E \to A$	$\gamma_{AB} + \gamma_{BD} + \gamma_{DC} + \gamma_{CE} + \gamma_{EA}$	$a_1 \cdot b_3 \cdot d_2 \cdot c_4 \cdot e_0$
$A \to B \to D \to E \to C \to A$	$\gamma_{AB} + \gamma_{BD} + \gamma_{DE} + \gamma_{EC} + \gamma_{CA}$	$a_1 \cdot b_3 \cdot d_4 \cdot e_2 \cdot c_0$
$A \to B \to E \to C \to D \to A$	$\gamma_{AB} + \gamma_{BE} + \gamma_{EC} + \gamma_{CD} + \gamma_{DA}$	$a_1 \cdot b_4 \cdot e_2 \cdot c_3 \cdot d_0$
$A \to B \to E \to D \to C \to A$	$\gamma_{AB} + \gamma_{BE} + \gamma_{ED} + \gamma_{DC} + \gamma_{CA}$	$a_1 \cdot b_4 \cdot e_3 \cdot d_2 \cdot c_0$
$A \to C \to B \to D \to E \to A$	$\gamma_{AC} + \gamma_{CB} + \gamma_{BD} + \gamma_{DE} + \gamma_{EA}$	$a_2 \cdot c_1 \cdot b_3 \cdot d_4 \cdot e_0$
$A \to C \to B \to E \to D \to A$	$\gamma_{AC} + \gamma_{CB} + \gamma_{BE} + \gamma_{ED} + \gamma_{DA}$	$a_2 \cdot c_1 \cdot b_4 \cdot e_3 \cdot d_0$
$A \to C \to D \to B \to E \to A$	$\gamma_{AC} + \gamma_{CD} + \gamma_{DB} + \gamma_{BE} + \gamma_{EA}$	$a_2 \cdot c_3 \cdot d_1 \cdot b_4 \cdot e_0$
$A \to C \to D \to E \to B \to A$	$\gamma_{AC} + \gamma_{CD} + \gamma_{DE} + \gamma_{EB} + \gamma_{BA}$	$a_2 \cdot c_3 \cdot d_4 \cdot e_1 \cdot b_0$
$A \to C \to E \to B \to D \to A$	$\gamma_{AC} + \gamma_{CE} + \gamma_{EB} + \gamma_{BD} + \gamma_{DA}$	$a_2 \cdot c_4 \cdot e_1 \cdot b_3 \cdot d_0$
$A \to C \to E \to D \to B \to A$	$\gamma_{AC} + \gamma_{CE} + \gamma_{ED} + \gamma_{DB} + \gamma_{BA}$	$a_2 \cdot c_4 \cdot e_3 \cdot d_1 \cdot b_0$
$A \to D \to B \to C \to E \to A$	$\gamma_{AD} + \gamma_{DB} + \gamma_{BC} + \gamma_{CE} + \gamma_{EA}$	$a_3 \cdot d_1 \cdot b_2 \cdot c_4 \cdot e_0$
$A \to D \to B \to E \to C \to A$	$\gamma_{AD} + \gamma_{DB} + \gamma_{BE} + \gamma_{EC} + \gamma_{CA}$	$a_3 \cdot d_1 \cdot b_4 \cdot e_2 \cdot c_0$
$A \to D \to C \to B \to E \to A$	$\gamma_{AD} + \gamma_{DC} + \gamma_{CB} + \gamma_{BE} + \gamma_{EA}$	$a_3 \cdot d_2 \cdot c_1 \cdot b_4 \cdot e_0$
$A \to D \to C \to E \to B \to A$	$\gamma_{AD} + \gamma_{DC} + \gamma_{CE} + \gamma_{EB} + \gamma_{BA}$	$a_3 \cdot d_2 \cdot c_4 \cdot e_1 \cdot b_0$
$A \to D \to E \to B \to C \to A$	$\gamma_{AD} + \gamma_{DE} + \gamma_{EB} + \gamma_{BC} + \gamma_{CA}$	$a_3 \cdot d_4 \cdot e_1 \cdot b_2 \cdot c_0$
$A \to D \to E \to C \to B \to A$	$\gamma_{AD} + \gamma_{DE} + \gamma_{EC} + \gamma_{CB} + \gamma_{BA}$	$a_3 \cdot d_4 \cdot e_2 \cdot c_1 \cdot b_0$
$A \to E \to B \to C \to D \to A$	$\gamma_{AE} + \gamma_{EB} + \gamma_{BC} + \gamma_{CD} + \gamma_{DA}$	$a_4 \cdot e_1 \cdot b_2 \cdot c_3 \cdot d_0$
$A \to E \to B \to D \to C \to A$	$\gamma_{AE} + \gamma_{EB} + \gamma_{BD} + \gamma_{DC} + \gamma_{CA}$	$a_4 \cdot e_1 \cdot b_3 \cdot d_2 \cdot c_0$
$A \to E \to C \to B \to D \to A$	$\gamma_{AE} + \gamma_{EC} + \gamma_{CB} + \gamma_{BD} + \gamma_{DA}$	$a_4 \cdot e_2 \cdot c_1 \cdot b_3 \cdot d_0$
$A \to E \to C \to D \to B \to A$	$\gamma_{AE} + \gamma_{EC} + \gamma_{CD} + \gamma_{DB} + \gamma_{BA}$	$a_4 \cdot e_2 \cdot c_3 \cdot d_1 \cdot b_0$
$A \to E \to D \to B \to C \to A$	$\gamma_{AE} + \gamma_{ED} + \gamma_{DB} + \gamma_{BC} + \gamma_{CA}$	$a_4 \cdot e_3 \cdot d_1 \cdot b_2 \cdot c_0$
$A \to E \to D \to C \to B \to A$	$\gamma_{AE} + \gamma_{ED} + \gamma_{DC} + \gamma_{CB} + \gamma_{BA}$	$a_4 \cdot e_3 \cdot d_2 \cdot c_1 \cdot b_0$

Table 3.3: Hamiltonian cycles of the directed 4-city graph with their edgeweight summation and expected diagonal element products (3.12).

Rearranged Indices (Base 5)	Base 10	Base 2
12340	970	001111001010
12403	978	001111010010
13420	1110	010001010110
13042	1022	001111111110
14302	1202	010010110010
14023	1138	010001110010
23140	1670	011010000110
24103	1778	011011110010
24310	1830	011100100110
20341	1346	010101000010
23401	1726	011010111110
20413	1358	010101001110
32410	2230	100010110110
34012	2382	100101001110
34120	2410	100101101010
30421	1986	011111000010
32041	2146	100001100010
30142	1922	011110000010
42301	2826	101100001010
43021	2886	101101000110
43102	2902	101101010110
40312	2582	101000010110
42013	2758	101011000110
40123	2538	100111101010

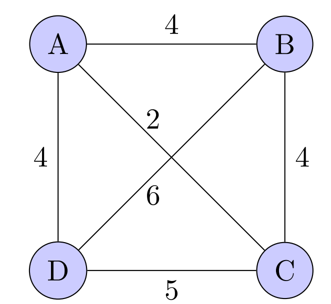
Table 3.4: Eigenstates of matrix U (3.11), containing the normalized hamiltonian cycle edge weight sum of the directed 4-city graph

Chapter 4

Simulations

4.1 An Undirected 4-City Graph

Lets consider the following example of a symmetric 4-city system. In this undirected graph we need to look at $(4-1)!/2 = 3$ hamiltonian cycles. The constraint for our BTSP in this case will involve $\gamma < 6$:



$$w = \{w_{AB}, w_{AC}, w_{AD}, w_{BC}, w_{CD}, w_{BD}\} = \{4, 2, 4, 4, 5, 6\}$$

4.1.1 Algorithm Construction

We will follow the instructions highlighted at the begining of chapter 3. We start by normalizing our edge weights. We need to sort our all edge weights in descending order as in equation 3.2:

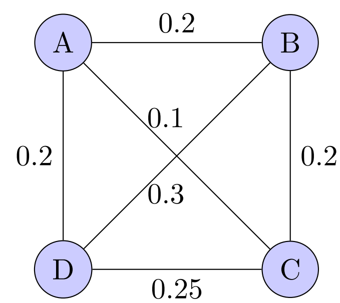
$$w' = \{6, 5, 4, 4, 4, 2\}$$

Then we need to retrieve the sum S as in equation 3.3

$$S = \sum_{i=1}^{4} w'_i = 6 + 5 + 4 + 4 = 19$$

From here we can normalize our edgeweights as in 3.4, we can set $\epsilon = 1$

$$\tilde{w} = \frac{\{4, 2, 4, 4, 5, 6\}}{20} = \{0.2, 0.1, 0.2, 0.2, 0.25, 0.3\}$$



Now we need to construct the unitary operator and eigenstates. Our matrix U and U' diagonals will look like the following:

$$u = \begin{bmatrix} 1 \\ e^{i2\pi(0.2)} \\ e^{i2\pi(0.1)} \\ e^{i2\pi(0.2)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.2)} \\ 1 \\ e^{i2\pi(0.2)} \\ e^{i2\pi(0.3)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.1)} \\ e^{i2\pi(0.2)} \\ 1 \\ e^{i2\pi(0.25)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.2)} \\ e^{i2\pi(0.3)} \\ e^{i2\pi(0.25)} \\ 1 \end{bmatrix}$$

$$u' = \begin{bmatrix} 1 \\ e^{i2\pi(0.2)} \\ e^{i2\pi(0.1)} \\ e^{i2\pi(0.2)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.2)} \\ 1 \\ e^{i2\pi(0.2)} \\ e^{i2\pi(0)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.1)} \\ e^{i2\pi(0.2)} \\ 1 \\ e^{i2\pi(0.25)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.2)} \\ e^{i2\pi(0)} \\ e^{i2\pi(0.25)} \\ 1 \end{bmatrix}$$

To construct our controlled matrices we can use the block matrix structure shown in 2.1. the number of diagonal elements in U and U' is 4^4 thus we need 8 eigenstate qubits to represent all 256 states:

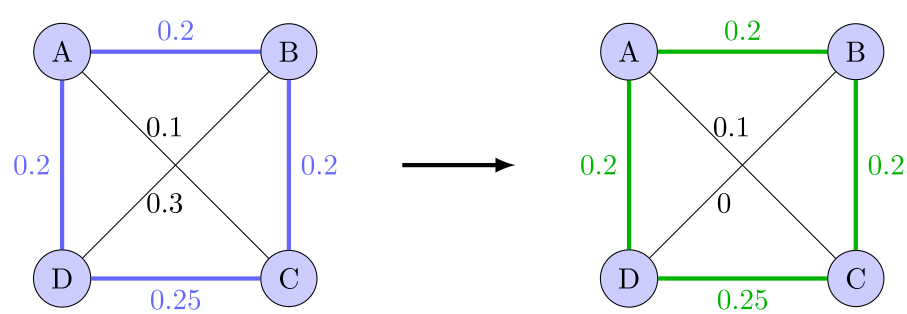
$$CU = \begin{bmatrix} \mathbb{I}_8 & 0 \\ 0 & U \end{bmatrix}, \quad CU' = \begin{bmatrix} \mathbb{I}_8 & 0 \\ 0 & U' \end{bmatrix}$$

Because we are dealing with the symmetric case. Based on Table 3.1 we can simply use the results and conversions from the first three cycles. Thus we will be estimating phases using the following eigenstates:

$$|108\rangle = |01101100\rangle$$
$$|114\rangle = |01110010\rangle$$
$$|180\rangle = |10110100\rangle$$

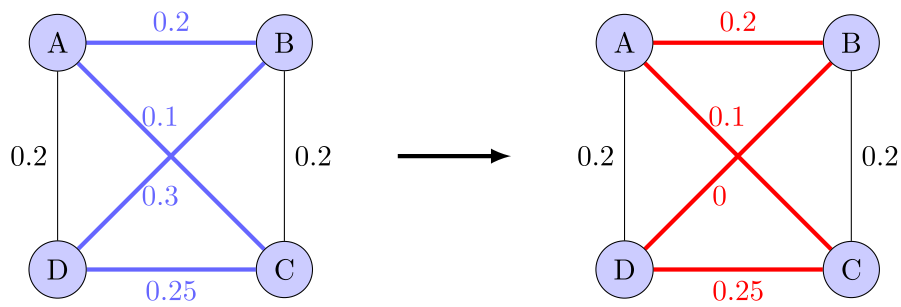
And expect the following phases:

Cycle 1: $A \to B \to C \to D \to A$



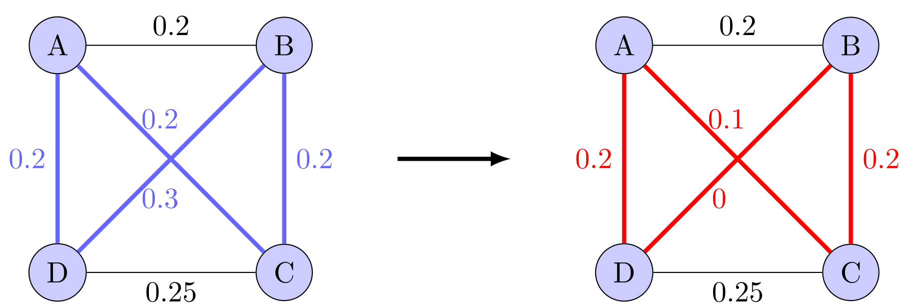
$$u_{108} = e^{i2\pi(\gamma_{AB}+\gamma_{BC}+\gamma_{CD}+\gamma_{DA})} = e^{i2\pi(0.85)}$$
$$u'_{108} = e^{i2\pi(\gamma_{AB}+\gamma_{BC}+\gamma_{CD}+\gamma_{DA})} = e^{i2\pi(0.85)}$$

Cycle 2: $A \to B \to D \to C \to A$



$$u_{114} = e^{i2\pi(\gamma_{AB}+\gamma_{BD}+\gamma_{DC}+\gamma_{CA})} = e^{i2\pi(0.85)}$$
$$u'_{114} = e^{i2\pi(\gamma_{AB}+\gamma_{BD}+\gamma_{DC}+\gamma_{CA})} = e^{i2\pi(0.55)}$$

Cycle 3: $A \to C \to B \to D \to A$



$$u_{180} = e^{i2\pi(\gamma_{AC}+\gamma_{CB}+\gamma_{BD}+\gamma_{DA})} = e^{i2\pi(0.80)}$$
$$u'_{180} = e^{i2\pi(\gamma_{AC}+\gamma_{CB}+\gamma_{BD}+\gamma_{DA})} = e^{i2\pi(0.50)}$$

4.1.2 Results: Simulations with Qiskit

We use Qiskit, an open source framework for quantum circuits to run simulations. Fig. 4.1 shows us the circuit for our first hamiltonian cycle initialized in eigenstate $|01101100\rangle$. We will run a similiar circuit for the other two hamiltonian cycles with the only change being the eigenstate initialization. We conduct an ideal simulation implying our results are not impacted by noise. Each circuit by default is run 1024 times which we can use as a quasi-probability distribution.

