

Exponential Quantum Speedup for the Traveling Salesman Problem*

Anant Sharma

*Centre for Quantum Engineering, Research and Education (CQuERE)
TCG Centres for Research and Education in Science and Technology*

Kolkata 700091, India.
anantsharma2410@gmail.com

Nupur Deshpande

Department of Physics

Indian Institute of Science Education and Research

Tirupati 517507, India.

rajeshdeshpande@students.iisertirupati.ac.in

Sanchita Ghosh

*Centre for Quantum Engineering, Research and Education (CQuERE)
TCG Centres for Research and Education in Science and Technology*

Kolkata 700091, India.
sanchita.ghosh14@gmail.com

Sreetama Das

*Istituto Nazionale di Ottica (CNR-INO)
50125 Florence, Italy.*

*Department of Physics and Astronomy
University of Florence*

50019 Sesto Fiorentino, Italy.

sreetama.das@ino.cnr.it

Shibdas Roy

*Centre for Quantum Engineering, Research and Education (CQuERE)
TCG Centres for Research and Education in Science and Technology*

Kolkata 700091, India.

Academy of Scientific and Innovative Research (AcSIR)

Ghaziabad 201002, India.

roy.shibdas@gmail.com

Abstract

The traveling salesman problem is the problem of finding out the shortest route in a network of cities, that a salesman needs to travel to cover all the cities, without visiting the same city more than once. This problem is known to be NP -hard with a brute-force complexity of $O(N^N)$ or $O(N^{2N})$ for N number of cities. This problem is equivalent to finding out the shortest Hamiltonian cycle in a given graph, if at least one Hamiltonian cycle exists in it. Quantum algorithms for this problem typically provide with a quadratic speedup only, using Grover's search, thereby having a complexity of $O(N^{N/2})$ or $O(N^N)$. We present a bounded-error quantum polynomial-time (BQP) algorithm for solving the problem, providing with an exponential speedup. The overall complexity of our algorithm is $O(N^3 \log(N)\kappa/\epsilon + 1/\epsilon^3)$, where the errors ϵ are $O(1/\text{poly}(N))$, and κ is the not-too-large condition number of the matrix encoding all Hamiltonian cycles.

Index Terms

Traveling Salesperson Problem, Hamiltonian Cycle Problem, Quantum Algorithm, Exponential Speedup.

I. INTRODUCTION

Logistics and complex supply chain related problems that require optimization are challenging to solve. The Traveling Salesman Problem (TSP) is the most commonly explored

use case of combinatorial optimization. The problem appears simple: find the shortest path in a graph that visits each node exactly once and returns to its origin. It is an NP -hard problem, where NP stands for nondeterministic polynomial-time [1]. The hardest of all problems in NP complexity class are NP -complete, while problems that are at least as hard as NP -complete problems and can lie outside NP are NP -hard. The real-world applications of TSP extend to domains, such as transportation, manufacturing, and network design.

Classically, the problem has been tackled by exact as well as heuristic algorithms. Notably, seminal work in linear programming in Ref. [2] introduced cutting planes, laying the groundwork for branch and cut methods [3]–[5], and branch and bound algorithms [6], [7]. In particular, Ref. [8] discussed an implementation of the method from Ref. [2], suitable for TSP instances having a million or more cities. There are other approaches to solve TSP in the literature, such as a thermodynamic approach to find approximate solutions using a Monte Carlo algorithm in Ref. [9].

With the advent of quantum computing and the possibility of solving combinatorial optimization problems faster than classical methods, TSP became a test bed for ample Noisy Intermediate Scale Quantum (NISQ)-era algorithms. Both gate-based approaches and annealer-based approaches have been tested extensively for TSP. Refs. [10]–[12] use annealer-based

*S. D. acknowledges financial support from the European Union's Horizon 2020 research and innovation programme under FET-OPEN Grant Agreement No. 828946 (PATHOS) and from the European Commission's Horizon Europe Framework Programme under the Research and Innovation Action Grant Agreement No. 101070546 (MUQUABIS).

approaches for the problem. For example, while Ref. [10] explored the use of Quadratic Unconstrained Binary Optimization (QUBO) models in solving TSP through quantum annealing algorithms and Graph Neural Networks (GNN), Ref. [11] proposed a path-integral Monte Carlo quantum annealing scheme. By contrast, gate-based approaches include the use of Quantum Approximate Optimization Algorithm (QAOA) [13], and Variational Quantum Eigensolvers (VQE) [14]. Fault-Tolerant Quantum Computing (FTQC) algorithms use approaches based on Grover's search to solve the problem with a quadratic speedup [15]–[18]. In Ref. [16], the eigenstates corresponding to Hamiltonian cycles in the graph are treated as given, but in practice, finding all the Hamiltonian cycles in a graph itself is an NP -complete problem.

In this work, we develop a gate-based FTQC BQP algorithm that solves TSP with exponential speedup. We achieved this by using a novel quantum circuit involving controlled swap gates to yield all candidate Hamiltonian cycles of a given graph of N nodes, quantum phase estimation to capture the sums of edges of these Hamiltonian cycles, and density matrix exponentiation to find the shortest Hamiltonian cycle. The algorithm complexity is $O(N^3 \log(N)\kappa/\epsilon + 1/\epsilon^3)$, that is polynomial in N , when the errors ϵ are polynomially but not exponentially small in N , as required for the overall error probability of our algorithm to be less than or equal to $1/3$,

$$\begin{aligned}
U = & e^{i\phi_{00}}|00\rangle\langle 00| + e^{i\phi_{01}}|01\rangle\langle 01| + e^{i\phi_{02}}|02\rangle\langle 02| + e^{i\phi_{03}}|03\rangle\langle 03| \\
& + e^{i\phi_{10}}|10\rangle\langle 10| + e^{i\phi_{11}}|11\rangle\langle 11| + e^{i\phi_{12}}|12\rangle\langle 12| + e^{i\phi_{13}}|13\rangle\langle 13| \\
& + e^{i\phi_{20}}|20\rangle\langle 20| + e^{i\phi_{21}}|21\rangle\langle 21| + e^{i\phi_{22}}|22\rangle\langle 22| + e^{i\phi_{23}}|23\rangle\langle 23| \\
& + e^{i\phi_{30}}|30\rangle\langle 30| + e^{i\phi_{31}}|31\rangle\langle 31| + e^{i\phi_{32}}|32\rangle\langle 32| + e^{i\phi_{33}}|33\rangle\langle 33|.
\end{aligned} \tag{2}$$

