

Quantum Alternating Operator Ansatz for Solving the Minimum Exact Cover Problem

Sha-Sha Wang¹, Hai-Ling Liu¹, Su-Juan Qin¹, Fei Gao^{1,*} and Qiao-Yan Wen^{1†}

¹ *State Key Laboratory of Networking and Switching Technology,
Beijing University of Posts and Telecommunications, Beijing 100876, China*
(Dated: November 29, 2022)

The minimum exact cover (MEC) is a common combinatorial optimization problem, with wide applications in tail-assignment and vehicle routing. In this paper, we adopt quantum alternating operator ansatz (QAOA+) to solve MEC problem. In detail, to obtain a trivial feasible solution, we first transform MEC into a constrained optimization problem with two objective functions. Then, we adopt the linear weighted sum method to solve the above constrained optimization problem and construct the corresponding target Hamiltonian. Finally, to improve the performance of this algorithm, we adopt parameters fixing strategy to simulate, where the experimental instances are 6, 8, and 10 qubits. The numerical results show that the solution can be obtained with high probability when level p of the algorithm is low. Besides, we optimize the quantum circuit by removing single-qubit rotating gates R_Z . We found that the number of quantum gates is reduced by np for p -level optimized circuit. Furthermore, p -level optimized circuit only needs p parameters, which can achieve an experimental effect similar to original circuit with $2p$ parameters.

I. INTRODUCTION

Quantum computers have computational advantages over classical computers by exploiting quantum effects, providing polynomial or even exponential speedups for specific problems, such as integer factorization [1], unstructured data search [2], solving linear equations [3], linear regression [4, 5], support vector machine [6], dimension reduction [7–10], matrix computation [11–14], anomaly detection [15] and cryptanalysis [16]. However, the current quantum hardware devices only support a limited number of physical qubits and limited gate fidelity, which makes the above quantum algorithms unable to be implemented on near-term devices.

Recently, quantum approximation optimization algorithm (QAOA) [17], a hybrid quantum-classical algorithm, which can be implemented on a near-term noisy intermediate-scale quantum (NISQ) device [18]. QAOA has successfully solved many combinatorial optimization problems, such as Max Cut [19, 20], Minimum Vertex Cover [21], Correlation Clustering [22].

The minimum exact cover (MEC) is a constrained optimization problem, with wide applications in the tail-assignment and vehicle routing. Some scholars solved this problem using QAOA [23–25] and achieved good results. However, their algorithms need to search for the target solution in the overall Hilbert space. This will lead to inefficiency in the search for solutions, and also invalid solutions are obtained.

To overcome the above problems, quantum alternating operator ansatz (QAOA+) [31, 32] was proposed. It can make the search for solutions more efficient, and the probability of obtaining invalid solutions is zero. QAOA+ has

been applied to many combinatorial optimization problems, such as Graph-Coloring [33], Maximum Independent Set [34], Max- k Vertex Cover [35], Graph Matching [36], Lattice Protein Folding [37]. However, there is no relevant research to solve MEC using QAOA+.

In this paper, we solve the MEC problem using QAOA+. Specifically, we first transform MEC problem into a constrained optimization problem with two objective functions to obtain a trivial feasible solution. Then, we adopt the linear weighted sum method to solve the above constrained optimization problem, and construct the corresponding target Hamiltonian. Finally, we perform numerical experiments with 6, 8, and 10 qubits by using the ProjectQ quantum software development. The numerical results show that the solution can be obtained with high probability, even though level p of the algorithm is low. Besides, we remove n single-qubit rotating gates R_Z to optimize quantum circuit. We found that the number of quantum gates is reduced by np for p -level optimized circuit.

It is worth emphasizing that our algorithm adopts the linear sum method to solve the constrained optimization problem with two objective functions. This may inspire using QAOA+ to solve multi-objective constrained optimization problems.

This paper is organized as follows. In Sec. II, QAOA+ is reviewed. In Sec. III, we apply QAOA+ to solve MEC problem. In Sec. IV, numerical results and analysis are given. Finally, the summary and prospects are given in Sec. V.

II. REVIEW OF QAOA+

Considering the optimization problem (F, f) , where F is the feasible set and $f : F \rightarrow \mathbb{R}$ is the objective function to be optimized. Let \mathcal{F} be the Hilbert space of dimension $|F|$, whose standard basis is $\{|x\rangle : x \in F\}$. As a hybrid

* gaof@bupt.edu.cn

† wqy@bupt.edu.cn

quantum-classical algorithm, QAOA+ [31] is often used to solve combinatorial optimization problems. The specific process of QAOA+ is as follows.

First, we should be able to create an initial state $|x\rangle, x \in F$ which is a trivial feasible solution, or the uniform superposition state of trivial feasible solutions. Second, the phase-separation operator $U(H_P, \gamma) = e^{-\gamma H_P}$ which depends on the objective function f , and the mixing operator $U(H_M, \beta) = e^{-\beta H_M}$ which depends on F and its structure are applied alternately to $|x\rangle$, where γ and β are real parameters, and H_M and H_P are the mixing Hamiltonian and the target Hamiltonian, respectively. It worth noting that $U(H_M, \beta)$ needs to meet two conditions: 1) preserve the feasible subspace; 2) provide transitions between all pairs of feasible spaces, see Ref.[31] for details.

The alternating sequence continues for a total of p times with different variational parameters $\vec{\gamma} = (\gamma_1, \gamma_2, \dots, \gamma_p)$ and $\vec{\beta} = (\beta_1, \beta_2, \dots, \beta_p)$, where $\gamma_i \in [0, 2\pi]$, $\beta_i \in [0, \pi]$, such that the final variational state becomes

$$|\psi_p(\vec{\gamma}, \vec{\beta})\rangle = U(H_M, \beta_p)U(H_P, \gamma_p) \cdots U(H_P, \gamma_1)|x\rangle. \quad (1)$$

The variational parameters are optimized on classical computers. The structure of the QAOA+ is shown in Fig. 1. The objective of the classical optimizer is to find the optimal parameters $(\vec{\gamma}^*, \vec{\beta}^*)$, which are obtained by maximizing the expected value of the target Hamiltonian

$$(\vec{\gamma}^*, \vec{\beta}^*) = \arg \max_{\vec{\gamma}, \vec{\beta}} F_p(\vec{\gamma}, \vec{\beta}), \quad (2)$$

where $F_p(\vec{\gamma}, \vec{\beta}) = \langle \psi_p(\vec{\gamma}, \vec{\beta}) | H_P | \psi_p(\vec{\gamma}, \vec{\beta}) \rangle$.