We can see in Fig. 4.2 our 3-qubit phase estimation for the first cycle with the highest counts is 111 111. The left set of binary digits refer to the phase estimated after our constrained is satisfied and similiarly the right is for estimation before. We can convert these binary digits to their decimal representation:

$$\text{Cycle 1}: \quad 0.111,\ 0.111 = 0.875,\ 0.875$$

We can perform a similiar analysis for the other two cycles:

$$\text{Cycle 2}: \quad 0.100,\ 0.111 = 0.500,\ 0.875$$
$$\text{Cycle 3}: \quad 0.110,\ 0.111 = 0.875,\ 0.750$$

From each cycle we can look at the two largest states (counts?) and summarize it in table 4.1. This table also shows us higher order qubit estimation, 4 & 5.

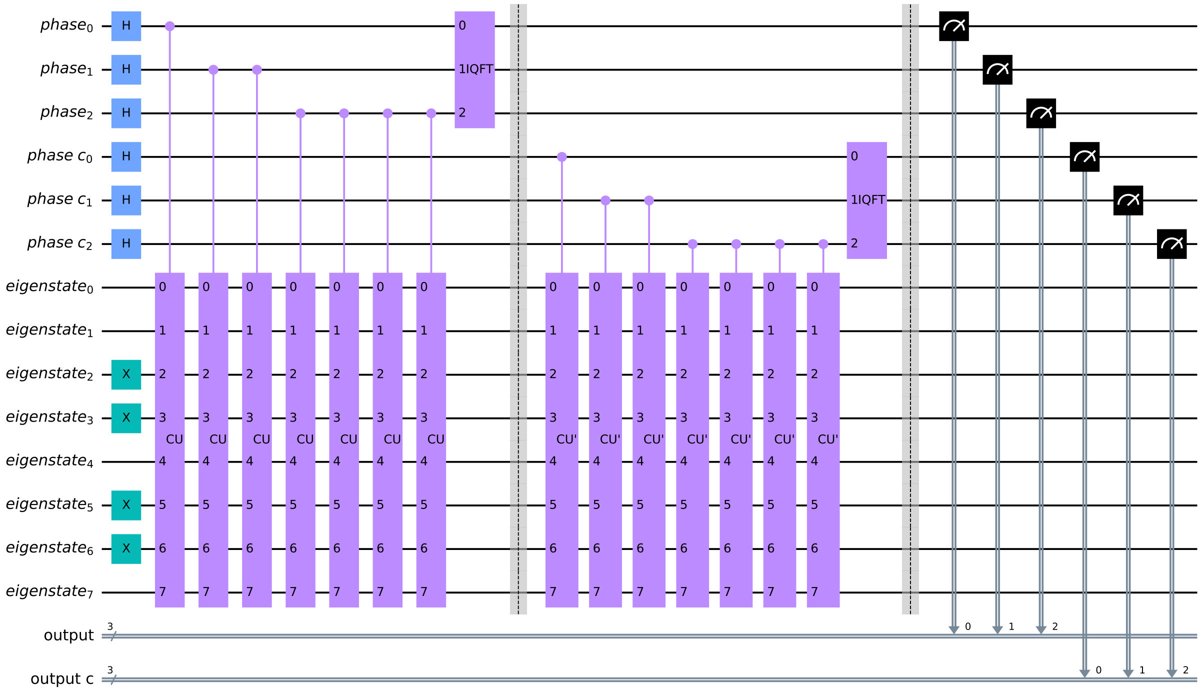


Figure 4.1: the quantum circuit for the BTSP: 3 qubit phase estimation is performed measuring the hamiltonian cycle $A \to B \to C \to D \to A$, using the corresponding eigenstate is $|01101100\rangle$. Due to Qiskit convention on qubit ordering, the eigentate is initialized in reverse. The CU gate denotes the control unitary matrix containing all the hamiltonian cycles. The CU' gate inhabits the same cycles but before it was constructed, all edgeweights not satisfying the constraint, $\geq \alpha$, were set to zero. We have two sets of 3 qubits to be measured and stored in to classical registers labelled 'output' and 'output c'.

Cycle	Expected	Phase Qubits	Highest Counts	Prob.	2nd Highest Counts	Prob.
1	0.85, 0.85	3	0.875, 0.875	77%	0.75, 0.875	6%
		4	0.875, 0.875	34%	0.875, 0.8125	16%
		5	0.84375, 0.84375	77%	0.84375, 0.875	5%
2	0.55, 0.85	3	0.5, 0.875	50%	0.625, 0.875	24%
		4	0.5625, 0.875	49%	0.5625, 0.8125	24%
		5	0.5625, 0.84375	51%	0.53125, 0.84375	21%
3	0.50, 0.80	3	0.5, 0.75	58%	0.5, 0.875	27%
		4	0.5, 0.8125	88%	0.5, 0.75	6%
		5	0.5, 0.8125	58%	0.5, 0.78125	26%

Table 4.1: Simulation results for the 4-city graph. N refers to the number of phase qubits, 1st and 2nd refer to the most probable and second most probable measurement, along with their associated probabilities on their right