However, some edges from among all the possible $2 \times {}^N C_2$ number of edges may not exist in the actual given graph. We would, then, precompute the sum of all the up to $2 \times {}^N C_2$ number of edges in the graph. Call this sum s , computing which is cheap and efficient even classically. Then, we would encode the phase factor for every edge that does not exist in the graph, including ϕ_{kk} , as equal to s in the unitary U .

$$\begin{aligned}
|\nu\rangle = & |01122330\rangle : \varphi_\nu = \phi_{01} + \phi_{12} + \phi_{23} + \phi_{30} : 0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 0, \\
|\nu\rangle = & |03322110\rangle : \varphi_\nu = \phi_{03} + \phi_{32} + \phi_{21} + \phi_{10} : 0 \rightarrow 3 \rightarrow 2 \rightarrow 1 \rightarrow 0, \\
|\nu\rangle = & |02211330\rangle : \varphi_\nu = \phi_{02} + \phi_{21} + \phi_{13} + \phi_{30} : 0 \rightarrow 2 \rightarrow 1 \rightarrow 3 \rightarrow 0, \\
|\nu\rangle = & |03311220\rangle : \varphi_\nu = \phi_{03} + \phi_{31} + \phi_{12} + \phi_{20} : 0 \rightarrow 3 \rightarrow 1 \rightarrow 2 \rightarrow 0, \\
|\nu\rangle = & |01133220\rangle : \varphi_\nu = \phi_{01} + \phi_{13} + \phi_{32} + \phi_{20} : 0 \rightarrow 1 \rightarrow 3 \rightarrow 2 \rightarrow 0, \\
|\nu\rangle = & |02233110\rangle : \varphi_\nu = \phi_{02} + \phi_{23} + \phi_{31} + \phi_{10} : 0 \rightarrow 2 \rightarrow 3 \rightarrow 1 \rightarrow 0.
\end{aligned} \tag{3}$$

Notice that there are ${}^N P_N = N! = 4! = 24$ number of possible permutations of four different vertices $|0\rangle, |1\rangle, |2\rangle, |3\rangle$. For example, the eigenstates $|01122330\rangle$ and $|23300112\rangle$ represent the same Hamiltonian cycle, but the starting points

and κ is the condition number of the matrix encoding all Hamiltonian cycles of the graph.

II. METHOD

Consider that an arbitrary directed graph is given, with N vertices that are connected by edges. Then, there can be a maximum of $2 \times {}^N C_2 = 2 \times N!/(2(N-2)!) = N(N-1)$ number of edges in the graph. A Hamiltonian cycle, if one exists in the graph, would have exactly N vertices and N edges. We here want to find a quantum algorithm that would take time, polynomial in N , to solve the problem of finding out the shortest Hamiltonian cycle, if one exists, in the graph.

We start with $\lceil \log N \rceil$ number of qubits. For example, if we have 4 vertices in a graph, we would use 2 qubits that can have 4 levels: $|0\rangle = |00\rangle, |1\rangle = |01\rangle, |2\rangle = |10\rangle, |3\rangle = |11\rangle$. We create a unitary operator U , that encodes the distances of all the edges into the phase factors of their eigenstates:

$$U = \sum_{j,k=0}^{N-1} e^{i\phi_{jk}} |jk\rangle\langle jk|, \tag{1}$$

where ϕ_{jk} is the distance between city j to city k . The phase factor ϕ_{jk} is equal to the phase factor ϕ_{kj} in case of an undirected graph. For example, if we have $N = 4$, i.e., cities represented by index values $j = 0, 1, 2, 3$, then we create the following diagonal unitary matrix:

If we now have $V = U^{\otimes N}$, then there are $N!$ number of eigenstates, that can be possible Hamiltonian cycles from among a total of N^{2N} number of eigenstates of V , of which $(N-1)!$ Hamiltonian cycles are unique. For example, for $N = 4$, there are a total of 4^8 number of eigenstates of V , but we have the following $(4-1)! = 6$ eigenstates representing unique Hamiltonian cycles starting from city 0.

are different, i.e. cities 0 and 2, respectively. So, there are N number of same Hamiltonian cycles, but simply rotated with respect to each other, for each of the $(N-1)!$ unique Hamiltonian cycles, amounting to a total of $N!$ Hamiltonian

cycle eigenstates of V for a fully-connected directed graph.

Now, we initialize N number of data registers, each of $\lceil \log N \rceil$ qubits, to $|0\rangle, |1\rangle, |2\rangle, \dots, |N-1\rangle$, respectively. Then, we create all possible permutations of $0, 1, 2, \dots, N-1$ by using ${}^N C_2$ number of single-qubit ancilla registers, each initialized to the state $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, and applying $\lceil \log N \rceil$ number of controlled swap gates on each of every combination of two data registers with one ancilla register as the control qubit. Please see the required circuit in Figure 1.