We define the success probability as the probability of finding the optimal solution

$$P_{success} = |\langle x_{sol} | \psi_p(\vec{\gamma}, \vec{\beta}) \rangle|^2, \quad (3)$$

where x_{sol} is the solution to the problem.

III. APPLY QAOA+ TO SOLVE MEC PROBLEM

In this section, we first introduce MEC. Then, MEC is transformed into a constrained optimization problem with two objective functions. Finally, we solve MEC using QAOA+.

A. MEC

MEC [25] is shown as follows: considering the sets $X = \{x_1, \dots, x_m\}$ and $S = \{S_1, \dots, S_n\}$, where $S_i \subset X (i = 1, \dots, n)$, such that

$$X = \bigcup_{i=1}^n S_i. \quad (4)$$

A subset S^* of S , it is called an exact cover (EC) of X when elements of S^* are disjoint sets and union of the elements of S^* is X . S^* with the least number of elements is called MEC (MEC is not unique).

MEC problem can be expressed as follows [25]

$$\min \sum_{i=1}^n s_i, \quad (5)$$

$$s.t. \sum_{i: x_j \in S_i} s_i = 1, \quad \forall x_j \in X, \quad (6)$$

$$s_i, s_j \in \{0, 1\}, \quad (7)$$

where s_i is the label of set S_i . The objective function Eq. (5) is to minimize the number of sets, subject to constraints Eq. (6) ensuring that the elements of X are covered only once, i.e., EC.

Some algorithms [23–25] have been proposed to solve this problem using QAOA. The key point of QAOA is to construct the target Hamiltonian which includes solutions of the MEC problem. For constrained optimization problems, the common method is to incorporate hard constraints into the target function as a penalty item, and then convert the target function into a target Hamiltonian [25–30]. However, their algorithms need to search for the target solutions in the overall Hilbert space. This will lead to inefficiency in the search for solutions, and also invalid solutions are obtained. QAOA+ limits the state of system to the feasible space of constrained optimization problems. This makes the search for solutions more efficient, and the probability of obtaining invalid solutions is zero. And, the initial state $|x\rangle$ of the system is required to be a trivial feasible solution to the problem. However, EC is the feasible space for the MEC problem, which has no trivial solution.

To create a feasible initial state $|x\rangle$, we first give the following analysis according to the describe of MEC problem. Suppose an EC $S^* = \{S_l, \dots, S_k\}$, where $2 \leq l, k \leq n$ (without regard to $S_i = X$), we can conclude that elements of S^* are disjoint sets, and $|S_l| + \dots + |S_k| = |X|$ can be obtained. S^* with the least number of elements is called MEC. Then, let $\omega_i = |S_i|$, the MEC problem transformed into the following optimization problem with two objective functions

$$\min \sum_{i=1}^n s_i, \quad (8)$$

$$\max \sum_{i=1}^n \omega_i s_i, \quad (9)$$

$$s.t. \quad s_i + s_j \leq 1, S_i \cap S_j \neq \emptyset, \quad (10)$$

$$s_i, s_j \in \{0, 1\}, \quad (11)$$

where s_i and s_j are the label of sets S_i and S_j respectively. The objective function Eq. (8) is to minimize the number of sets and the objective function Eq. (9) is to maximize the sum of the weights of sets, subject to constraints Eq. (10) ensuring that two sets S_i, S_j cannot be

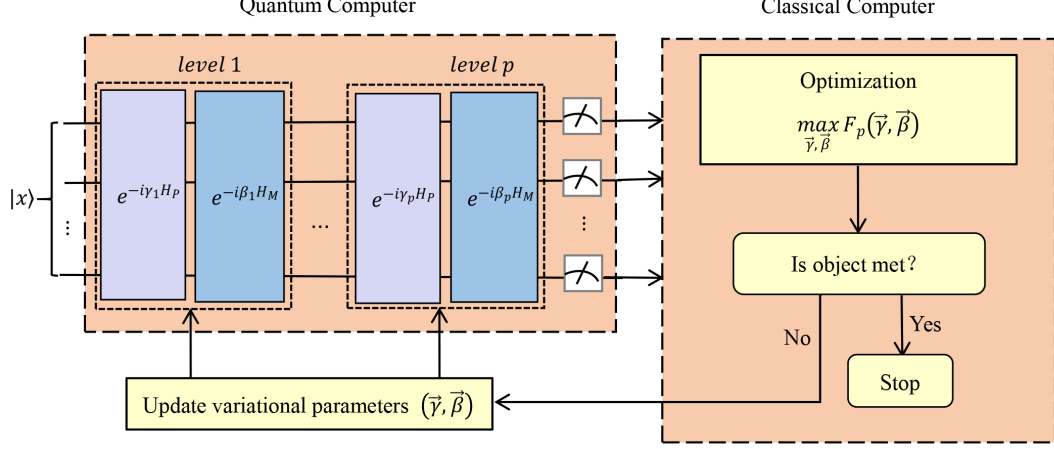


FIG. 1. Schematic of the QAOA+ [23]. The quantum processor consists of three parts: initial state, phase-separation operators $U(H_P, \gamma)$, and mixing-operators $U(H_M, \beta)$. The variational parameters are optimized on classical computers. The quantum computer is used to evaluate the expectation value of the objective function.

selected simultaneously, where $S_i \cap S_j \neq \emptyset$. Noting that Eq. (8) needs to be optimized on the premise of meeting Eq. (9).