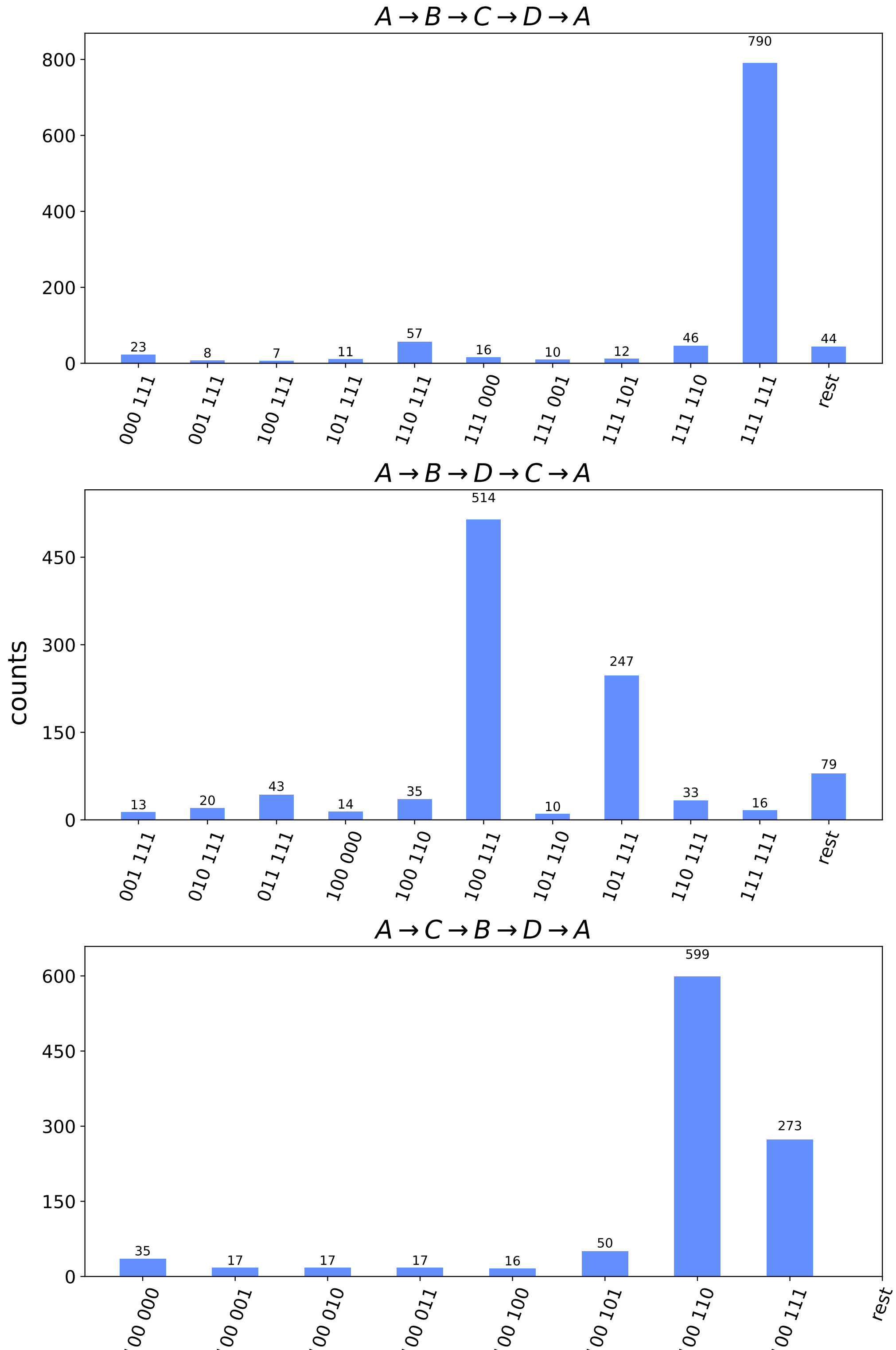


Figure 4.2: 3-qubit phase estimation for the 4-city graph

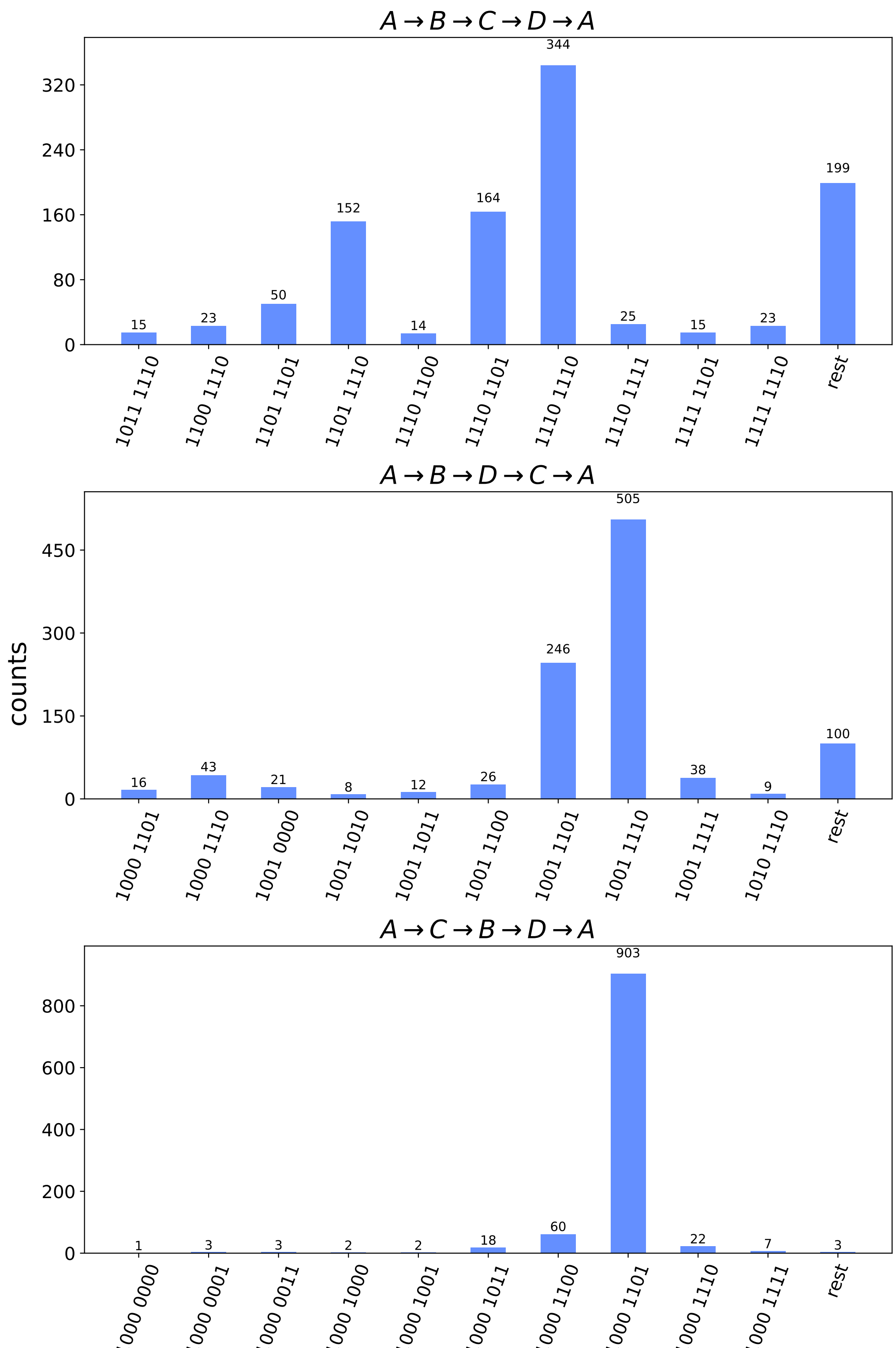


Figure 4.3: 4-qubit phase estimation for the 4-city graph

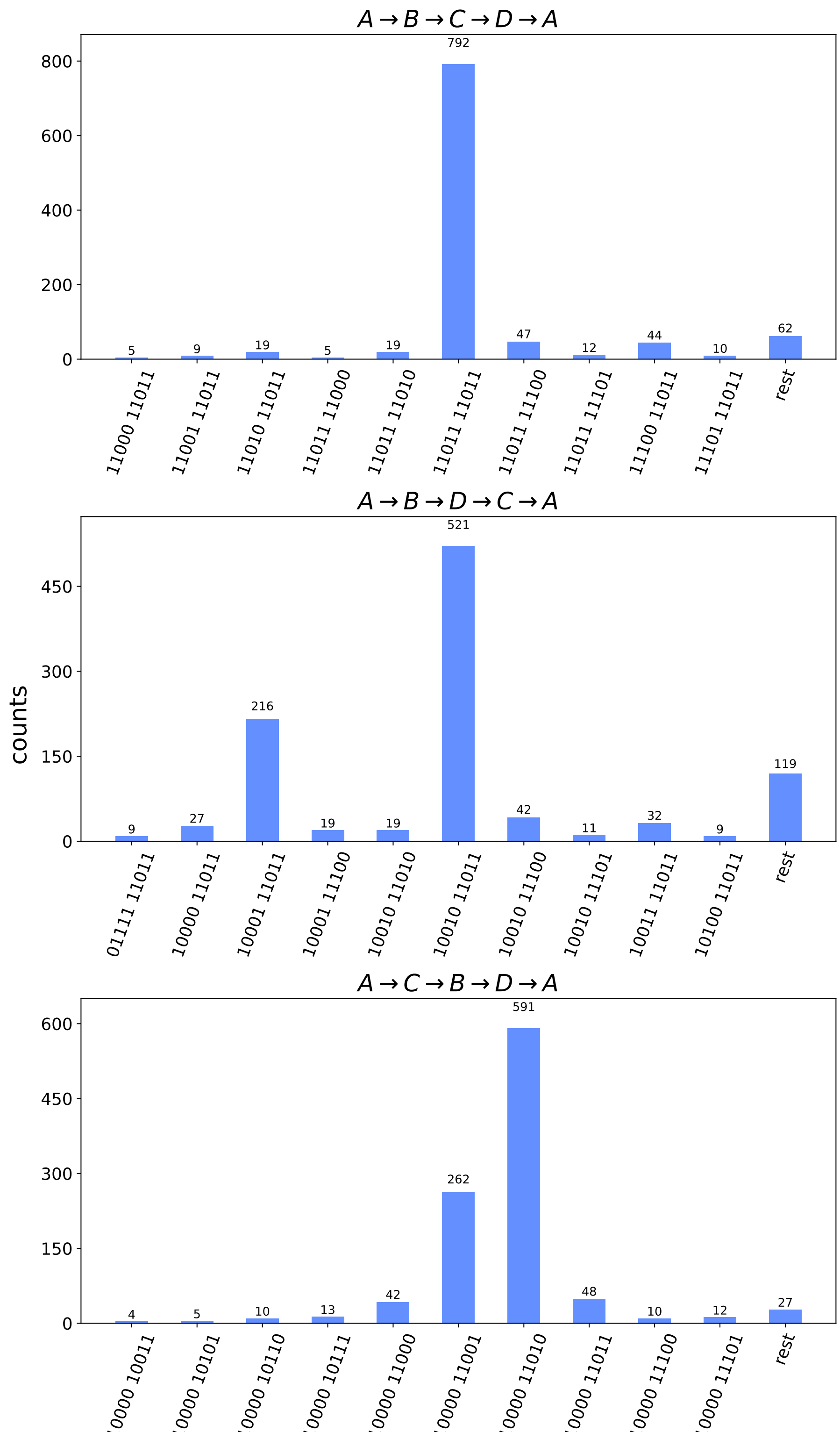
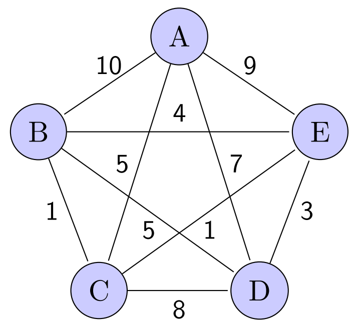


Figure 4.4: 5-qubit phase estimation for the 4-city graph

4.2 An Undirected 5-City Graph

Lets consider the following example of a symmetric 5-city system. In this undirected graph we need to look at $(5-1)!/2 = 12$ hamiltonian cycles. The constraint for our BTSP in this case will involve $\gamma < 9$:



4.2.1 Algorithm Construction

We will follow the instructions highlighted at the begining of chapter 3. We start by normalizing our edge weights. We need to sort our all edge weights in descending order as in equation 3.2:

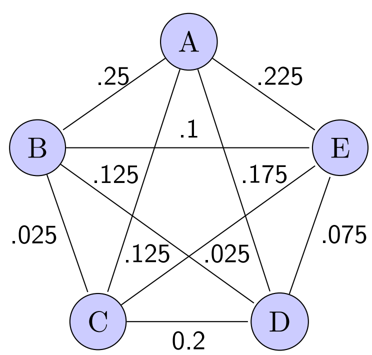
$$w' = \{10, 9, 8, 7, 5, 5, 4, 3, 1, 1\}$$

Then we need to retrieve the sum S as in equation 3.3

$$S = \sum_{i=1}^{5} w'_i = 10 + 9 + 8 + 7 + 5 = 39$$

From here we can normalize our edgeweights as in 3.4, we can set $\epsilon = 1$

$$\tilde{w} = \frac{\{10, 9, 8, 7, 5, 5, 4, 3, 1, 1\}}{40} = \{0.25, 0.225, 0.2, 0.175, 0.125, 0.125, 0.1, 0.075, 0.025, 0.025\}$$



Now we need to construct the unitary operator and eigenstates. Our matrix U and U' diagonals will look like the following:

$$u = \begin{bmatrix} 1 \\ e^{i2\pi(0.25)} \\ e^{i2\pi(0.125)} \\ e^{i2\pi(0.175)} \\ e^{i2\pi(0.225)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.25)} \\ 1 \\ e^{i2\pi(0.025)} \\ e^{i2\pi(0.125)} \\ e^{i2\pi(0.1)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.125)} \\ e^{i2\pi(0.025)} \\ 1 \\ e^{i2\pi(0.2)} \\ e^{i2\pi(0.025)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.175)} \\ e^{i2\pi(0.125)} \\ e^{i2\pi(0.2)} \\ 1 \\ e^{i2\pi(0.075)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.225)} \\ e^{i2\pi(0.1)} \\ e^{i2\pi(0.025)} \\ e^{i2\pi(0.075)} \\ 1 \end{bmatrix}$$

$$u' = \begin{bmatrix} 1 \\ e^{i2\pi(0)} \\ e^{i2\pi(0.125)} \\ e^{i2\pi(0.175)} \\ e^{i2\pi(0)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0)} \\ 1 \\ e^{i2\pi(0.025)} \\ e^{i2\pi(0.125)} \\ e^{i2\pi(0.1)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.125)} \\ e^{i2\pi(0.025)} \\ 1 \\ e^{i2\pi(0.2)} \\ e^{i2\pi(0.025)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0.175)} \\ e^{i2\pi(0.125)} \\ e^{i2\pi(0.2)} \\ 1 \\ e^{i2\pi(0.075)} \end{bmatrix} \otimes \begin{bmatrix} e^{i2\pi(0)} \\ e^{i2\pi(0.1)} \\ e^{i2\pi(0.025)} \\ e^{i2\pi(0.075)} \\ 1 \end{bmatrix}$$

The number of diagonal elements in U and U' is $5^5 = 3125$ thus we need atleast 12 eigenstate qubits to represent all 3125 states. We will have left over states ($2^{12} - 5^5 = 971$). Thus to accomodate this issue we need to add 1s to the end of the diagonal of matrices U and U'. With this method we do not affect the eigenstates. Then we can construct our block matrix structure shown in 2.1 to create the controlled gates:

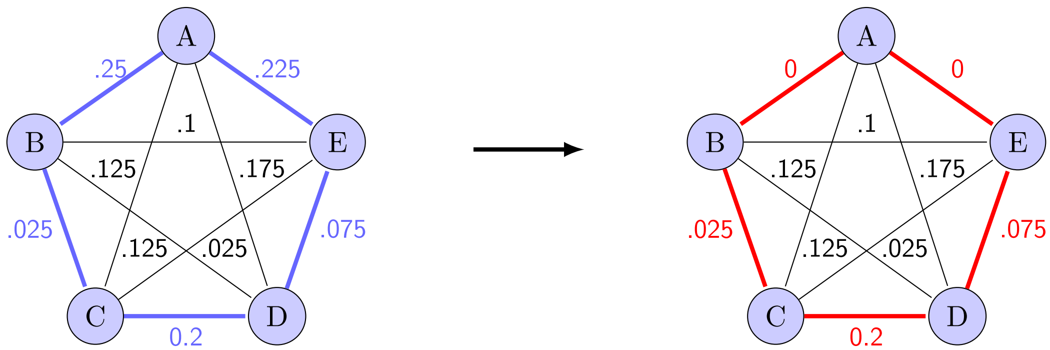
$$\mathrm{diag}(U) = [u, \mathrm{ones}(971)], \quad \mathrm{diag}(U') = [u', \mathrm{ones}(971)] \tag{4.1}$$
$$CU = \begin{bmatrix} \mathbb{I}_{12} & 0 \\ 0 & U \end{bmatrix}, \quad CU' = \begin{bmatrix} \mathbb{I}_{12} & 0 \\ 0 & U' \end{bmatrix}$$

Because we are dealing with the symmetric case, we will only use half of the eigenstates listed in Table 3.3:

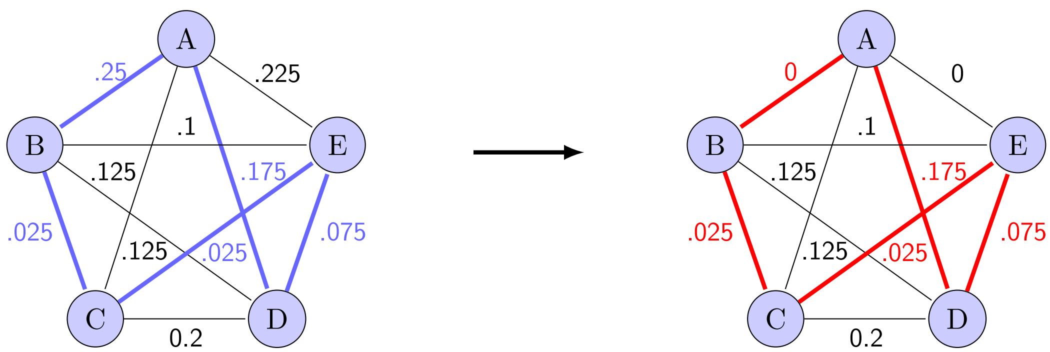
$$|970\rangle = |001111001010\rangle$$
$$|978\rangle = |001111010010\rangle$$
$$|1110\rangle = |010001010110\rangle$$
$$|1022\rangle = |001111111110\rangle$$
$$|1202\rangle = |010010110010\rangle$$
$$|1138\rangle = |010001110010\rangle$$
$$|1670\rangle = |011010000110\rangle$$
$$|1778\rangle = |011011110010\rangle$$
$$|1830\rangle = |011100100110\rangle$$
$$|1726\rangle = |011010111110\rangle$$
$$|2230\rangle = |100010110110\rangle$$
$$|2410\rangle = |100101101010\rangle$$

And expect the following phases:

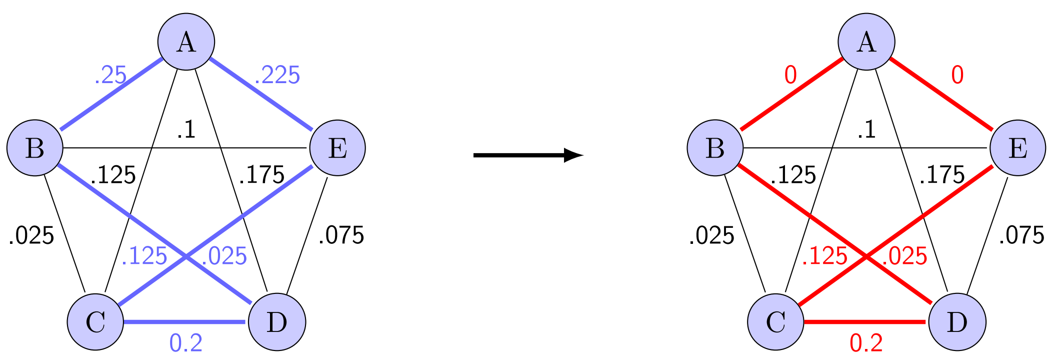
Cycle 1: $A \rightarrow B \rightarrow C \rightarrow D \rightarrow E \rightarrow A$. $\quad u_{970} = e^{i2\pi(0.775)}, \quad u'_{970} = e^{i2\pi(0.3)}$