We will then have the following state in the data registers, upon tracing out the ancilla registers, with $\sum_{\mu} \beta_{\mu}^2 = 2^N C_2$:

$$\rho = \frac{1}{2^N C_2} \sum_{\mu} \beta_{\mu}^2 |\mu\rangle \langle \mu|. \quad (4)$$

We, then, expand the state ρ from an N -register state to a $2N$ -register state. For example, for $N = 4$, we augment a state $|0123\rangle$ to the state $|01122330\rangle$, so that it forms a valid eigenstate for the unitary V . We can augment the N -register state by adding N new registers, each of $\lceil \log N \rceil$ qubits initialised to $|0\rangle$, at appropriate places, and applying $CNOT$ gates to create adjacent copies of every register in ρ . This way, we will now have terms like $|01122330\rangle$ replacing $|0123\rangle$ (for $N = 4$) in ρ . Please see Figure 2. Call this new state σ , so that we have, with $\sum_{\nu} \beta_{\nu}^2 = 2^N C_2$:

$$\sigma = \frac{1}{2^N C_2} \sum_{\nu} \beta_{\nu}^2 |\nu\rangle \langle \nu|. \quad (5)$$

We use this state σ as the input eigenstates to perform quantum phase estimation of the unitary V , to obtain the following state at the output:

$$\gamma = \frac{1}{2^N C_2} \sum_{\nu} \beta_{\nu}^2 |\tilde{\varphi}_{\nu}\rangle \langle \tilde{\varphi}_{\nu}| \otimes |\nu\rangle \langle \nu|. \quad (6)$$

The state γ then has all the valid Hamiltonian cycle eigenstates $|\nu\rangle$, along with the estimates $\tilde{\varphi}_{\nu}$ of their corresponding sums φ_{ν} of weights of constituent edges ϕ_{jk} .

Notice that we use the improved quantum phase estimation method from Ref. [19] in the phase estimation of V , and so, we would have the time variable $t = O(\eta\kappa/\varepsilon)$ (the factor $\eta\kappa$ arises as a result of using $C = \eta\kappa$ in the controlled rotation later) when simulating the unitary U in the beginning by exponentiating a diagonal matrix Φ , such that $U = e^{i\Phi t}$. The matrix Φ to exponentiate to obtain unitary U of (2) is:

$$\begin{aligned} \Phi = & \phi_{00}|00\rangle\langle 00| + \phi_{01}|01\rangle\langle 01| + \phi_{02}|02\rangle\langle 02| + \phi_{03}|03\rangle\langle 03| \\ & + \phi_{10}|10\rangle\langle 10| + \phi_{11}|11\rangle\langle 11| + \phi_{12}|12\rangle\langle 12| + \phi_{13}|13\rangle\langle 13| \\ & + \phi_{20}|20\rangle\langle 20| + \phi_{21}|21\rangle\langle 21| + \phi_{22}|22\rangle\langle 22| + \phi_{23}|23\rangle\langle 23| \\ & + \phi_{30}|30\rangle\langle 30| + \phi_{31}|31\rangle\langle 31| + \phi_{32}|32\rangle\langle 32| + \phi_{33}|33\rangle\langle 33|, \end{aligned}$$

which, being diagonal, and so, sparse, U can be simulated efficiently [19], [20]. Here, $\varepsilon/2$ is the estimation precision error in trace distance, and so, the maximum probability of estimation error. We use $\varepsilon = O(1/\text{poly}(N))$ to let time t to simulate U be polynomial, and not exponential, in N , as long as the error probability of our overall algorithm is below $1/3$.

In order to find the shortest Hamiltonian cycle, we add to γ an ancilla qubit, initialized in the state $(|0\rangle\langle 0| + |1\rangle\langle 1|)/2$, and rotate it, conditioned on $|\tilde{\varphi}_{\nu}\rangle$, to get, with $\alpha_{\nu}^2 := \beta_{\nu}^2/2^N C_2$:

$$\begin{aligned} \xi = & \sum_{\nu} \alpha_{\nu}^2 |\tilde{\varphi}_{\nu}\rangle \langle \tilde{\varphi}_{\nu}| \otimes |\nu\rangle \langle \nu| \\ & \otimes [(1 - C^2 \tilde{\varphi}_{\nu}^2)|0\rangle\langle 0| + C^2 \tilde{\varphi}_{\nu}^2 |1\rangle\langle 1|]. \end{aligned} \quad (7)$$

We ensure that all the eigenphases φ_{ν} are between 0 and 1 by initially dividing all edges ϕ_{jk} by $\hat{\varphi}_{\max}$, that is taken as the sum of the N largest edges as an estimate of φ_{\max} . If our estimate $\hat{\varphi}_{\max}$ is equal to φ_{\max} and if the phase estimation was perfect, then we have the minimum $\tilde{\varphi}_{\nu}$, which is $\tilde{\varphi}_{\min}$, equal to the inverse of the not-too-large condition number (of the matrix of which $\tilde{\varphi}_{\nu}$'s are the eigenvalues), $1/\kappa = \tilde{\varphi}_{\min}/\tilde{\varphi}_{\max}$. This would mean that the ancilla qubit above will be rotated from $|0\rangle$ only for $\tilde{\varphi}_{\min}$ that is equal to $1/\kappa$, if we use $C = \kappa$, since the probability $C^2 \tilde{\varphi}_{\nu}^2$, attached to $|1\rangle$, will be equal to 1 only for $\tilde{\varphi}_{\min}$. In other words, the ancilla qubit will not be rotated at all for any $\tilde{\varphi}_{\nu}$, other

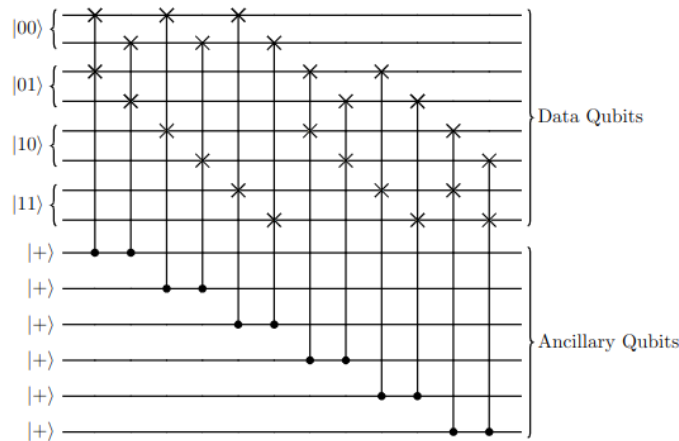


Figure 1. Quantum circuit to create a superposition of all permutations of $0, 1, 2, \dots, N-1$ for $N = 4$.