The linear weighted sum method [38] is the simplest method to solve the multi-objective optimization problem. According to importance of each objective function to determine the corresponding weight, this method transforms the multi-objective into single-objective optimization problem. We adopt the linear weighted sum method to solve the above optimization problem, and transform it into a single-objective optimization problem

$$\max \quad \lambda_1 f_1 - \lambda_2 f_2, \quad (12)$$

$$\text{s.t.} \quad s_i + s_j \leq 1, S_i \cap S_j \neq \emptyset, \quad (13)$$

$$s_i, s_j \in \{0, 1\}, \quad (14)$$

where $\lambda_1 > \lambda_2 > 0$, $f_1 = \sum_{i=1}^n \omega_i s_i$, $f_2 = \sum_{i=1}^n s_i$.

B. QAOA+ FOR MEC

The QAOA+ mapping comprises phase-separation operators $U(H_P, \gamma)$, mixing operators $U(H_M, \beta)$, and initial state $|x\rangle$ for MEC problem. $U(H_P, \gamma) = e^{-i\gamma H_P}$ depends on Eq. (12). $U(H_M, \beta) = e^{-i\beta H_M}$ depends on Eq. (13) and its structure. According to Eq. (13), the initial state $|0\rangle^{\otimes n}$ can be chosen, which is a trivial feasible solution. Next, we need to construct the mixing Hamiltonian H_M and the target Hamiltonian H_P .

To construct H_M , inspired by [30], we construct a graph in which set $S_i (i = 1, \dots, n)$ is regarded as a vertex. There is an edge between two vertices S_i, S_j if and only if $S_i \cap S_j \neq \emptyset$. Therefore, the constraint Eq. (13) is equivalent to solving independent sets on the graph.

Given an independent set S' ($s_i = 1$ if and only if $S_i \in S'$, else $s_i = 0$), to maintain the property of the independent set, the following rules should be met when

adding and deleting vertices [31]: 1) the neighbors of S_i are marked as $S_{i1}, S_{i2}, \dots, S_{il}$, adding a vertex $S_i \notin S'$ so that the new point set is still an independent set only if none of the neighbors $S_{i1}, S_{i2}, \dots, S_{il}$ of S_i are already in S' , i.e., $s_{i1} = s_{i2} = \dots = s_{il} = 0$; 2) removing any vertex $S_j \in S'$ without affecting the feasibility of the state. Hence, a bit-flip operation at a vertex, controlled by its neighbors, suffices both to remove and add vertices while maintaining the independence property.

The mixing Hamiltonian H_M is expressed as follows

$$H_M = \sum_{i=1}^n \sum_{m_i=1}^{m_i} |s_{i1}s_{i2}\dots s_{il}\rangle \langle s_{i1}s_{i2}\dots s_{il}| \otimes X_i, \quad (15)$$

where $m_i = \prod_{k=1}^l (1 - s_{ik})$.

The objective function $f = \lambda_1 \sum_{i=1}^n \omega_i s_i - \lambda_2 \sum_{i=1}^n s_i$, and target Hamiltonian H_P is obtained by replacing s_i with $\frac{1 - \sigma_i^Z}{2}$

$$H_P = \lambda_1 \sum_{i=1}^n \omega_i \frac{1 - \sigma_i^Z}{2} - \lambda_2 \sum_{i=1}^n \frac{1 - \sigma_i^Z}{2}, \quad (16)$$

where $\lambda_1 > \lambda_2 > 0$, σ_i^Z represents Pauli-Z operation on i th qubit.

IV. NUMERICAL SIMULATION

We study instances for three different problem sizes of the MEC problem given in Table I, corresponding to 6, 8, and 10 qubits, respectively.

A. Discussion about weights

In multi-objective problems, the weight of each index is one of the important factors that affect the accuracy

TABLE I. Information about the MEC problem instances

$ X $	$ S $	Number of instances	Number of solutions for each instance
12	6	10	1
16	8	10	1
20	10	10	1

of the results. Next, we discuss the weight λ_i ($i = 1, 2$) of MEC in two cases and fix λ_1 and λ_2 .

The MEC is expressed as the following optimization problem

$$\max f, \quad (17)$$

$$\text{s.t. } s_i + s_j \leq 1, S_i \cap S_j \neq \emptyset, \quad (18)$$

$$s_i, s_j \in \{0, 1\}, \quad (19)$$

where $\lambda_1 > \lambda_2 > 0$, $f = \lambda_1 \sum_{i=1}^n \omega_i s_i - \lambda_2 \sum_{i=1}^n s_i$.

Suppose the set A is a MEC (solution of MEC problem), and the corresponding objective function is $f_A = \lambda_1 m - \lambda_2 m'$, where $m = |X|$, $m' = |A|$. Suppose the set B is not MEC, and its corresponding objective function is $f_B = \lambda_1 t - \lambda_2 t'$, where $t \leq m$, $t' = |B|$. Based on the above assumptions, we can obtain $f_A > f_B$. Next, we will consider that B is an EC or not, and discuss weight λ_i in two situations.

If set B is an EC, we can obtain $t = m$, $t' > m'$. The inequality $f_A > f_B$ is always true with $\lambda_i > 0$ ($i = 1, 2$). If set B is not an EC, we can get $t < m$, and then deduce $\frac{\lambda_1}{\lambda_2} > \frac{m'-t'}{m-t}$.

To determine the appropriate values of λ_1 and λ_2 , the range of function $f = \lambda_1 f_1 - \lambda_2 f_2$ is limited to $(0, 1]$

$$0 < n\lambda_2 f_1 - \lambda_2 f_2 \leq 1. \quad (20)$$

Because of $n f_1 - f_2 > 0$, we can deduce $0 < \lambda_2 \leq \frac{1}{n f_1 - f_2}$, where $f_1 \leq m$, $f_2 \geq 2$ (without regard to $S_i = X$). Further, $0 < \lambda_2 \leq \frac{1}{nm-2}$ can be obtained. Without losing generality, we can make $\lambda_2 = \frac{1}{nm-2}$ in this paper. And then, we make $\frac{\lambda_1}{\lambda_2} = n$ according to $\frac{m'-t'}{m-t} < n$ (n is number of qubits).