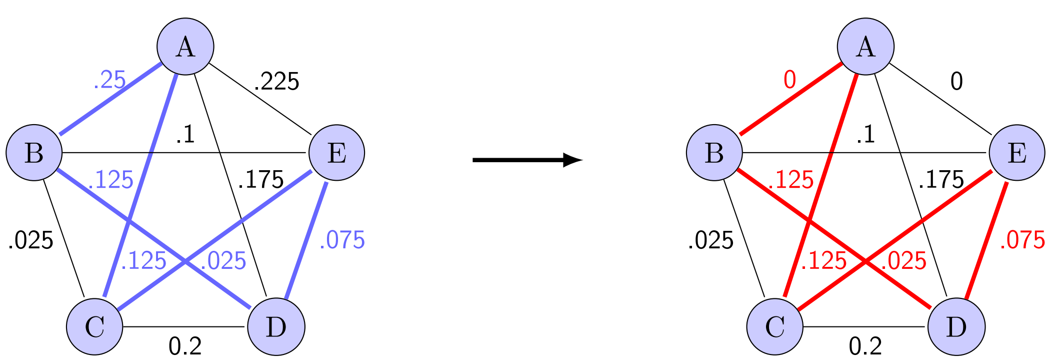
Cycle 2: $A \to B \to C \to E \to D \to A$. $u_{978} = e^{i2\pi(0.55)}$, $u'_{978} = e^{i2\pi(0.3)}$



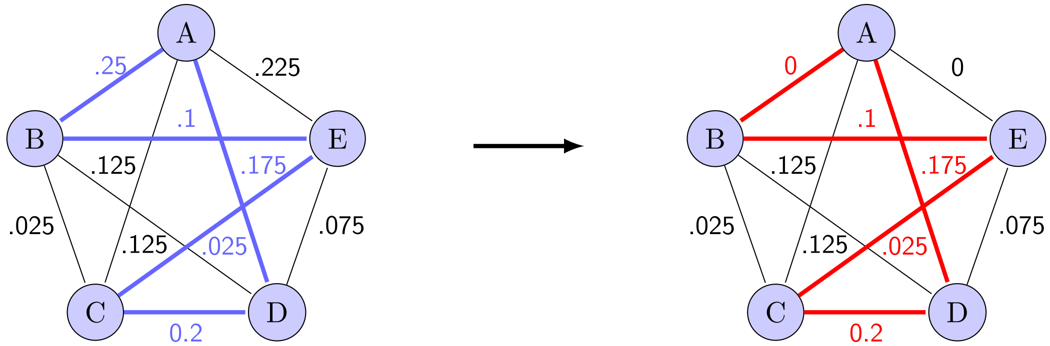
Cycle 3: $A \to B \to D \to C \to E \to A$. $u_{1110} = e^{i2\pi(0.825)}$, $u'_{1110} = e^{i2\pi(0.35)}$



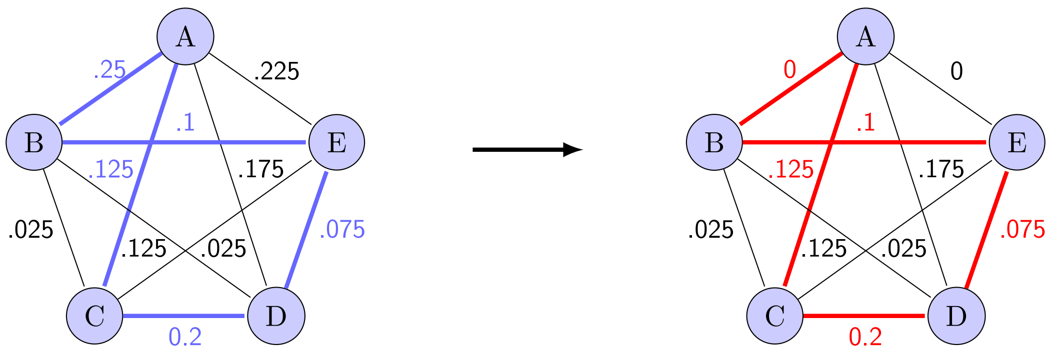
Cycle 4: $A \to B \to D \to E \to C \to A$. $u_{1022} = e^{i2\pi(0.6)}$, $u'_{1022} = e^{i2\pi(0.35)}$



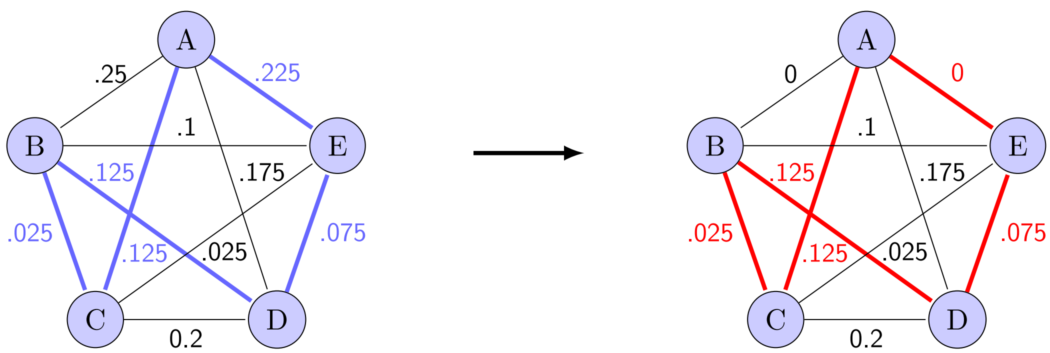
Cycle 5: $A \to B \to E \to C \to D \to A$. $u_{1202} = e^{i2\pi(0.75)}$, $u'_{1202} = e^{i2\pi(0.5)}$



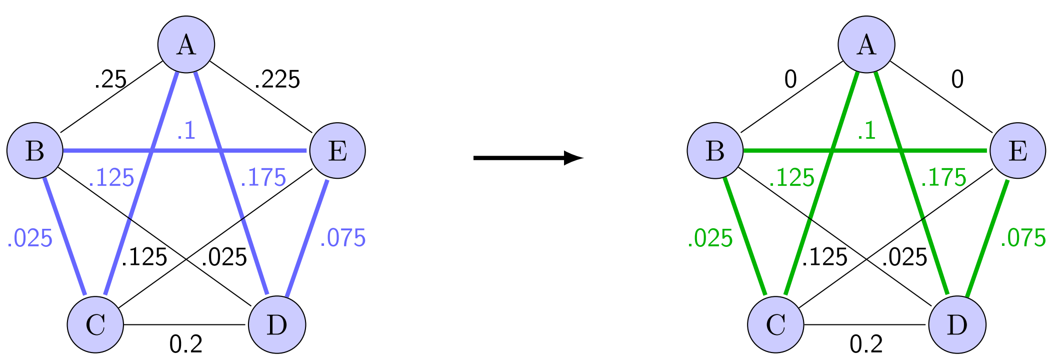
Cycle 6: $A \to B \to E \to D \to C \to A.$ $\qquad u_{1138} = e^{i2\pi(0.75)}, \qquad u'_{1138} = e^{i2\pi(0.5)}$



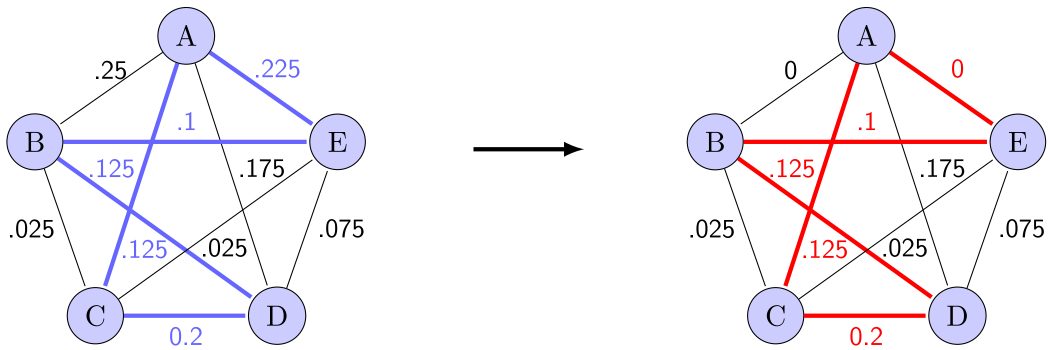
Cycle 7: $A \to C \to B \to D \to E \to A.$ $\qquad u_{1670} = e^{i2\pi(0.575)}, \qquad u'_{1670} = e^{i2\pi(0.35)}$



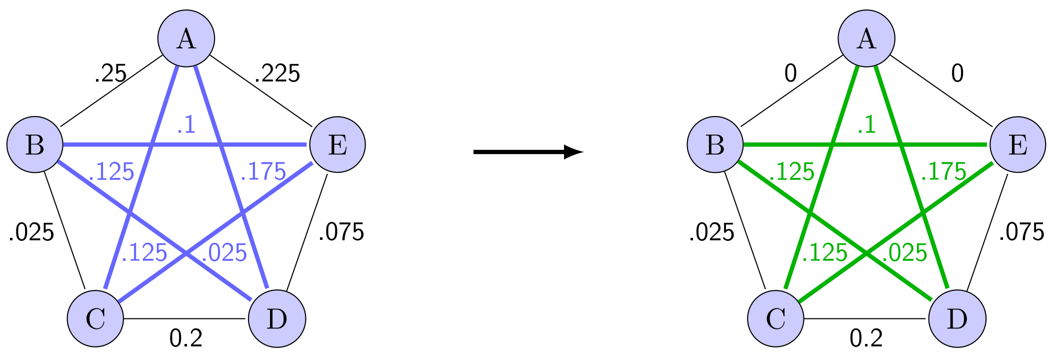
Cycle 8: $A \to C \to B \to E \to D \to A.$ $\qquad u_{1778} = e^{i2\pi(0.5)}, \qquad u'_{1778} = e^{i2\pi(0.5)}$



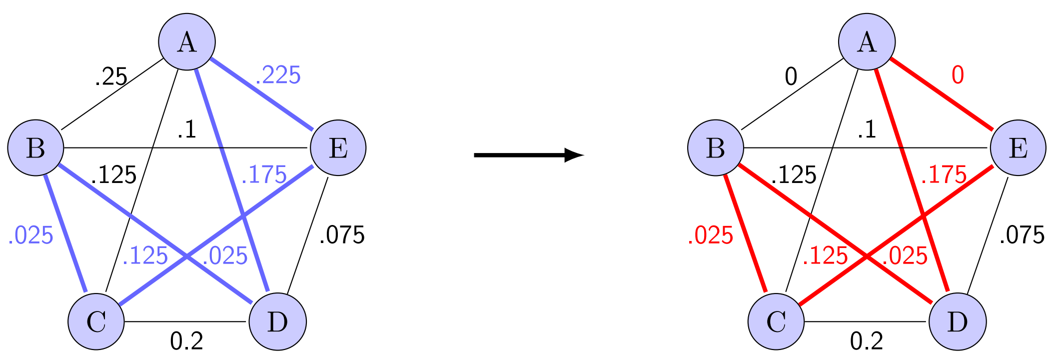
Cycle 9: $A \to C \to D \to B \to E \to A.$ $\qquad u_{1830} = e^{i2\pi(0.775)}, \qquad u'_{1830} = e^{i2\pi(0.55)}$



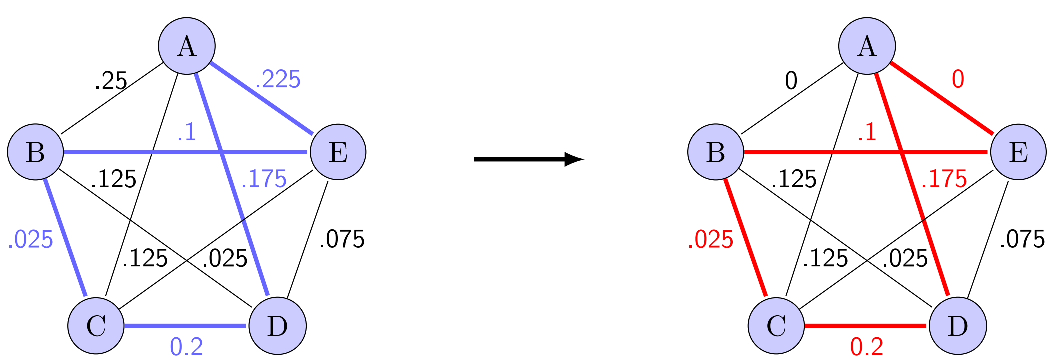
Cycle 10: $A \to C \to E \to B \to D \to A$. $\qquad u_{1726} = e^{i2\pi(0.55)}, \qquad u'_{1726} = e^{i2\pi(0.55)}$



Cycle 11: $A \to D \to B \to C \to E \to A$. $\qquad u_{2230} = e^{i2\pi(0.575)}, \qquad u'_{2230} = e^{i2\pi(0.35)}$



Cycle 12: $A \to D \to C \to B \to E \to A$. $\qquad u_{2410} = e^{i2\pi(0.725)}, \qquad u'_{2410} = e^{i2\pi(0.5)}$



4.2.2 Results: Simulations with Qiskit

Fig. 4.5 shows us the circuit for our first hamiltonian cycle initialized in eigenstate $|970\rangle = |001111001010\rangle$. We will run a similiar circuit for the other two hamiltonian cycles with the only change being the eigenstate initialization. We conduct an ideal simulation implying our results are not impacted by noise. Each circuit by default is run 1024 times which we can use as a quasi-probability distribution.