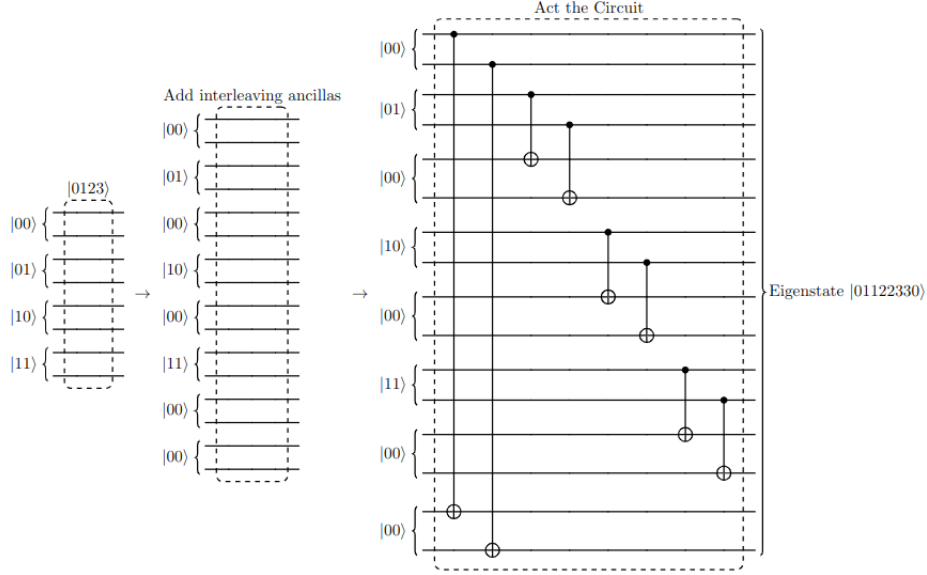


Figure 2. Quantum circuit to augment terms like $|0123\rangle$ in ρ to $|01122330\rangle$ in σ for $N = 4$.

than $\tilde{\varphi}_{\min}$. However, since $\hat{\varphi}_{\max}$ would almost always be an overestimate of φ_{\max} , we would have $1/\kappa$ rather larger than $\tilde{\varphi}_{\min}$, more so when the variance in the given edges is large, or there are missing edges initially assigned a value of s . This is why we use an extra multiplicative factor η , that we discuss later, to ensure that only $\tilde{\varphi}_{\min}$ is likely going to be less than or equal to $1/(\eta\kappa)$. So, in order to find and separate out $\tilde{\varphi}_{\min}$, we choose above $C = \eta\kappa$, so that the ancilla qubit is rotated from $|0\rangle$ only for $\tilde{\varphi}_{\min}$ that is less than or equal to $1/(\eta\kappa)$. We will discuss shortly how to guess the value of $\eta\kappa$ to use.

We then need to find and output the Hamiltonian cycle $|\nu\rangle$, that corresponds to $\tilde{\varphi}_{\min}$. Notice that if $C\tilde{\varphi}_{\min} = O(1)$, then the probability of obtaining 1 as the outcome of measuring the ancilla qubit above can be as small as $O(N/2^{N C_2}) = O(1/2^{O(N^2)})$, which is more than exponentially small in N . So, we cannot efficiently perform a postselection on the outcome being 1 of measuring the ancilla like in Ref. [19], to obtain the below desired state from the state ξ in (7):

$$\zeta = \sum_{\tilde{\varphi}_{\min}} \frac{\alpha_{\nu}^2 C^2 \tilde{\varphi}_{\nu}^2}{\lambda_{\min}} |\tilde{\varphi}_{\nu}\rangle \langle \tilde{\varphi}_{\nu}| \otimes |\nu\rangle \langle \nu|, \quad (8)$$

where if only $\tilde{\varphi}_{\min}$ is less than $1/(\eta\kappa) = 1/C$, then we would have N terms in the summation, all of which are the same Hamiltonian cycles (with the same sum of weights of edges), just rotated with respect to each other, so that $\lambda_{\min} := \sum_{\tilde{\varphi}_{\min}} \alpha_{\nu}^2 C^2 \tilde{\varphi}_{\nu}^2$. We would not use amplitude amplification either, as used in Ref. [19], since it gives only a quadratic speedup, while we want to get exponential speedup.

Instead, in order to get the above state ζ in (8), we first exponentiate the ancilla qubit (call it ϱ) from (7) to get the unitary $Y = e^{i\varrho\tau}$, and perform phase estimation on Y for eigenstate $|1\rangle$. We create Y by repeatedly applying the below

to state ϱ of ancilla ‘‘anc’’ and another state ς [21], [22]:

$$\text{Tr}_{\text{anc}} [e^{iS\Delta\tau} (\varrho \otimes \varsigma) e^{-iS\Delta\tau}] = \varsigma - i\Delta\tau [\varrho, \varsigma] + O(\Delta\tau^2). \quad (9)$$

Here, S is the swap operator, which is sparse and so, $e^{iS\Delta\tau}$ can be performed efficiently [19], [20]. Also, here, $\tau = n\Delta\tau$, where $n = O(\tau^2/\epsilon)$ is the required number of copies of ϱ , and so, the required number of times (9) needs to be repeated to obtain a simulation of Y with an error of ϵ . The phase estimation process requires controlled- $e^{i\varrho\tau}$ operations, that can be performed by simply using conditional swap instead of swap operation above for varying times τ (see Ref. [21]).