B. Low levels: patterns in optimal variational parameters

The patterns in the optimal variational parameters for MaxCut have been observed in Ref.[39], where it was found that there is a linear relationship between the parameters and the level p . Based on observed linear patterns, two heuristic optimization strategies are proposed, which significantly speed up the classical optimization of QAOA. The optimal parameter pattern is a useful guide in the selection and design of heuristic strategies. Before studying the performance of the QAOA+, we need to observe the patterns of optimal variational parameters at low level, namely up to $p = 5$.

To find the optimal variational parameters for $1 \leq p \leq 5$, the gradient-based Broyden-Fletcher-Goldfarb-Shanno (BFGS) [40–43] is adopted in this paper. It is a commonly used local optimization algorithm, which is repeated with sufficiently many random initial parameters to find the global optimum.

After performing numerical simulations for 10 instances of MEC problem with 6-qubit using QAOA+, we present the optimal variational parameters $(\vec{\gamma}^*, \vec{\beta}^*)$ from $p = 3$ up to $p = 5$ as shown in Fig. 2. The optimal parameters do not follow the linear pattern as in Ref.[39] so the interpolation optimization cannot be performed. Recently, parameters fixing strategy [44], a straightforward, yet practically effective, is proposed to improve the performance of QAOA at large circuit depths. The optimal parameters $(\gamma_1^*, \dots, \gamma_{p-1}^*, \beta_1^*, \dots, \beta_{p-1}^*)$ at level $p-1$ to be further optimized as they are passed into QAOA of p -level as the initial parameters. Hence, the initial parameters at level p will be $(\gamma_1^*, \dots, \gamma_{p-1}^*, \gamma_p, \beta_1^*, \dots, \beta_{p-1}^*, \beta_p)$, where γ_p and β_p are random parameters. Inspired by this, we will investigate whether this strategy can improve the performance of QAOA+.

C. Analysis of success probability

Based on the discussion of optimal variational parameter patterns in the previous section, we intend to use random initialization and parameters fixing strategy to study the performance of QAOA+. From the starting point of generation, we run the BFGS optimization method for this algorithm.

In Fig. 3(a), the mean success probability, as a function of level p , is plotted with random initialization parameters method, over all instances for the three different problem sizes. It is observed that the mean success probability increased slowly with the increase of level p overall in all 30 instances.

To investigate whether parameters fixing strategy can improve the performance of QAOA+, we select an instance from each problem size, and simulate them up to $p = 7$ using random initialization and parameters fixing strategy respectively. In Fig. 3(b), we plot the mean success probability using the random initialization for these three instances. It is observed that for 6-qubit and 8-qubit, the solution can be obtained with a probability close to 100% with $p = 7$. In Fig. 3(c), we plot the mean success probability using the parameters fixing strategy for these three instances. When $p > 2$, the parameters fixing strategy outperforms the random initialization run for these three examples. The solution can be obtained with a probability close to 100% for 6 and 8 qubits, even though level p of the algorithm is low.

The numerical results show that the solution can be obtained with high probability by using parameters fixing strategy, even though level p of the algorithm is low. Hence, we can conclude that the parameters fixing strategy can make the algorithm have better performance, at

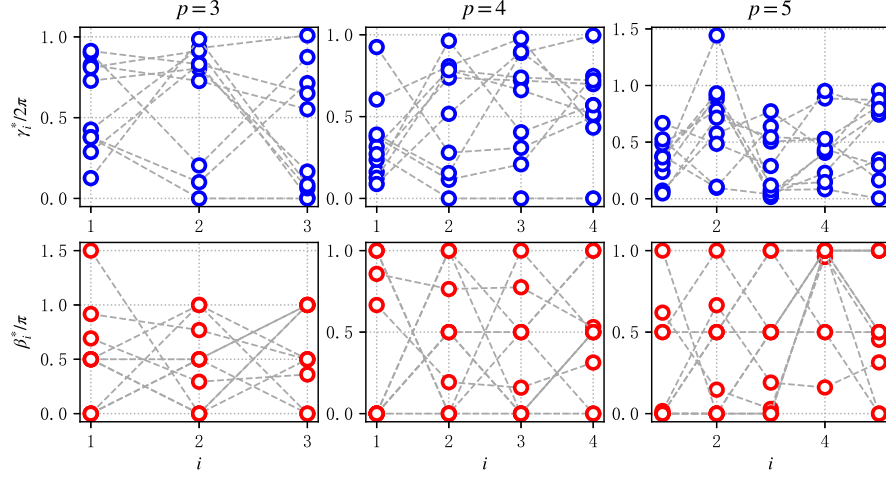


FIG. 2. Optimal QAOA+ variational parameters for 10 instances with 6-qubit, for $3 \leq p \leq 5$. In the above figure, each dashed line connects parameters for one instance. For each instance and each p , we use the classical BFGS optimization method from 1000 random initial variational parameters, and keep the best parameters.

least true for the MEC problem instances used in our work.