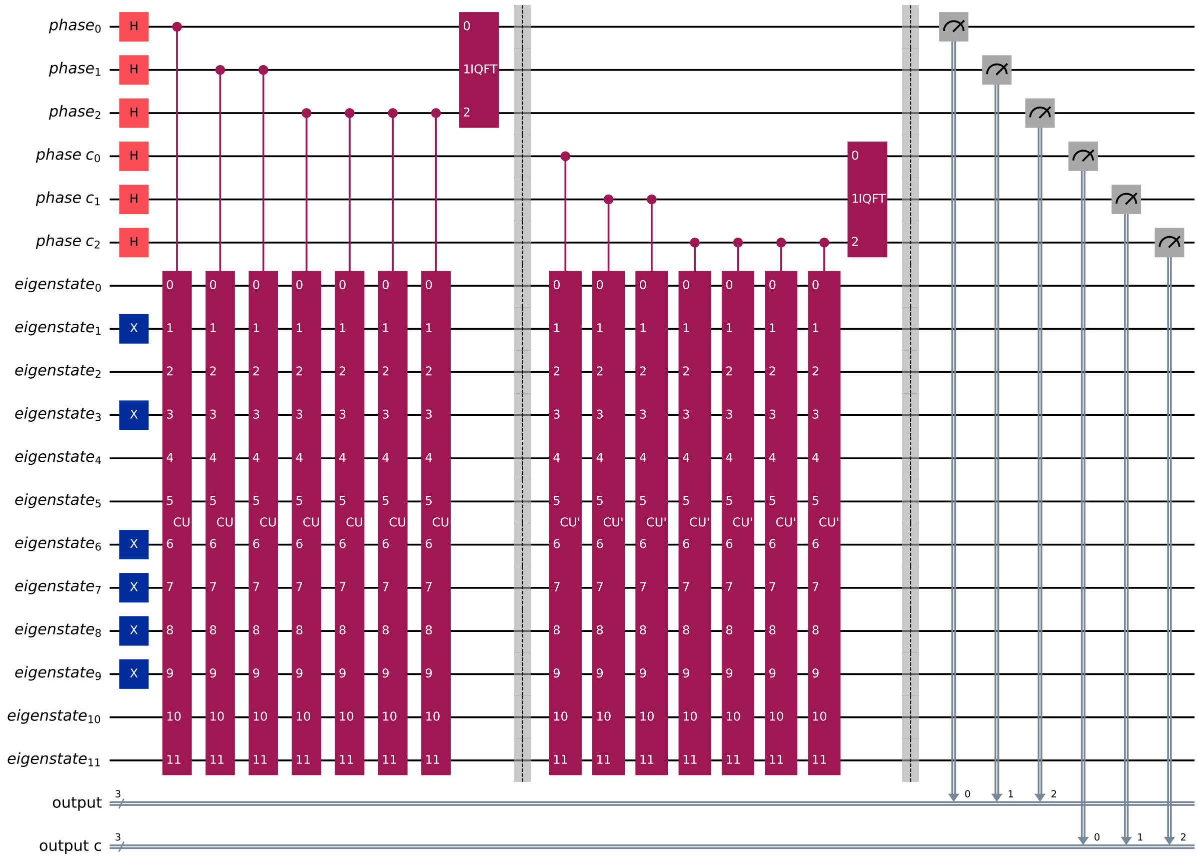


Figure 4.5: the quantum circuit for the BTSP: 3 qubit phase estimation is performed measuring the hamiltonian cycle $A \to B \to C \to D \to E \to A$, using the corresponding eigenstate is $|970\rangle = |001111001010\rangle$. Due to Qiskit convention on qubit ordering, the eigentate is initialized in reverse. The CU gate denotes the control unitary matrix containing all the hamiltonian cycles. The CU' gate inhabits the same cycles but before it was constructed, all edgeweights not satisfying the constraint, $\geq \alpha$, were set to zero. We have two sets of 3 qubits to be measured and stored in to classical registers labelled 'output' and 'output c'.

As we did for the 4-city graph, we present the top two counts (states?) for each hamiltonian cycle. 4-qubit estimation was performed as well. This results can be found in table 4.2.

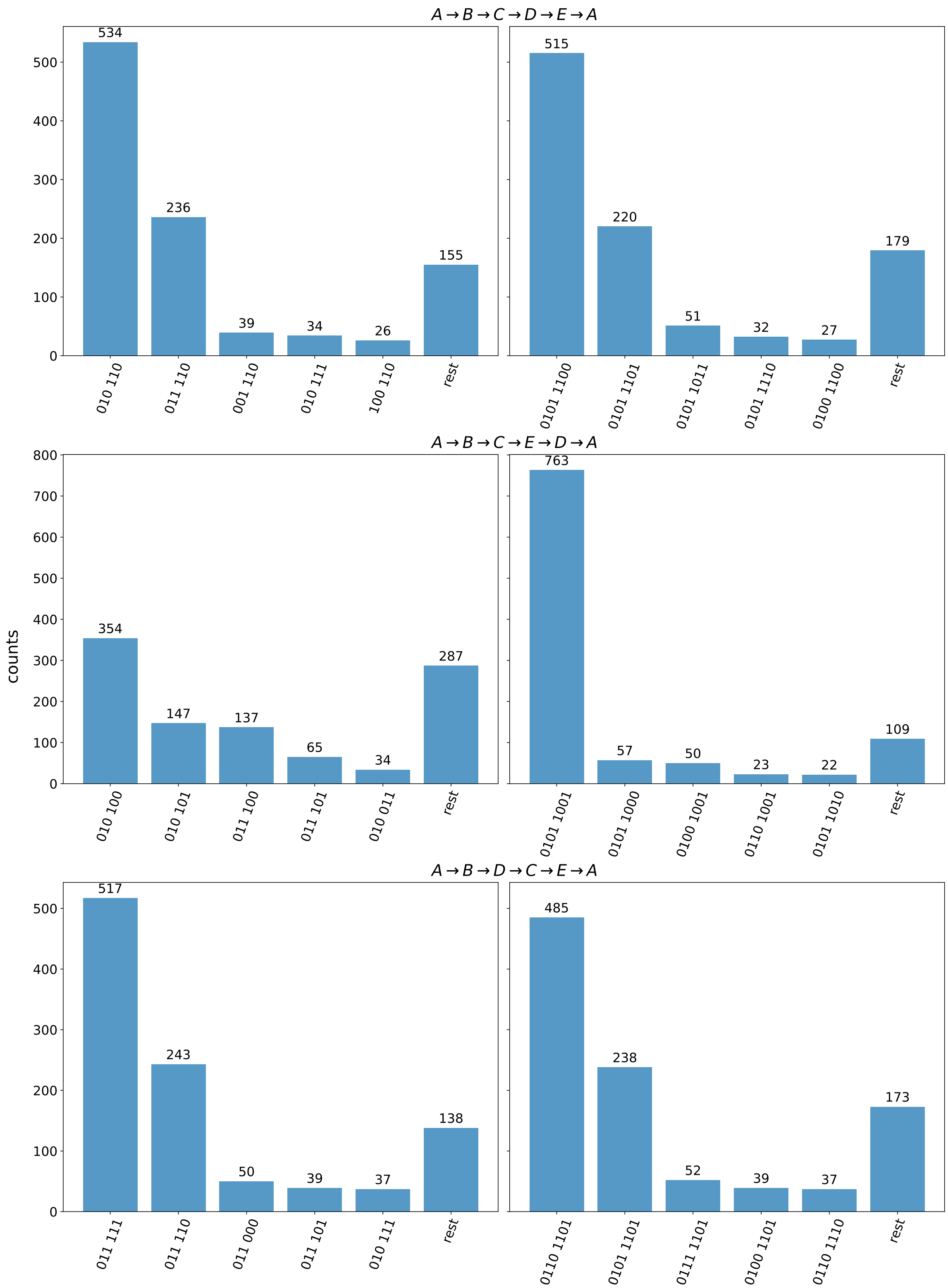


Figure 4.6: 3 qubit (left column) & 4 qubit (right column) phase estimation for the 5-city graph. Hamiltonian cycles: 1 to 3

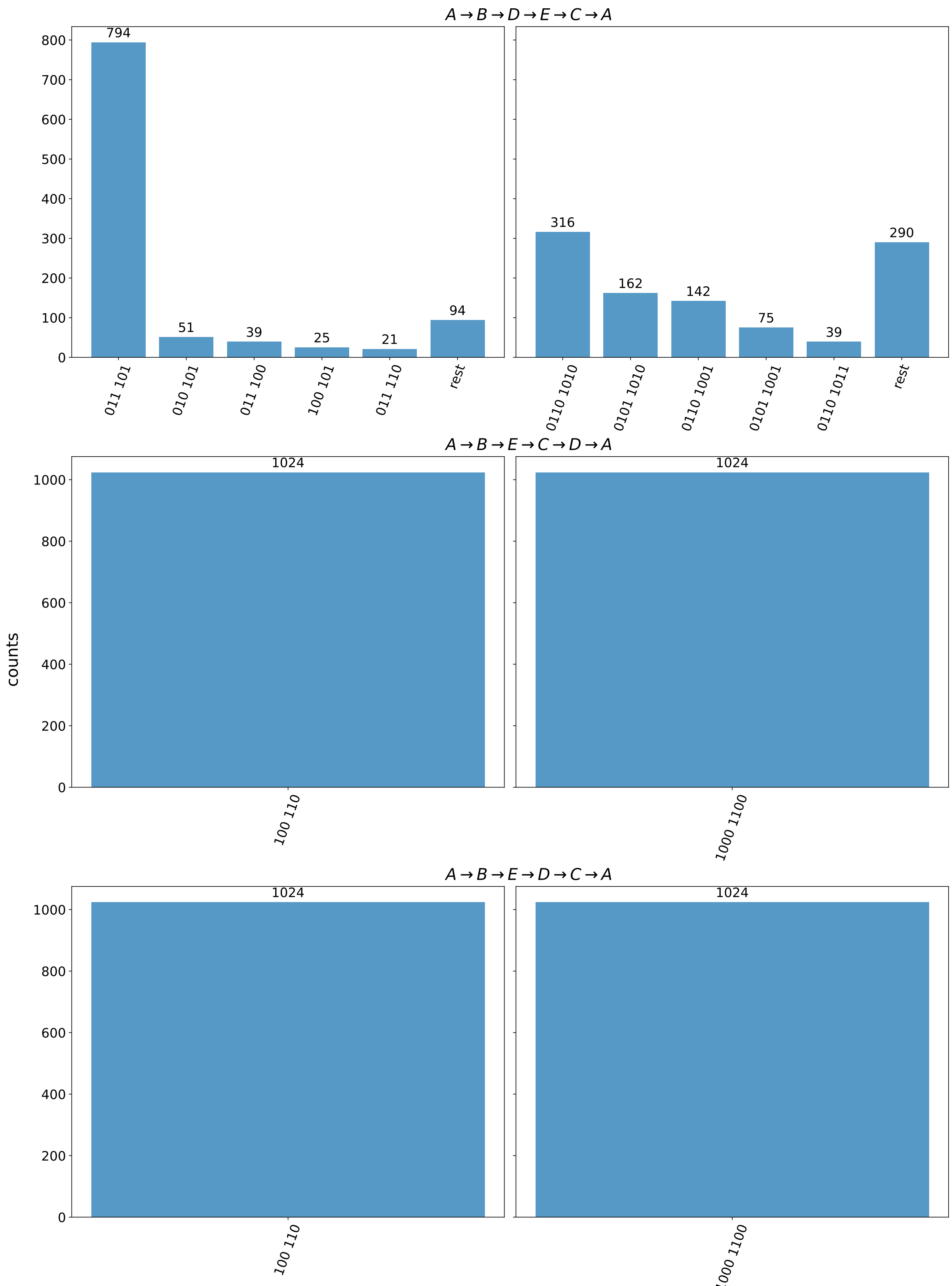


Figure 4.7: 3 qubit (left column) & 4 qubit (right column) phase estimation for the 5-city graph. Hamiltonian cycles: 4 to 6