The phase estimate so obtained would be $\tilde{\lambda}_{\min}$, using which we further apply a rotation to the ancilla qubit in (7), to get:

$$\chi = \sum_{\nu} \alpha_{\nu}^2 |\tilde{\varphi}_{\nu}\rangle \langle \tilde{\varphi}_{\nu}| \otimes |\nu\rangle \langle \nu| \otimes \left[\left(1 - \frac{C^2 \tilde{\varphi}_{\nu}^2}{\tilde{\lambda}_{\min}} \right) |0\rangle \langle 0| + \frac{C^2 \tilde{\varphi}_{\nu}^2}{\tilde{\lambda}_{\min}} |1\rangle \langle 1| \right], \quad (10)$$

where since the eigenvalue of the eigenstate $|1\rangle$ of the ancilla qubit is evidently $\sum_{\nu} \frac{\alpha_{\nu}^2 C^2 \tilde{\varphi}_{\nu}^2}{\tilde{\lambda}_{\min}} = 1$, we get the eigenvalue of the eigenstate $|0\rangle$ of the ancilla qubit to be $\sum_{\nu} \alpha_{\nu}^2 \left(1 - \frac{C^2 \tilde{\varphi}_{\nu}^2}{\tilde{\lambda}_{\min}} \right) = \sum_{\nu} \alpha_{\nu}^2 - \sum_{\tilde{\varphi}_{\min}} \frac{\alpha_{\nu}^2 C^2 \tilde{\varphi}_{\nu}^2}{\tilde{\lambda}_{\min}} = 1 - 1 = 0$. Thus, the above state, upon tracing out the ancilla qubit, is just the desired state ζ from (8), where every $\tilde{\varphi}_{\nu}$ is equal to $\tilde{\varphi}_{\min}$, so that measuring the two registers yield the outputs, $\tilde{\varphi}_{\min}$ and an eigenstate ν , corresponding to the desired shortest Hamiltonian cycle in the graph. Clearly, if $\tilde{\varphi}_{\min}$ so obtained is larger than $s/\hat{\varphi}_{\max}$, the eigenstate ν so obtained would not be a desired Hamiltonian cycle, since it would have at least one missing edge assigned a normalised value of $s/\hat{\varphi}_{\max}$. So, we can decide that there is no Hamiltonian cycle in the given graph. Otherwise, our algorithm would output the obtained

values of ν and $\tilde{\varphi}_{\min} \times \hat{\varphi}_{\max}$ as the shortest Hamiltonian cycle of the graph, and the sum of its edges, respectively.

Note that the controlled rotation in (7) is achieved by considering two ancilla qubits, denoted by A and B , initialised in the state $|0_A 0_B\rangle$, and then rotating this state, conditioned on phase estimates $|\tilde{\varphi}_\nu\rangle$, and ignoring one of the ancilla qubits:

$$\xi = \text{Tr}_B \left\{ \sum_{\nu} \alpha_{\nu}^2 |\tilde{\varphi}_\nu\rangle \langle \tilde{\varphi}_\nu| \otimes |\nu\rangle \langle \nu| \otimes |\Phi_{AB}\rangle \langle \Phi_{AB}| \right\}, \quad (11)$$

where $|\Phi_{AB}\rangle := \sqrt{1 - C^2 \tilde{\varphi}_\nu^2} |0_A 0_B\rangle + C \tilde{\varphi}_\nu |1_A 1_B\rangle$. In order to simulate the unitary Y , we perform density matrix exponentiation of the state ϱ of the ancilla qubit (as pointed out earlier), that requires $n = O(\tau^2/\epsilon)$ copies of ϱ . Clearly, we can obtain two copies of ϱ from above, one by ignoring the qubit B , and the other by ignoring the qubit A , but undoing the action of $e^{i s \tau}$ on ϱ in between. Thus, we get the desired n copies of ϱ , required for simulation of Y , by considering n ancilla qubits, initialised in the state $|0^{\otimes n}\rangle$, and then rotating this state, conditioned on phase estimates $|\tilde{\varphi}_\nu\rangle$:

$$\vartheta = \sum_{\nu} \alpha_{\nu}^2 |\tilde{\varphi}_\nu\rangle \langle \tilde{\varphi}_\nu| \otimes |\nu\rangle \langle \nu| \otimes |\psi\rangle \langle \psi|, \quad (12)$$

where $|\psi\rangle := \sqrt{1 - C^2 \tilde{\varphi}_\nu^2} |0^{\otimes n}\rangle + C \tilde{\varphi}_\nu |1^{\otimes n}\rangle$. With n ancilla qubits, the state corresponding to χ of (10) is:

$$\Theta = \sum_{\nu} \alpha_{\nu}^2 |\tilde{\varphi}_\nu\rangle \langle \tilde{\varphi}_\nu| \otimes |\nu\rangle \langle \nu| \otimes |\Psi\rangle \langle \Psi|, \quad (13)$$

where $|\Psi\rangle := \sqrt{1 - \frac{C^2 \tilde{\varphi}_\nu^2}{\lambda_{\min}}} |0^{\otimes n}\rangle + \frac{C \tilde{\varphi}_\nu}{\sqrt{\lambda_{\min}}} |1^{\otimes n}\rangle$.