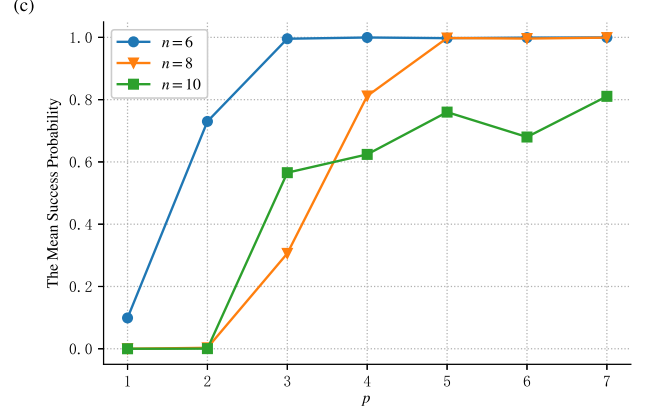
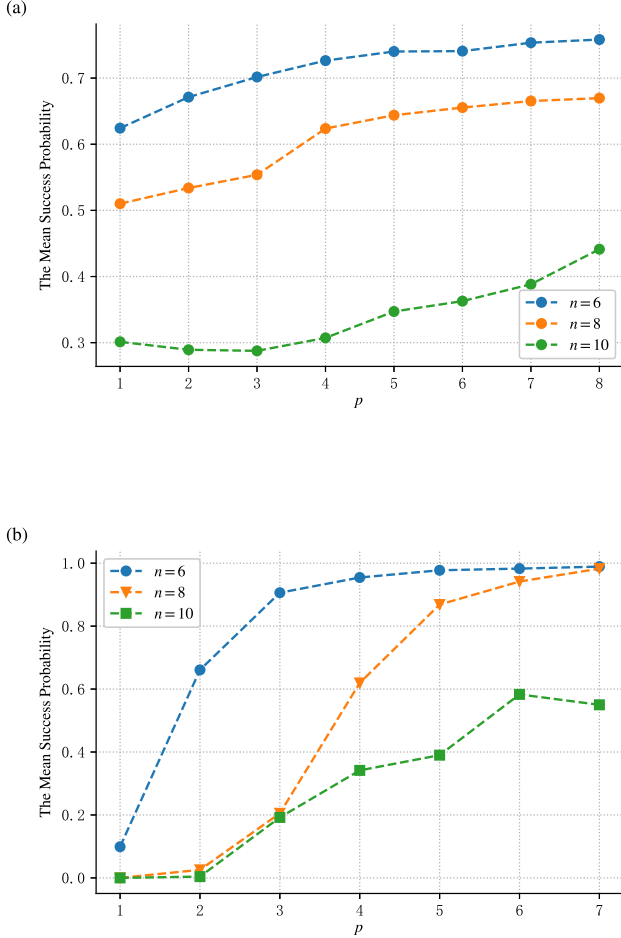


FIG. 3. (a) The mean success probability, as a function of level p averaged, is plotted using random initialization method, over all instances for the three different problem sizes. (b) The mean success probability as a function of level p for one selected instance from each problem size is plotted using random initialization method. (c) The mean success probability is plotted using the parameters fixing strategy, for one selected instance from each problem size.

D. Quantum circuit optimization

The QAOA+ mapping comprises phase-separation operators $U(H_P, \gamma)$, mixing operators $U(H_M, \beta)$, and initial state $|x\rangle$ for MEC problem. Based on H_M and H_P , the corresponding circuits of $U(H_M, \beta)$ are multiqubit-controlled- $R_X(2\beta)$ gates, and the corresponding circuits of $U(H_P, \gamma)$ are n single-qubit rotating gates R_Z . For example: $X = \{1, \dots, 12\}$ and $S = \{S_1, \dots, S_6\}$, where $S_1 = \{1, 2, 4, 5, 6, 8, 9, 10\}$, $S_2 = \{1, 4, 6, 7\}$, $S_3 = \{5, 8, 9, 11, 12\}$, $S_4 = \{4, 7, 8, 9, 10, 11, 12\}$, $S_5 =$

$\{2, 3, 4, 5, 6, 7, 11, 12\}$, $S_6 = \{3, 10, 12\}$. The corresponding figure is constructed, as shown in Fig. 4.

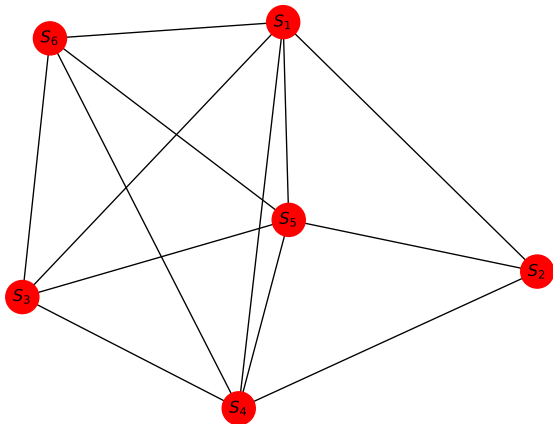


FIG. 4. Graph representation of the instance.

Based on discussion about weight $\lambda_i (i = 1, 2)$, let $\lambda_2 = \frac{1}{nm-2} = 1/70$, $\lambda_1 = n\lambda_2 = 6/70$, the overall 1-level quantum circuit diagram of QAOA+ mapping is given, as shown in Fig. 5. Since single-qubit rotating gate R_Z only changes the phase, we consider removing n single-qubit rotating gates R_Z , as shown in Fig. 6. We find that this new p -level circuit only needs p parameters, and the number of quantum gates is reduced by np . To study the ability of p -level circuit shown in Fig. 6 to find a solution, in Fig. 7, the comparison of mean success probability is plotted using random initialization method, for these two p -level circuits. The results show that p -level circuit requires only p parameters, which can achieve an experimental effect similar to the original circuit with $2p$ parameters. The number of quantum gates

is reduced by np for p -level optimized circuit.

V. SUMMARY AND PROSPECTS

To summarize, we solved the MEC problem with QAOA+. The results show that the solution can be obtained with high probability, even though level p of the algorithm is low. In detail, we first transform the MEC into a constrained optimization problem with two objective functions. Then, we adopt the linear weighted sum method to solve the above constrained optimization problem and construct the corresponding target Hamiltonian. Finally, inspired by the parameter fixed strategy, we use this strategy to simulate instances with 6, 8, and 10 qubits. The numerical results show that the solution can be obtained with a probability close to 100% for 6 and 8 qubits, even though level p of the algorithm is low. Besides, we optimize the quantum circuit by removing single-qubit rotating gates R_Z . The results show that the number of quantum gates is reduced by np for p -level optimized circuit. Furthermore, p -level optimized circuit only needs p parameters, which can achieve an experimental effect similar to original circuit with $2p$ parameters.

In this paper, we adopt the linear sum method to solve the constrained optimization problem with two objective functions, and get good results. It is hoped that our algorithm can bring more inspiration for solving multi-objective optimization problems.