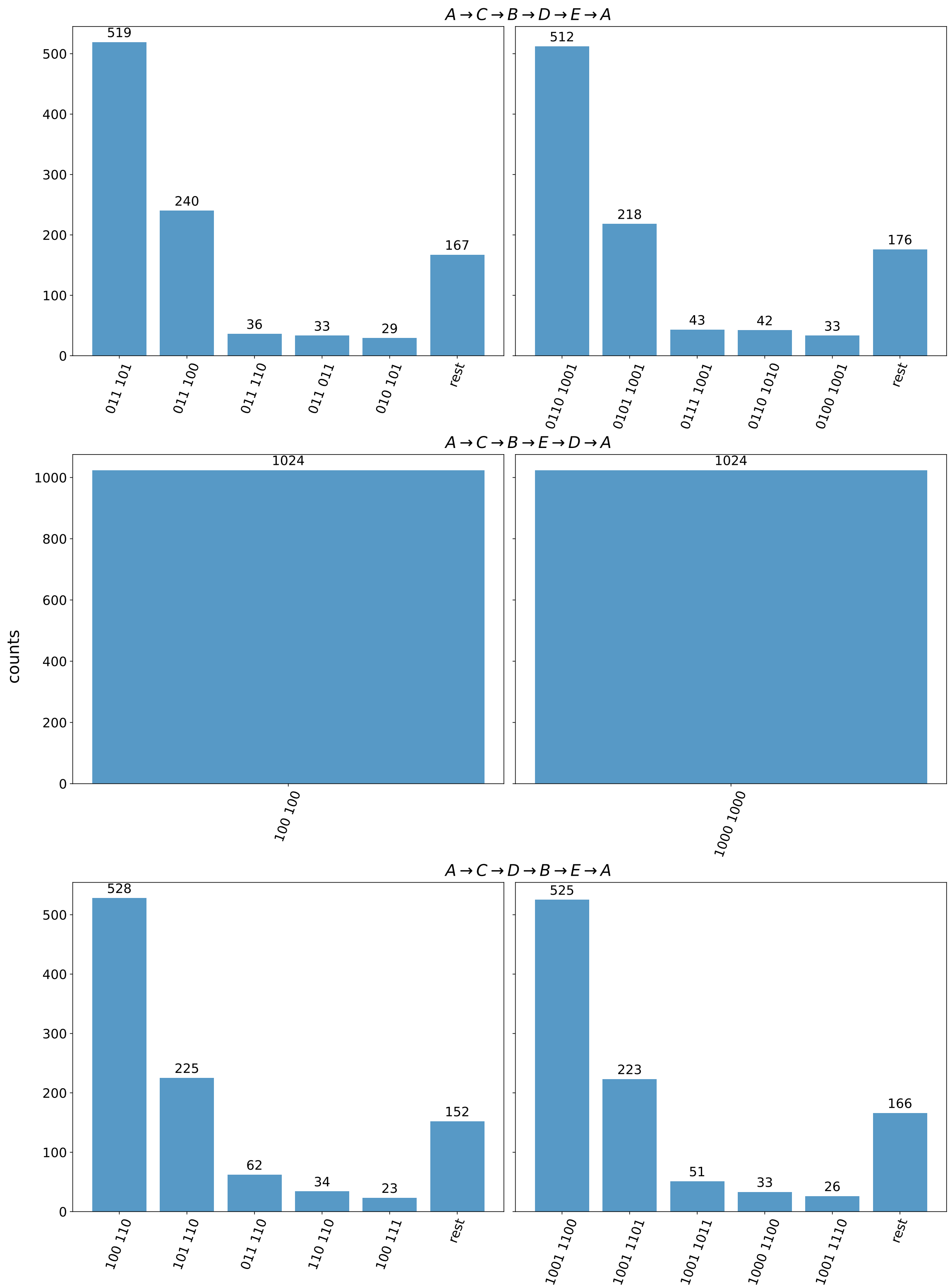


Figure 4.8: 3 qubit (left column) & 4 qubit (right column) phase estimation for the 5-city graph. Hamiltonian cycles: 7 to 9

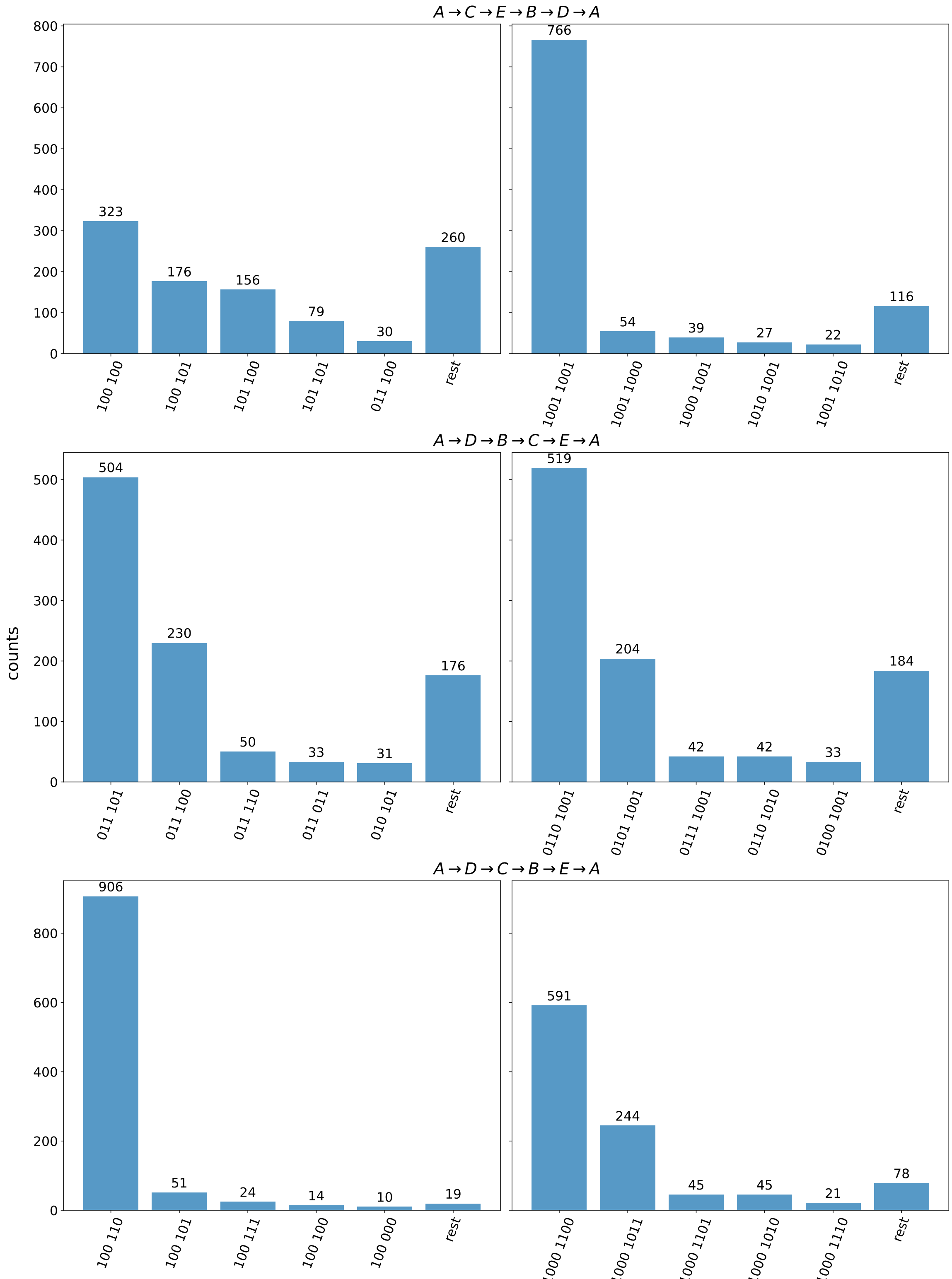


Figure 4.9: 3 qubit (left column) & 4 qubit (right column) phase estimation for the 5-city graph. Hamiltonian cycles: 10 to 12

Cycle	Expected	Phase Qubits	Highest Counts	Prob.	2nd Highest Counts	Prob.
1	0.3, 0.775	3	0.25, 0.75	52%	0.375, 0.75	23%
		4	0.3125, 0.75	50%	0.3125, 0.8125	21%
2	0.3, 0.55	3	0.25, 0.5	35%	0.25, 0.625	14%
		4	0.3125, 0.5625	75%	0.3125, 0.5	6%
3	0.35, 0.825	3	0.375, 0.875	50%	0.375, 0.75	24%
		4	0.375, 0.8125	47%	0.3125, 0.8125	23%
4	0.35, 0.6	3	0.375, 0.625	78%	0.25, 0.625	5%
		4	0.375, 0.625	31%	0.3125, 0.625	16%
5	0.5, 0.75	3	0.5, 0.75	100%		
		4	0.5, 0.75	100%		
6	0.5, 0.75	3	0.5, 0.75	100%		
		4	0.5, 0.75	100%		
7	0.35, 0.575	3	0.375, 0.625	51%	0.375, 0.5	23%
		4	0.375, 0.5625	50%	0.3125, 0.5625	21%
8	0.5, 0.5	3	0.5, 0.5	100%		
		4	0.5, 0.5	100%		
9	0.55, 0.775	3	0.5, 0.75	52%	0.625, 0.75	22%
		4	0.5625, 0.75	51%	0.5625, 0.8125	22%
10	0.55, 0.55	3	0.5, 0.5	32%	0.5, 0.625	17%
		4	0.5625, 0.5625	75%	0.5625, 0.5	5%
11	0.35, 0.575	3	0.375, 0.625	49%	0.375, 0.5	22%
		4	0.375, 0.5625	51%	0.3125, 0.5625	20%
12	0.50, 0.725	3	0.5, 0.75	88%	0.5, 0.625	5%
		4	0.5, 0.75	58%	0.5, 0.6875	24%

Table 4.2: Simulation results for the 5-city graph. N refers to the number of phase qubits, 1st and 2nd refer to the most probable and second most probable measurement, along with their associated probabilities on their right.

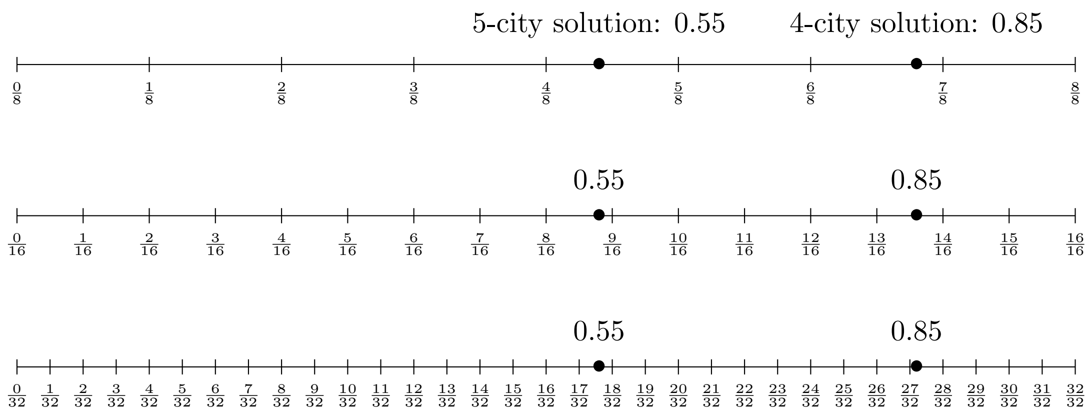
Chapter 5

Discussion

Referring to table 4.1. We can see cycle 1 represents our solution for our 4-city problem, as our expected phase estimation before and after the constraint satisfaction are both equal to 0.85. With 3-qubit estimation we were able to achieve a 77% quasi-probability of measuring the state: $0.875, 0.875$. Where we can conclude the most probable result indicates the cycle is a solution. One might expect a better quasi-probability as we increase the number of phase qubits, as it should perform a finer estimate of our phases. But as we see with 4-qubit estimation our quasi-probability or the most measured state: 0.875, 0.875, has dropped to 34%. This still is the state with the most counts that indicates our two phases are equal and this a solution. And a further 5-qubit estimation reverts the quasi-probability for the most measured state, in this case: 0.84375, 0.84375, to 77%. We can conclude from this that increases the number of phase qubits does not necessarily increase the probability of measuring a single state. To further elaborate on why this is the case, we can look at the representation of 0.85 in binary:

$$0.11011001100110011...$$

Because the binary representation of 0.85 is recurring, there is no point in which our estimation will be able to measure the value with perfect accuracy. We face a similiar issue with our 5-city simulation where cycle 10 represents our solution. The phase we try to estimate is 0.55, which is also recurring in binary. In both cases, we can only establish a very good approximate value. We can further illustrate this by looking at the resolution of 3,4, & 5 qubit estimation below and refer to FIG. 2.3 to understand the probabilities.

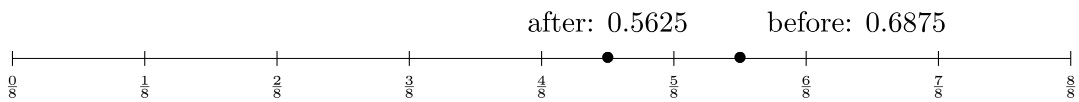


An easy way to interpret the number lines is that when the value is close to a specific step, that step is more likely to be measured. If it is perfectly inbetween two steps, we get the best possible approximation is either the lower bound or the upper bound both with the exact same probability, $P_b \approx 40\%$. It is important to note, that we are measuring two independent phases for each hamiltonian cycle, thus our best approximation will be $P_b^2 \approx 16\%$.

We can see for the 4-qubit estimation, the introduction of a more precise value of $13/16$ increased its probability of being measured as a good approximation for 0.85 and in turn decreased the probabiliy of $7/8 = 14/16$ being measured. Performing 5-qubit estimation does improve our results but does not justify the computational cost considering we achieved similiar results with 3-qubit estimation. We see a similiar issue with our results for the 5-city problem, we only simulated 3 and 4-qubit estimation but had we done 5, our confidence in the result would have decreased.

Unless we obtain a fortunate solution as in cycle 8 of the 5-city problem (FIG. 4.8), where our phase (0.5) can be respresented exactly, we need to run phase estimation a number of times from which we can use the mode of our results as the solution. And as we've discussed earlier, using a larger number of phase qubits does not neccesarily improve your confidence in the result. If we only consider the states with the highest counts in Tables 4.1, 4.1, then our results perfectly predict the solutions and non-solutions.