We discuss an *empirical* way to guess $C = \eta\kappa$. The *mid-range* of the means (of N edges) of the Hamiltonian cycles is normally close or equal to the *mean* M of all edges. We use an extra scaling factor $\omega/(2N)$, to offset our overestimate $\hat{\varphi}_{\max}$ of φ_{\max} , to get: $(\varphi_{\min}/N + \hat{\varphi}_{\max}/N)/2 = \omega M/(2N)$, with $\omega = \max(2N, (e! = 0)\theta)$, where $\theta = {}^N C_2$ for undirected graphs, $\theta/2 = {}^N C_2$ for directed graphs, e is number of too large (at least ten times the smallest edge) or missing edges. So, a guess of $1/\kappa$ is $1/\hat{\kappa} = \omega M/\hat{\varphi}_{\max} - 1$. We use $\eta = \Omega/\varpi$, if $\omega > 2N$, $\eta = (\Omega/\varpi) \cdot (\omega/(2N))$, if $\omega > 4N$, else $\eta = 1$, if $\omega = 2N$, where Ω is the sum of all edges including missing edges, ϖ is the sum of all edges excluding missing or too large edges. Usually, $1/C = 1/(\eta\hat{\kappa})$ would be below, and yet close to, the *normalised* φ_{\min} , so that we repeat our algorithm a few times, slightly raising $1/C$ each time till we capture $\tilde{\varphi}_{\min}$ only. This empirical method rarely fails; see [23].

III. ALGORITHM

- 1) We create the unitary $U = e^{i\Phi t}$ encoding all weights of edges ϕ_{jk} , where $\Phi = \sum_{j,k=0}^{N-1} \frac{\phi_{jk}}{\hat{\varphi}_{\max}} |jk\rangle \langle jk|$, s is the sum of all given edges, and $\hat{\varphi}_{\max}$ is the sum of the largest N edges of the graph, after replacing any missing edge by s . We create N copies of U to yield $V = U^{\otimes N}$.
- 2) We initialize N number of data registers of $\lceil \log N \rceil$ qubits each to $|0\rangle, |1\rangle, |2\rangle, \dots, |N-1\rangle$, respectively.

We generate all permutations of $0, 1, 2, \dots, N-1$ using ${}^N C_2$ number of single-qubit ancilla registers, each initialized to $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, and applying $\lceil \log N \rceil$ number of controlled swap gates on each combination of two data registers with one ancilla as control qubit.

- 3) The first register has the state $\rho = \frac{1}{2^{N C_2}} \sum_{\mu} \beta_{\mu}^2 |\mu\rangle \langle \mu|$, where $\sum_{\nu} \beta_{\nu}^2 = 2^{N C_2}$. We augment this N -register state by adding N ancilla registers each of $\lceil \log(N) \rceil$ qubits in state $|0\rangle$ and acting $CNOT$ gates to get a $2N$ -register state $\sigma = \frac{1}{2^{N C_2}} \sum_{\nu} \beta_{\nu}^2 |\nu\rangle \langle \nu|$, where $\sum_{\nu} \beta_{\nu}^2 = 2^{N C_2}$.
- 4) We perform quantum phase estimation [19] on V using σ as input to get $\gamma = \frac{1}{2^{N C_2}} \sum_{\nu} \beta_{\nu}^2 |\varphi_{\nu}\rangle \langle \varphi_{\nu}| \otimes |\nu\rangle \langle \nu|$.
- 5) We add to the state γ an ancilla register of n qubits, initialized in the state $|0^{\otimes n}\rangle$, and rotate it, conditioned on $|\varphi_{\nu}\rangle$, to get the state $\vartheta = \sum_{\nu} \alpha_{\nu}^2 |\tilde{\varphi}_\nu\rangle \langle \tilde{\varphi}_\nu| \otimes |\nu\rangle \langle \nu| \otimes |\psi\rangle \langle \psi|$, where $\alpha_{\nu}^2 := \beta_{\nu}^2 / 2^{N C_2}$, $|\psi\rangle := \left[\sqrt{1 - C^2 \tilde{\varphi}_\nu^2} |0^{\otimes n}\rangle + C \tilde{\varphi}_\nu |1^{\otimes n}\rangle \right]$ and C is set to $\eta\kappa$.
- 6) We exponentiate the effective state ϱ of each ancilla qubit, using n copies of ϱ from n ancilla qubits, to get a unitary $Y := e^{i\varrho\tau}$, and perform phase estimation on Y for the eigenstate $|1\rangle$. If the phase estimate for $|1\rangle$ is 0, we repeat step 5 with a slightly smaller value of C , and then repeat this step, until we can capture $\tilde{\varphi}_{\min}$ in step 5 and get $\hat{\lambda}_{\min}$ as the phase estimate in this step.
- 7) We further apply a rotation to the ancilla register in the state ϑ from step 5, using $\hat{\lambda}_{\min}$ obtained in step 6, to get $\Theta = \sum_{\nu} \alpha_{\nu}^2 |\tilde{\varphi}_\nu\rangle \langle \tilde{\varphi}_\nu| \otimes |\nu\rangle \langle \nu| \otimes |\Psi\rangle \langle \Psi|$, where $|\Psi\rangle := \left[\sqrt{1 - \frac{C^2 \tilde{\varphi}_\nu^2}{\lambda_{\min}}} |0^{\otimes n}\rangle + \frac{C \tilde{\varphi}_\nu}{\sqrt{\lambda_{\min}}} |1^{\otimes n}\rangle \right]$. So, upon tracing out the ancilla register $|\Psi\rangle$ from Θ , we get $\zeta = \sum_{\tilde{\varphi}_{\min}} \frac{\alpha_{\nu}^2 C^2 \tilde{\varphi}_\nu^2}{\lambda_{\min}} |\tilde{\varphi}_\nu\rangle \langle \tilde{\varphi}_\nu| \otimes |\nu\rangle \langle \nu|$, as $\sum_{\nu} \frac{\alpha_{\nu}^2 C^2 \tilde{\varphi}_\nu^2}{\lambda_{\min}} = 1$.
- 8) Measure the two registers in the state ζ from step 7 to get $\tilde{\varphi}_{\min}$ and a ν . If $\tilde{\varphi}_{\min}$ is larger than $s/\hat{\varphi}_{\max}$, output the decision that there is no Hamiltonian cycle in the graph. Otherwise, output the obtained values of ν and $\tilde{\varphi}_{\min} \times \hat{\varphi}_{\max}$ as the desired shortest Hamiltonian cycle of the graph, and the sum of its edges, respectively.