ACKNOWLEDGMENTS

We thank Shijie Pan, Linchun Wan, and Xiumei Zhao for useful discussions on the subject. This work is supported by the Beijing Natural Science Foundation (Grant No. 4222031), the National Natural Science Foundation of China (Grant Nos. 61976024, 61972048, 62272056), and the 111 Project B21049.

-
- [1] P. W. Shor, Algorithms for quantum computation: Discrete logarithms and factoring, in *Proceedings 35th Annual Symposium on Foundations of Computer Science*, pp. 124-134 (1994).
 - [2] L. K. Grover, Quantum mechanics helps in searching for a needle in a haystack, *Phys. Rev. Lett.* **79** (2), 325-328 (1997).
 - [3] A. W. Harrow, A. Hassidim, and S. Lloyd, Quantum algorithm for linear systems of equations, *Phys. Rev. Lett.* **103** (15), 150502 (2009).
 - [4] C. H. Yu, F. Gao, C. Liu, D. Huynh, M. Reynolds, and J. Wang, Quantum algorithm for visual tracking, *Phys. Rev. A* **99**, 022301 (2019).
 - [5] C. H. Yu, F. Gao, and Y. Q. Wen, An improved quantum algorithm for ridge regression, *IEEE Trans. Know. Data Eng.* **33** (3), 858-866 (2021).
 - [6] R. Patrick, M. Masoud, and L. Seth, Quantum support vector machine for big data classification, *Phys. Rev. Lett.* **113** (13), 130503 (2014).
 - [7] S. Lloyd, M. Mohseni, and P. Rebentrost, Quantum principal component analysis, *Nature Physics* **10**, 631 (2014).
 - [8] S. J. Pan, L. C. Wan, H. L. Liu, Q. L. Wang, S. J. Qin, Q. Y. Wen, and F. Gao, Improved quantum algorithm for A-optimal projection, *Phys. Rev. A* **102** (5), 052402 (2020).
 - [9] S. J. Pan, L. C. Wan, H. L. Liu, Y. S. Wu, S. J. Qin, Q. Y. Wen, and F. Gao, Quantum algorithm for neighborhood preserving embedding, *Chinese Physics B* **31**, 060304 (2022).
 - [10] Y. M. Li, H. L. Liu, S. J. Pan, S. J. Qin, F. Gao, and Q.

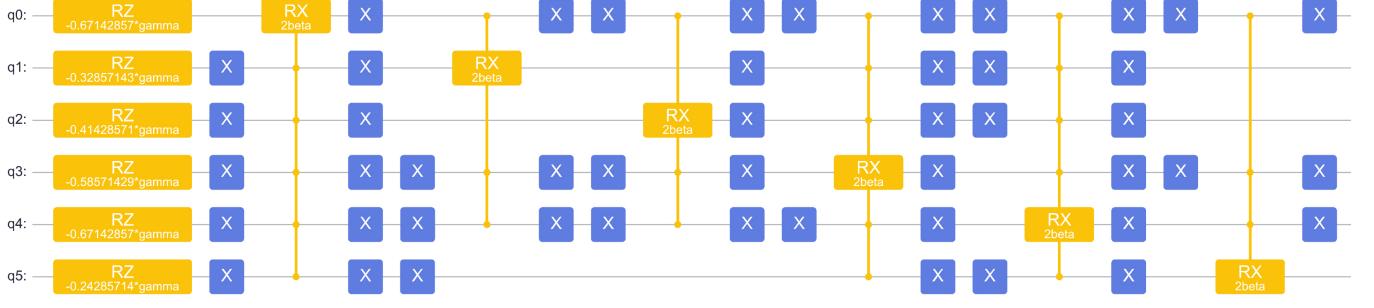


FIG. 5. The overall 1-level quantum circuit diagram of QAOA+ mapping.

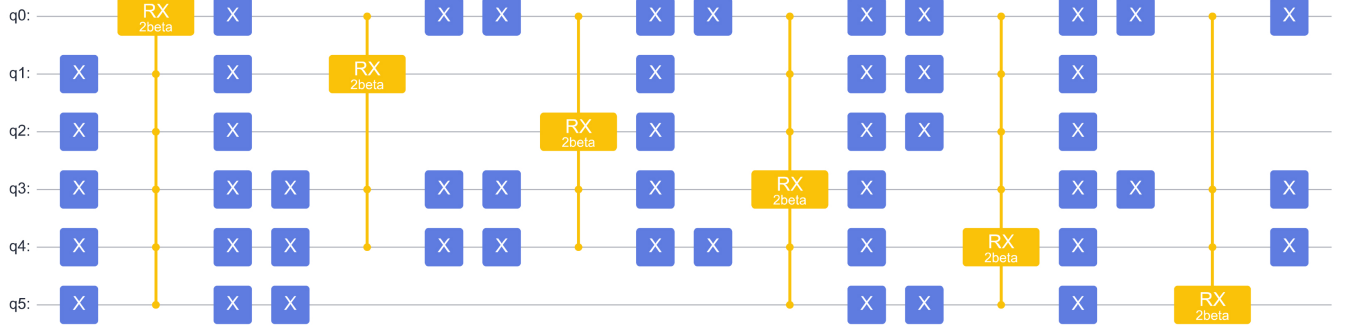


FIG. 6. The new 1-level quantum circuit after removing the single-qubit rotating gates R_Z .

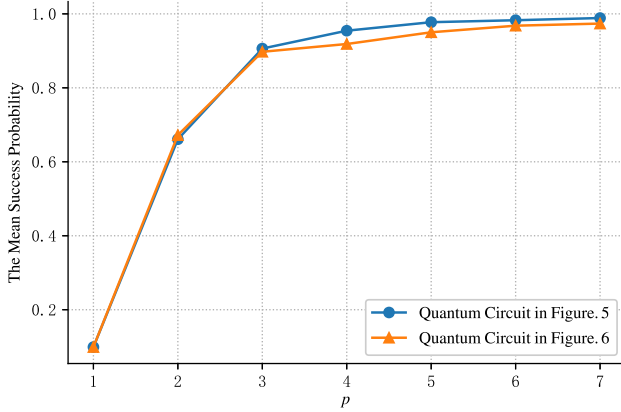


FIG. 7. The comparison of mean success probability corresponding to these two circuits.