The question we need to ask is now is how many phase qubits are needed correctly identify a solution or non-solution based on the most frequent state measured? And the answer is we need to make sure the resolution of our phase qubits is larger than the constraint value, α, of the problem (Eq. 3.1). Lets consider a non-solution where the reduction to the phase is exactly the resolution of 3-qubit estimation, 0.125:



Based on our best approximation, we are likely to obtain any of the four following results most frequently with $P_b^2 \approx 16\%$:

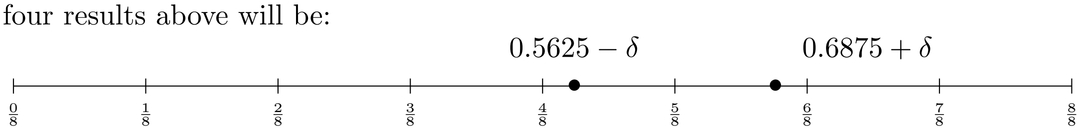
$$P_1 : 0.625, 0.625$$

$$P_2 : 0.500, 0.625$$

$$P_3 : 0.625, 0.750$$

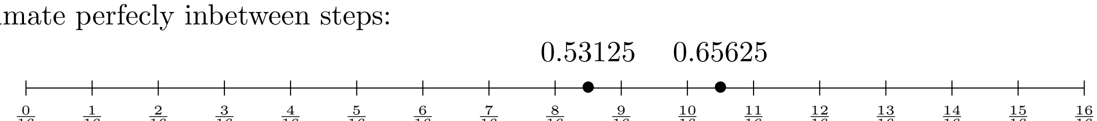
$$P_4 : 0.500, 0.750$$

Here we can see we run a risk of selecting P_1. By extending the distance between our phases, we reduce the probability of measuring 0.625 and we can qualitatively predict how probable our four results above will be:



$$P_1 < P_2 = P_3 < P_4$$

We actually simulated a similiar case in cycle 7 of our 5-city problem (FIG. 4.8), where the least probable result of the top 4 states, indicated the cycle was a solution. If $\delta << 1$, we would have to run our circuit many times over to appropriately measure the non-solution as the most frequent result. Otherwise we run the risk again of predicting a solution with P_1 as it would be very close to P_4. A safe bet would be to have a phase resolution atleast twice the constraint value. Lets illustrate this again by inconveniently placing the phases we hope to estimate perfecly inbetween steps:



We now run zero risk of the four most probable states indicating a solution. As our measurement will likely collapse to any of these four options with $P_b^2 \approx 16\%$:

$$P_1 : 0.5000, 0.6250$$

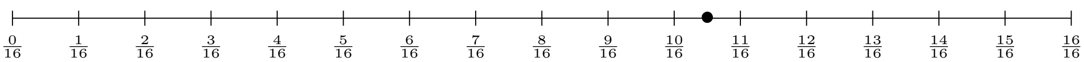
$$P_2 : 0.5000, 0.6875$$

$$P_3 : 0.5625, 0.6250$$

$$P_4 : 0.5625, 0.6875$$

And we can also show in the case of a solution, two of the four states will show it is a solution and the other two will not, but we can confidently say it is simply a rounding error since our constraint value would reduce a phase by much more. We can illustrate this considering the phase 0.65625:

before & after: 0.65625



$$P_1 : 0.6250, 0.6250$$

$$P_2 : 0.6250, 0.6875$$

$$P_3 : 0.6875, 0.6250$$

$$P_4 : 0.6875, 0.6875$$

We can also discuss the number of eigenstate qubits needed. Our method asks us to construct a matrix of size $N^N \times N^N$, where N represents the number of cities. This does result in a unitary matrix however, it cannot be neccesarily represented by an exact number of qubits.We saw this issue in our 5-city problem, where we introduced ones at the end of the matrix (Eq.4.1). If n represents the number of qubits we need and m represents the number of cities, we need to solve the equation:

$$2^n = m^m$$

$$n = m\log_2(m)$$

With this we can conclude the number of eigenstate qubits needed will scale polynomially where it $< m^2$. For example in the case of 5 cities, $n \approx 11.6$ and we round up to 12 qubits.

Because we run through all hamiltonian cycles to solve this problem our time complexity remains $O((N-1)!)$. We can however solve this decision problem by running all hamiltonian cycles in parallel reducing our execution time but the tradeoff would be introducing exponential space complexity, $O((N-1)!)$.

Bibliography

[1] P.W. Shor. Algorithms for quantum computation: discrete logarithms and factoring. In *Proceedings 35th Annual Symposium on Foundations of Computer Science*, pages 124–134, 1994.

[2] Lov K. Grover. A fast quantum mechanical algorithm for database search, 1996.

[3] John Larusic. A heuristic for solving the bottleneck traveling salesman problem. 2005.

[4] Ravi Ramakrishnan, Prabha Sharma, and Abraham P. Punnen. An efficient heuristic algorithm for the bottleneck traveling salesman problem. *Opsearch*, 46(3):275–288, 09 2009. Copyright - Operational Research Society of India 2009; Last updated - 2023-08-22.

[5] A. Yu. Kitaev. Quantum measurements and the abelian stabilizer problem, 1995.

[6] Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, 2000.

[7] Phase-estimation and factoring: Ibm quantum learning.

[8] Karthik Srinivasan, Saipriya Satyajit, Bikash K. Behera, and Prasanta K. Panigrahi. Efficient quantum algorithm for solving travelling salesman problem: An ibm quantum experience, 2018.

Appendix A

Hamiltonian Cycles and Locating Eigenstates Code

The code detailed in this section can be used to generate the information found in Tables 3.1, 3.2, 3.3 and 3.4, which construct the Hamiltonian cycles and locate the eigenstates.

[1]:
```python
from itertools import permutations
import numpy as np

def hamiltonian_cycles(cities, symmetric = False):
    'returns a list of all possible hamiltonian cycles for a given list of cities'
    start = cities[0]
    cycles = []
    for permutation in permutations(cities[1:]):
        cycle = start + ''.join(permutation) + start
        if symmetric:
            if cycle[::-1] not in cycles:
                cycles.append(cycle)
        else:
            cycles.append(cycle)
    return cycles

def map_indices(cities, symmetric = False):
    'returns all the hamiltonian cycles and the indices'
    cycles = hamiltonian_cycles(cities, symmetric = symmetric)
    index_map = {cities[i]: str(range(len(cities))[i]) for i in range(len(cities))}
    indices_cycles = []
    for cycle in cycles:
        indices_city = ''
        for city in cycle[1:]:
            indices_city += index_map[city]
        indices_cycles.append(indices_city)
    return cycles, indices_cycles

def sort_indices(cycles, indices_cycles):
    'sorts the indices'
    results = []
    for cycle, index in zip(cycles, indices_cycles):
        pairs = list(zip(cycle, index))
        sorted_pairs = sorted(pairs, key = lambda pair: pair[0]) # sorts by city name
        sorted_index = ''.join([pair[1] for pair in sorted_pairs])
        results.append([cycle, index, sorted_index])
    return results
```

[2]:
```python
cities = ['A', 'B', 'C', 'D', 'E']
cycles, indices_cycles = map_indices(cities, symmetric = True)
cycles, indices_cycles
```

[2]:
```
(['ABCDEA',
  'ABCEDA',
  'ABDCEA',
  'ABDECA',
  'ABECDA',
  'ABEDCA',
  'ACBDEA',
  'ACBEDA',
  'ACDBEA',
  'ACEBDA',
  'ADBCEA',
```

```
 'ADCBEA'],
['12340',
 '12430',
 '13240',
 '13420',
 '14230',
 '14320',
 '21340',
 '21430',
 '23140',
 '24130',
 '31240',
 '32140'])
```

[3]:
```python
table = sort_indices(cycles, indices_cycles)
print("cycle, index, sorted_index")
table
```

```
cycle, index, sorted_index
```

[3]:
```
[['ABCDEA', '12340', '12340'],
 ['ABCEDA', '12430', '12403'],
 ['ABDCEA', '13240', '13420'],
 ['ABDECA', '13420', '13042'],
 ['ABECDA', '14230', '14302'],
 ['ABEDCA', '14320', '14023'],
 ['ACBDEA', '21340', '23140'],
 ['ACBEDA', '21430', '24103'],
 ['ACDBEA', '23140', '24310'],
 ['ACEBDA', '24130', '23401'],
 ['ADBCEA', '31240', '32410'],
 ['ADCBEA', '32140', '34120']]
```

[4]:
```python
# Base 10 and 2 conversions
table = np.array(table)
indices = table[:,2]
base_10 = np.array([int(indices[i], len(cities)) for i in range(len(indices))])
base_2  = np.array(["{0:b}".format(base_10[i]) for i in range(len(base_10))])
table = np.append(table, base_10.reshape(-1,1), axis=1)
table = np.append(table, base_2.reshape(-1,1), axis=1)
print("cycle, index, sorted_index, base 10, base 2 \n",table)
```

```
cycle, index, sorted_index, base 10, base 2
 [['ABCDEA' '12340' '12340' '970' '1111001010']
 ['ABCEDA' '12430' '12403' '978' '1111010010']
 ['ABDCEA' '13240' '13420' '1110' '10001010110']
 ['ABDECA' '13420' '13042' '1022' '1111111110']
 ['ABECDA' '14230' '14302' '1202' '10010110010']
 ['ABEDCA' '14320' '14023' '1138' '10001110010']
 ['ACBDEA' '21340' '23140' '1670' '11010000110']
 ['ACBEDA' '21430' '24103' '1778' '11011110010']
 ['ACDBEA' '23140' '24310' '1830' '11100100110']
 ['ACEBDA' '24130' '23401' '1726' '11010111110']
 ['ADBCEA' '31240' '32410' '2230' '100010110110']
```

```
['ADCBEA' '32140' '34120' '2410' '100101101010']]
```

Appendix B

Simulation Code with Qiskit

The code detailed in this section demonstrates simulations for the four-city graph, as discussed in Section 4.1.2. This code can be extended to model the five-city graph presented in Section 4.2.2, and can be further adapted to accommodate even larger city graphs.

[1]:
```python
import numpy as np
from matplotlib import pyplot as plt
import math

# for circuit construction
from qiskit import QuantumCircuit, ClassicalRegister, QuantumRegister

# QFT circuit needed for phase estimation
from qiskit.circuit.library import QFT

# for creating custom gates
from qiskit import quantum_info as qi

# for simulation
from qiskit_aer import Aer
from qiskit import transpile
from qiskit.visualization import plot_histogram

# for storing data later
import pandas as pd
```

[2]:
```python
#4-city graph edge weights as described in chapter 4.1

w_1 = 4 # a <-> b
w_2 = 2 # a <-> c
w_3 = 4 # a <-> d
w_4 = 4 # b <-> c
w_5 = 5 # c <-> d
w_6 = 6 # b <-> d

weights = []

for i in range(1, 7):
    variable_name = "w_" + str(i)
    current_number = locals()[variable_name]
    weights.append(current_number)

#sorting edge weights
sorted_weights = np.sort(weights)[::-1]

# normalization factor
S = np.sum(sorted_weights[:4])

# epsilon
eps = 1

weights = weights / (S + eps)
weights
```

[2]:
```
array([0.2 , 0.1 , 0.2 , 0.2 , 0.25, 0.3 ])
```

[3]:
```python
## solutions
# A->B->C->D->A
```

```
# A->B->D->C->A
# A->C->B->D->A

print('solution 1: {:.2f}'.format(weights[0] + weights[3] + weights[4] + weights[2]))
print('solution 2: {}'.format(weights[0] + weights[5] + weights[4] + weights[1]))
print('solution 3: {}'.format(weights[1] + weights[3] + weights[5] + weights[2]))
print(" ")
print('solutions after max weight removed')
print('solution 1: {:.2f}'.format(weights[0] + weights[3] + weights[4] + weights[2]))
print('solution 2: {}'.format(weights[0]  + weights[4] + weights[1]))
print('solution 3: {}'.format(weights[1] + weights[3] + weights[2]))
```

```
solution 1: 0.85
solution 2: 0.85
solution 3: 0.8

solutions after max weight removed
solution 1: 0.85
solution 2: 0.55
solution 3: 0.5
```

[4]:
```
## Creating CU matrix

m = 8 # eigenvalue qubits
U111 = 1
U122 = np.exp(1j * weights[0] * 2 * np.pi)
U133 = np.exp(1j * weights[1] * 2 * np.pi)
U144 = np.exp(1j * weights[2] * 2 * np.pi)
U1 = np.diag([U111, U122, U133, U144])

U211 = np.exp(1j * weights[0] * 2 * np.pi)
U222 = 1
U233 = np.exp(1j * weights[3] * 2 * np.pi)
U244 = np.exp(1j * weights[5] * 2 * np.pi)
U2 = np.diag([U211, U222, U233, U244])

U311 = np.exp(1j * weights[1] * 2 * np.pi)
U322 = np.exp(1j * weights[3] * 2 * np.pi)
U333 = 1
U344 = np.exp(1j * weights[4] * 2 * np.pi)
U3 = np.diag([U311, U322, U333, U344])

U411 = np.exp(1j * weights[2] * 2 * np.pi)
U422 = np.exp(1j * weights[5] * 2 * np.pi)
U433 = np.exp(1j * weights[4] * 2 * np.pi)
U444 = 1
U4 = np.diag([U411, U422, U433, U444])

U = np.kron(np.kron(np.kron(U1,U2),U3),U4)
print(np.all(np.diag(U) != 0)) # confirming only the diagonal is being used.

Ugate = qi.Operator(U).to_instruction()
Ugate.label = "CU"
CUgate = Ugate.control()
```

True

[5]:
```
## confirming the eigenstates are correct

eigstatelist = ['01101100', #1230 A->B->C->D->A
                '01110010', #1302 A->B->D->C->A
                '10110100'] #2310 A->C->B->D->A

U_angles = np.diag(np.angle(U))/2/np.pi
eiglistint = [int(eigstatelist[i], 2) for i in range(len(eigstatelist))]

# converting from (-pi,pi) to (0,2pi)
sol_check = U_angles[eiglistint] + 1
sol_check
```