The improved quantum phase estimation method from Ref. [19], that we use above, is as follows. We start with an initial state $|\Lambda_0\rangle |u_j\rangle$, where $|u_j\rangle$ is the j -th eigenstate of the Hermitian matrix Γ , that we exponentiate, and $|\Lambda_0\rangle := \frac{\sqrt{2}}{\sqrt{T}} \sum_{\iota=0}^{T-1} \sin \frac{\pi(\iota+\frac{1}{2})}{T} |\iota\rangle$ for some large T . The state $|\Lambda_0\rangle$ can be prepared upto some error ϵ_{Λ} in time $\text{poly} \log(T/\epsilon_{\Lambda})$ (see Ref. [19]). We apply the conditional Hamiltonian evolution $\sum_{\iota=0}^{T-1} |\iota\rangle \langle \iota| \otimes e^{i\Gamma \iota t/T}$ on the initial state in both registers, and then apply inverse quantum Fourier transform on the first register to get the state $\sum_{q=0}^{T-1} v_{q|j} |q\rangle |u_j\rangle$. Defining the estimate \tilde{r}_q of the q -th eigenvalue r_q of Γ as $\tilde{r}_q := \frac{2\pi q}{t}$, we relabel the Fourier basis states $|q\rangle$ to get $\sum_{q=0}^{T-1} v_{q|j} |\tilde{r}_q\rangle |u_j\rangle$. If the phase estimation is perfect, we have $v_{q|j} = 1$ if $\tilde{r}_q = r_j$, and 0 otherwise. So, we get the state $|\tilde{r}_j\rangle |u_j\rangle$, from which we obtain the estimate of r_j upon measuring the first register.

IV. ALGORITHM COMPLEXITY

In Figure 1 for step 2, the swap gates on $\lceil \log N \rceil$ number of qubits of each data register are applied parallelly. Since there are ${}^N C_2$ number of such sets of swap gates, the complexity of this step is $O(N^2)$. The complexity is independent of N in Figure 2 for step 3, since all the $CNOT$ gates can be applied in parallel. In step 1, creating each copy of U has a complexity of $O(2 \log(N)t)$ [19], [20], since each eigenstate has $2 \log N$ qubits. Further, N copies of U , required for V , can be created in parallel. In step 4, we use improved quantum phase estimation from Ref. [19], the complexity of which is dominated by the inverse quantum Fourier transform involved, and is, thus, $O(\ell^2)$, if we use ℓ qubits in the phase estimate register. The use of improved quantum phase estimation in this step along with the controlled rotation with $C = \eta\kappa$ in step 5 require the time variable t in step 1 to be $O(\eta\kappa/\epsilon)$ (see Ref. [19]). In step 5, the complexity is polynomial for the controlled rotation of the ancilla register state, as in Ref. [19]. The circuit depth of the density matrix exponentiation in step 6 of the (single) ancilla qubit is $O(\log(2)n) = O(\tau^2/\epsilon) = O(1/\epsilon^3)$ [21], [22], where ϵ is the simulation error for Y , as also the precision error of phase estimation of Y for $|1\rangle$ for which $\tau = O(1/\epsilon)$. Here, ϵ is an error in trace distance, and so, determines the maximum probability of error in the simulation or estimation of Y [24]. Notice that the eigenvalue of ρ for the eigenstate $|1\rangle$ can be as low as $O(1/2^{O(N^2)})$, that can be indistinguishable from 0, if less than $O(N^2)$ qubits are used in the phase estimate register. However, using $O(N^2)$ number of qubits in the phase estimate register, the time variable in simulating Y would scale as $\tau = O(2^{O(N^2)})$. Nonetheless, since ϵ determines the maximum probability of error, we can use $\epsilon = O(1/\text{poly}(N))$, and not necessarily $\epsilon = O(1/2^{O(N^2)})$, so that the time τ required to simulate unitary Y is polynomial, and not exponential, in N , as long as the overall cumulative probability of error of our algorithm does not exceed $1/3$. The complexities of steps 7 and 8 can be ignored evidently. Thus, the overall time complexity of our algorithm is $O(2 \log(N)t)$, which yields $O(\log(N)\eta\kappa/\epsilon) \leq O(N^3 \log(N)\kappa/\epsilon)$, taking $\epsilon = \epsilon$ for simplicity, with $\epsilon = O(1/\text{poly}(N))$, and $\eta \leq O(N^3)$. This is because the complexity of step 1 is dominant amongst all steps of the algorithm, if it suffices to have $\epsilon \geq O(1/N)$. Notice that we need some classical preprocessing of all the input weights of the edges of the graph, e.g. computing $\hat{\varphi}_{\max}$ by summing the N largest edges, for which we need to sort the data, that is expensive. If we use merge sort algorithm to sort the ${}^N C_2$ number of edges, the time complexity would be $O({}^N C_2 \log({}^N C_2)) = O(N^2 \log(N))$, which is still less than $O(N^3 \log(N)\kappa/\epsilon)$. However, if $\epsilon \leq O(1/N^2)$, the complexity of step 6 is dominant, and the overall complexity of our algorithm is at least $O(\epsilon^{-3}) = O(N^6)$, that is an exponential speedup over the brute-force complexity of $O(N^N)$ for undirected graphs [1], or $O(N^{2N})$ for directed graphs for TSP.