Y. Wen, Quantum discriminative canonical correlation analysis, arXiv:2206.05526.

- [11] L. C. Wan, C. H. Yu, S. J. Pan, F. Gao, Q. Y. Wen, and S. J. Qin, Asymptotic quantum algorithm for the Toeplitz systems, *Phys. Rev. A* **97**, 062322 (2018).
- [12] H. L. Liu, S. J. Qin, L. C. Wan, C. H. Yu, S. J. Pan, F. Gao, and Q. Y. Wen, A quantum algorithm for solving eigenproblem of the Laplacian matrix of a fully connected weighted graph, arXiv:2203.14451.

- [13] L. C. Wan, C. H. Yu, S. J. Pan, S. J. Qin, F. Gao, and Q. Y. Wen, Block-encoding-based quantum algorithm for linear systems with displacement structures, *Phys. Rev. A* **104**, 062414 (2021).
- [14] H. L. Liu, C. H. Yu, L. C. Wan, S. J. Qin, F. Gao, and Q. Y. Wen, Quantum mean centering for block-encoding-based quantum algorithm, *Physica A: Statistical Mechanics and its Applications* **607**, 128227 (2022).
- [15] M. Guo, H. Liu, Y. Li, W. Li, F. Gao, S. Qin, and Q. Wen, Quantum algorithms for anomaly detection using amplitude estimation, *Physica A: Statistical Mechanics and its Applications* **604** (3), 127936 (2022).
- [16] Z. Q. Li, B. B. Cai, H. W. Sun, H. L. Liu, L. C. Wan, S. J. Qin, Q. Y. Wen, and F. Gao, Novel quantum circuit implementation of Advanced Encryption Standard with low costs, *Sci. China-Phys. Mech. Astron.* **65**, 290311 (2022).
- [17] E. Farhi, J. Goldstone, and S. Gutmann, A quantum approximate optimization algorithm, arXiv:1411.4028.
- [18] P. Botsinis, D. Alanis, S. Feng, Z. Babar, H. V. Nguyen, D. Chandra, S. X. Ng, R. Zhang, and L. Hanzo, Quantum-assisted indoor localization for uplink mm-wave and downlink visible light communication systems, *IEEE Access* **5**, 23327-23351 (2017).
- [19] Z. Wang, S. Hadfield, Z. Jiang, and E. G. Rieffel, Quantum approximate optimization algorithm for maxcut: A fermionic view, *Physical Review A* **97**, 022304 (2018).
- [20] R. Herrman, L. Treffert, J. Ostrowski, P. C. Lotshaw, T. S. Humble, and G. Siopsis, Impact of graph structures for QAOA on maxcut, *Quantum Information Processing*

- 20** (9), 289 (2021).
- [21] Y. J. Zhang, X. D. Mu, X. W. Liu, X. Y. Wang, X. Zhang, K. Li, T. Y. Wu, D. Zhao, and C. Dong, Applying the quantum approximate optimization algorithm to the minimum vertex cover problem, *Applied Soft Computing*, **118**, 108554 (2022).
 - [22] J. R. Weggemans, A. Urech, A. Rausch, R. Spreeuw, R. Boucherie, F. Schreck, K. Schoutens, J. Minář, and F. Speelman, Solving correlation clustering with QAOA and a Rydberg qudit system: a full-stack approach, *Quantum* **6**, 687 (2022).
 - [23] P. Vikstål, M. Grnkvist, M. Svensson, M. Andersson, G. Johansson, and G. Ferrini, Applying the Quantum Approximate Optimization Algorithm to the Tail-Assignment Problem, *Phys. Rev. Applied* **14** (3), 034009 (2020).
 - [24] M. Svensson, M. Andersson, M. Grnkvist, P. Vikstål, D. Dubhashi, G. Ferrini, and G. Johansson, A Heuristic Method to solve large-scale Integer Linear Programs by combining Branch-and-Price with a Quantum Algorithm, arXiv:2103.15433.
 - [25] A. Lucas, Ising formulations of many NP problems, *Front. Phys.* **2**, 5 (2014).
 - [26] R. Biswas, et al., A NASA perspective on quantum computing: Opportunities and challenges, *Parallel Computing* **64**, 81-98 (2017).
 - [27] E. G. Rieffel, D. Venturelli, B. O’Gorman, M. B. Do, E. M. Prystay, and V. N. Smelyanskiy, A case study in programming a quantum annealer for hard operational planning problems, *Quantum Information Processing*, **14** (1), 1-36 (2015).
 - [28] S. Hadfield, On the representation of Boolean and real functions as Hamiltonians for quantum computing, arXiv:1804.09130.
 - [29] I. Hen and F. M. Spedalieri, Quantum Annealing for Constrained Optimization, *Phys. Rev. Applied* **5** (3), 034007 (2016).
 - [30] V. Choi, Different adiabatic quantum optimization algorithms for the NP-complete exact cover and 3SAT problems, arXiv:1010.1221.
 - [31] S. Hadfield, Z. Wang, B. O’Gorman, E. G. Rieffel, D. Venturelli, and R. Biswas, From the quantum approximate optimization algorithm to a quantum alternating operator ansatz, *Algorithms* **12** (2), 34 (2019).
 - [32] S. Hadfield, et al, Quantum Approximate Optimization with Hard and Soft Constraints, in *The Second International Workshop on Post-Moore’s Era Supercomputing*, pp. 15-21 (2017).
 - [33] Z. H. Wang, N. C. Rubin, J. M. Dominy, and E. G. Rieffel, XY mixers: Analytical and numerical results for the quantum alternating operator ansatz, *Phys. Rev. A* **10** (1), 012320 (2020).
 - [34] Z. H. Saleem, Max-independent set and the quantum alternating operator ansatz, *International Journal of Quantum Information* **18** (4), 2050011 (2020).
 - [35] J. Cook, S. Eidenbenz, and A. Brtschi, The Quantum Alternating Operator Ansatz on Max- k Vertex Cover, in *APS March Meeting*, **65**, 1 (2020).
 - [36] S. Chatterjee and D. Bera, Applying the Quantum Alternating Operator Ansatz to the Graph Matching Problem, arXiv:2011.11918.
 - [37] M. Fingerhuth, B. Tomá, and C. Ing, A quantum alternating operator ansatz with hard and soft constraints for lattice protein folding, arXiv:1810.13411.
 - [38] I. P. Stanimirović, M. L. Zlatanović, and M. D. Petković, On the linear weighted sum method for multi-objective optimization, *Facta Univ. Ser. Math. Inform.* **26**, 49-63 (2011).
 - [39] L. Zhou, S. T. Wang, S. Choi, H. Pichler, and M. D. Lukin, Quantum approximate optimization algorithm: Performance, mechanism, and implementation on near-term devices, *Phys. Rev. X* **10** (2), 021067 (2020).
 - [40] C. G. BROYDEN, The Convergence of a Class of Double-rank Minimization Algorithms 1. General Considerations, *IMA Journal of Applied Mathematics* **6**, 76 (1970).
 - [41] R. Fletcher, A new approach to variable metric algorithms, *The Computer Journal* **13**, 317 (1970).
 - [42] D. Goldfarb, A family of variable-metric methods derived by variational means, *Mathematics of Computation* **24**, 23 (1970).
 - [43] D. F. Shanno, Conditioning of quasi-Newton methods for function minimization, *Mathematics of Computation* **24**, 647 (1970).
 - [44] X. Lee, Y. Saito, D. Cai, and N. Asai, Parameters Fixing Strategy for Quantum Approximate Optimization Algorithm, in *2021 IEEE International Conference on Quantum Computing and Engineering*, pp. 10-16 (2021).
 - [45] M. Grönkvist, The Tail Assignment Problem, Ph.D. thesis, Chalmers University of Technology and Gteborg University (2005).
 - [46] T. L. Jacobs, L. A. Garrow, M. Lohatepanont, Frank S. Koppelman, G. M. Coldren, and H. W. Purnomo, Airline Planning and Schedule Development, in *Quantitative Problem Solving Methods in the Airline Industry*, pp. 35-39 (2012).
 - [47] M. Grönkvist and J. Kjerrström, Tail Assignment in Practice, in *Operations Research Proceedings 2004*, pp. 166-173 (2004).
 - [48] L. Martins, Applying Quantum Annealing to the Tail Assignment Problem, Ph.D. thesis, University of Porto (2020).
 - [49] R. M. Karp, Reducibility Among Combinatorial Problems, in *Complexity of Computer Computations*, pp. 85-103 (1972).