[5]:
```
array([0.85, 0.85, 0.8 ])
```

[6]:
```
### creating CU'
## removing edge-weight value 6 (normalized val = 0.3)
max_index = np.where(weights == 0.3)[0][0]
weights[max_index] = 0

U111 = 1
U122 = np.exp(1j * weights[0] * 2 * np.pi)
U133 = np.exp(1j * weights[1] * 2 * np.pi)
U144 = np.exp(1j * weights[2] * 2 * np.pi)
U1 = np.diag([U111, U122, U133, U144])

U211 = np.exp(1j * weights[0] * 2 * np.pi)
U222 = 1
U233 = np.exp(1j * weights[3] * 2 * np.pi)
U244 = np.exp(1j * weights[5] * 2 * np.pi)
U2 = np.diag([U211, U222, U233, U244])

U311 = np.exp(1j * weights[1] * 2 * np.pi)
U322 = np.exp(1j * weights[3] * 2 * np.pi)
U333 = 1
U344 = np.exp(1j * weights[4] * 2 * np.pi)
U3 = np.diag([U311, U322, U333, U344])

U411 = np.exp(1j * weights[2] * 2 * np.pi)
U422 = np.exp(1j * weights[5] * 2 * np.pi)
U433 = np.exp(1j * weights[4] * 2 * np.pi)
U444 = 1
U4 = np.diag([U411, U422, U433, U444])

Up = np.kron(np.kron(np.kron(U1,U2),U3),U4)
print(np.all(np.diag(Up) != 0))# confirming only the diagonal is being used.

UPgate = qi.Operator(Up).to_instruction()
UPgate.label = "CU'"
CUPgate = UPgate.control()
```

True

[7]:
```
U_angles = np.diag(np.angle(Up))/2/np.pi
eiglistint = [int(eigstatelist[i], 2) for i in range(len(eigstatelist))]

# converting from (-pi,pi) to (0,2pi)
sol_check = U_angles[eiglistint] + 1
sol_check[2] -= 1
sol_check
```

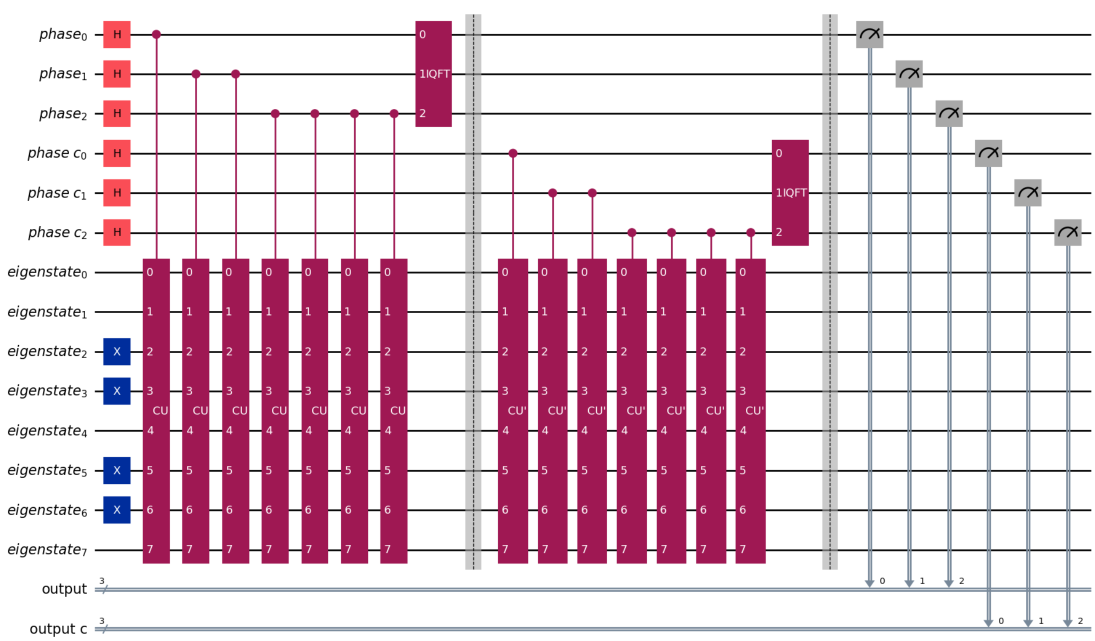
[7]:
```
array([0.85, 0.55, 0.5 ])
```

[8]:
```
def bitstring_converter(string):
    '''
    converts binary values < 1 to decimal
    specifically for the results retrieved
    from simulation
    '''
    values = []
    value = 0
    j = 0
    for i, v in enumerate(string):
        if v == '1':
            value += 1/(2**(i+1-j))
        elif v == " ":
            values.append(value)
            value = 0
            j = i+1
        if i == len(string)-1:
            values.append(value)
    return values[::-1]



def SingleHamiltonianCycle(eig, n):
    # we need a register for the eigenstate:
    eigst   = QuantumRegister(m, name = 'eigenstate')

    # we need two registers for the constrained problem:
    phase   = QuantumRegister(n, name = 'phase')
    phase_c = QuantumRegister(n, name = 'phase c')
    cr      = ClassicalRegister(n, 'output')
    cr_c    = ClassicalRegister(n, 'output c')

    # constructing the circuit (Initialization):
    qc = QuantumCircuit(phase, phase_c,eigst, cr,cr_c)

    # Apply H-Gates to phase qubits:
    for qubit in range(2*n):
        qc.h(qubit)

    for ind, val in enumerate(eig):
        if(int(val)):
            qc.x(ind + 2*n)
```

```python
    ## Phase Estimation
    eig_qubits = np.arange(0,m) + 2*n

    repetitions = 1
    for counting_qubit in range(2*n):
        if counting_qubit == n:
            repetitions = 1
            qc.append(QFT(num_qubits = n, inverse = True, do_swaps=True), phase)
            qc.barrier()
        applied_qubits = np.append([counting_qubit], [eig_qubits])
        for i in range(repetitions):
            if counting_qubit < n:
                qc.append(CUgate, list(applied_qubits)); # This is CU
            else:
                qc.append(CUPgate, list(applied_qubits));
        repetitions *= 2

    qc.append(QFT(num_qubits = n, inverse = True, do_swaps=True), phase_c)
    qc.barrier()

    qc.measure(phase,cr)
    qc.measure(phase_c,cr_c)

    return qc
```

[9]:
```python
n = 3 ## number of estimation qubits.

## A->B->C->D->A
eig = eigstatelist[0]
eig = eig[::-1] # needs to be reversed (Qiskit convention)
qc1 = SingleHamiltonianCycle(eig, n)
qc1.draw(fold=-1, output='mpl')
```

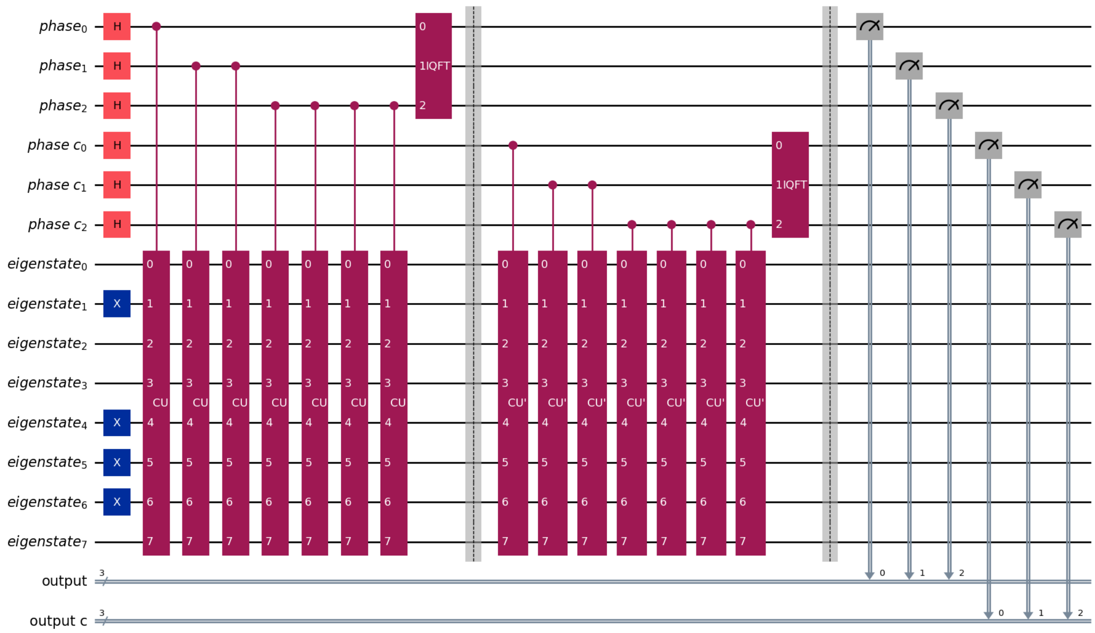
[9]:



[10]:
```
simulator = Aer.get_backend('qasm_simulator')
qc1 = transpile(qc1, simulator)
result = simulator.run(qc1).result()
counts1 = result.get_counts(qc1)
```

[11]:
```
## A->B->D->C->A
eig = eigstatelist[1]
eig = eig[::-1] # needs to be reversed (Qiskit convention)
qc2 = SingleHamiltonianCycle(eig, n)
qc2.draw(fold=-1, output='mpl')
```

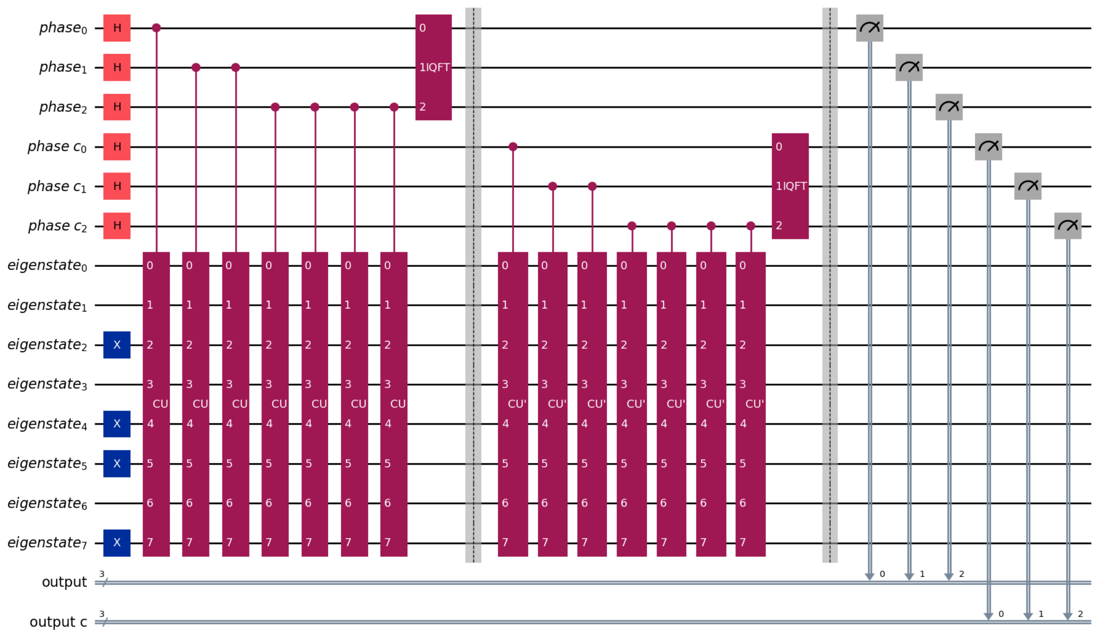
[11]:



[12]:
```
simulator = Aer.get_backend('qasm_simulator')
qc2 = transpile(qc2, simulator)
result = simulator.run(qc2).result()
counts2 = result.get_counts(qc2)
```

[13]:
```
## A->C->B->D->A
eig = eigstatelist[2]
eig = eig[::-1] # needs to be reversed (Qiskit convention)
qc3 = SingleHamiltonianCycle(eig, n)
qc3.draw(fold=-1, output='mpl')
```

[13]:



[14]:
```
simulator = Aer.get_backend('qasm_simulator')
qc3 = transpile(qc3, simulator)
result = simulator.run(qc3).result()
counts3 = result.get_counts(qc3)
```

[15]:
```
# quick check
# printing most probable values [before, after] constraint values removed
print('       before  after')
print('cycle 1', bitstring_converter(max(counts1, key=counts1.get)))
print('cycle 2', bitstring_converter(max(counts2, key=counts2.get)))
print('cycle 3', bitstring_converter(max(counts3, key=counts3.get)))
```

```
      before  after
cycle 1 [0.875, 0.875]
cycle 2 [0.875, 0.5]
cycle 3 [0.75, 0.5]
```

[16]:
```
fig, ax = plt.subplots(3, 1, figsize=(10, 17))
fig.subplots_adjust(hspace=10)
fig.supylabel('counts', fontsize=20)
plot_histogram(counts1, number_to_keep = 10, ax= ax[0])
plot_histogram(counts2, number_to_keep = 10, ax = ax[1])
plot_histogram(counts3, number_to_keep = 10, ax = ax[2])

ax[0].set_title('$A \\rightarrow B \\rightarrow C \\rightarrow D \\rightarrow A$',␣
 ↪fontsize = 20)
ax[1].set_title('$A \\rightarrow B \\rightarrow D \\rightarrow C \\rightarrow A$',␣
 ↪fontsize = 20)
```

```
ax[2].set_title('$A \\rightarrow C \\rightarrow B \\rightarrow D \\rightarrow A$',␣
↪fontsize = 20)

ax[0].set_ylabel('')
ax[1].set_ylabel('')
ax[2].set_ylabel('')
ax[2].grid(False)
plt.tight_layout()
plt.savefig('plots/'+ str(n) + 'qubit-4city_other.pdf')
plt.show()
```