To conclude, we provide for TSP a BQP algorithm of complexity $O(N^3 \log(N)\kappa/\epsilon + 1/\epsilon^3)$, where $\epsilon = O(1/\text{poly}(N))$.

REFERENCES

- [1] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*. Cambridge University Press, 2002.
- [2] G. Dantzig, R. Fulkerson, and S. Johnson, "Solution of a large-scale traveling-salesman problem," *Operations Research*, vol. 2, no. 4, pp. 393–410, November 1954.
- [3] M. Grötschel and O. Holland, "Solution of large-scale symmetric travelling salesman problems," *Mathematical Programming*, vol. 51, pp. 141–202, July 1991.
- [4] M. Padberg and G. Rinaldi, "A branch-and-cut algorithm for the resolution of large-scale symmetric traveling salesman problems," *SIAM Review*, vol. 33, no. 1, pp. 60–100, March 1991.
- [5] D. Applegate, R. Bixby, V. Chvátal, and W. Cook, "On the solution of traveling salesman problems," *Documenta Mathematica*, vol. 3, pp. 645–656, January 1998.
- [6] J. D. C. Little, K. G. Murty, D. W. Sweeney, and C. Karel, "An algorithm for the traveling salesman problem," *Operations Research*, vol. 11, no. 6, pp. 972–989, 1963.
- [7] M. Held and R. M. Karp, "The traveling-salesman problem and minimum spanning trees: Part II," *Mathematical Programming*, vol. 1, pp. 6–25, 1971.
- [8] D. Applegate, R. Bixby, V. Chvátal, and W. Cook, "Implementing the Dantzig-Fulkerson-Johnson algorithm for large traveling salesman problems," *Mathematical Programming*, vol. 97, pp. 91–153, 2003.
- [9] V. Černý, "Thermodynamical approach to the traveling salesman problem: An efficient simulation algorithm," *Journal of Optimization Theory and Applications*, vol. 45, pp. 41–51, January 1985.
- [10] H. He, "Quantum annealing and graph neural networks for solving TSP with QUBO," February 2024, arXiv:2402.14036.
- [11] R. Martoňák, G. E. Santoro, and E. Tosatti, "Quantum annealing of the traveling-salesman problem," *Physical Review E*, vol. 70, no. 5, p. 057701, November 2004.
- [12] E. Rodriguez, E. Osaba, and I. Oregi, "Analyzing the behaviour of D-Wave quantum annealer: fine-tuning parameterization and tests with restrictive Hamiltonian formulations," in *2022 IEEE Symposium Series on Computational Intelligence (SSCI)*, December 2022, pp. 938–946.
- [13] W. Qian, R. A. M. Basili, M. M. Eshaghian-Wilner, A. Khokhar, G. Luecke, and J. P. Vary, "Comparative study of variations in quantum approximate optimization algorithms for the traveling salesman problem," *Entropy*, vol. 25, no. 8, p. 1238, August 2023.
- [14] A. Matsuo, Y. Suzuki, I. Hamamura, and S. Yamashita, "Enhancing VQE convergence for optimization problems with problem-specific parameterized quantum circuits," *IEICE Transactions on Information and Systems*, vol. E106.D, pp. 1772–1782, November 2023.
- [15] J. Bang, J. Ryu, C. Lee, S. Yoo, J. Lim, and J. Lee, "A quantum heuristic algorithm for the traveling salesman problem," *Journal of the Korean Physical Society*, vol. 61, pp. 1944–1949, January 2013.
- [16] K. Srinivasan, S. Satyajit, B. K. Behera, and P. K. Panigrahi, "Efficient quantum algorithm for solving travelling salesman problem: An IBM quantum experience," May 2018, arXiv:1805.10928.
- [17] A. Moylett, N. Linden, and A. Montanaro, "Quantum speedup of the traveling-salesman problem for bounded-degree graphs," *Physical Review A*, vol. 95, no. 3, p. 032323, March 2017.
- [18] C. Tsyunsi and I. I. Beterov, "A quantum algorithm for solving the travelling salesman problem by quantum phase estimation and quantum search," *Journal of Experimental and Theoretical Physics*, vol. 137, pp. 210–215, September 2023.
- [19] A. W. Harrow, A. Hassidim, and S. Lloyd, "Quantum algorithm for linear systems of equations," *Physical Review Letters*, vol. 103, no. 15, p. 150502, October 2009.
- [20] D. W. Berry, G. Ahokas, R. Cleve, and B. C. Sanders, "Efficient quantum algorithms for simulating sparse Hamiltonians," *Communications in Mathematical Physics*, vol. 270, pp. 359–371, December 2006.
- [21] S. Lloyd, M. Mohseni, and P. Rebentrost, "Quantum principal component analysis," *Nature Physics*, vol. 10, pp. 631–633, July 2014.
- [22] M. Kjaergaard, M. E. Schwartz, A. Greene, G. O. Samach, A. Bengtsson, M. O’Keeffe *et al.*, "Demonstration of density matrix exponentiation using a superconducting quantum processor," *Physical Review X*, vol. 12, no. 1, p. 011005, January 2022.
- [23] Tests of our empirical method for TSP: <https://shorturl.at/nplN7>.
- [24] S. Kimmel, C. Y.-Y. Lin, G. H. Low, M. Ozols, and T. J. Yoder, "Hamiltonian simulation with optimal sample complexity," *npj Quantum Information*, vol. 3, no. 13, March 2017.