Appendix A: Multi-objective Constrained Optimization Problem

Airlines realize the optimal allocation of various production factors, through careful organization and production planning. Aircraft route allocation is an important part of the airline’s organization and production planning. A reasonable and effective aircraft route allocation scheme helps to ensure the core utilization of the airline’s resources, implement the airline’s development strategy, ensure the safety of the airline’s production and operation activities, and the realizability of the airline’s revenue and expenditure budget in the current year. For a long time, operational

research theory has been the source of innovation and development of international air transport industry, and has been widely used in the production and planning of various organizations of airlines, aviation revenue management and other fields. However, the airline network is one of the most complex networks in the world, and it is still developing rapidly. In the face of more and more complicated airline networks, the production and plans of airlines also pose great challenges to researchers.

The tail-assignment problem [45, 46] is an essential issue in the production planning of airlines. It is also one of the main contents in the operation control of airlines, where the goal is to decide which individual aircraft should operate which flight. By introducing the concept of route, the problem of aircraft-to-flight assignment is transformed into the problem of aircraft-to-route assignment. Each route starts and ends at the hub airport, and there are fixed departure and arrival times at the hub airport, thus reducing the scale and complexity of the problem. The tail-assignment problem is a combinatorial optimization problem essentially, which is NP-complete [49], and also a hot topic studied by scholars.

Now, let F denote the set of flights, and R the set of all legal routes. Denote by c_{r_i} the cost of route $r_i \in R$. Let a_{fr_i} be 1 if flight f is covered by route r_i and 0 otherwise. The decision variable x_{r_i} is 1 if route r_i should be used in the solution, and 0 otherwise. The tail-assignment problem [23, 24, 48] can now be formulated as

$$\min \sum_{i=1}^{|R|} c_{r_i} x_{r_i}, \quad (A1)$$

$$s.t. \sum_{r_i \in R} a_{fr_i} x_{r_i} = 1, \quad \forall f \in F, \quad (A2)$$

$$x_{r_i} \in \{0, 1\}, \quad \forall r_i \in R. \quad (A3)$$

The objective Eq. (A1) is to minimize the total cost of the selected routes, subject to constraints Eq. (A2) ensuring that the set of routes in a solution should contain flight f exactly once each flight. The model is an example of an exact cover problem, which is NP-complete [49].

According to the mathematical model of the MEC problem, the tail-assignment problem can also be expressed as the following

$$\min \sum_{i=1}^{|R|} c_{r_i} x_{r_i}, \quad (A4)$$

$$\max \sum_{i=1}^{|R|} \omega_{r_i} x_{r_i}, \quad (A5)$$

$$s.t. \quad x_{r_i} + x_{r_j} \leq 1, \quad r_i \cap r_j \neq \emptyset, \quad (A6)$$

$$x_{r_i}, x_{r_j} \in \{0, 1\}, \quad (A7)$$

where c_{r_i} represents the cost of r_i , and $\omega_{r_i} = |r_i|$. The objective Eq. (A4) is to minimize the total cost of the selected routes, and the objective Eq. (A5) is to maximize the sum of the weights of each route, subject to constraints Eq. (A6) ensuring that two routes with $r_i \cap r_j \neq \emptyset$ cannot be selected simultaneously.

In particular, we introduce a new target: the minimum number of aircraft (i.e., the minimum number of selected routes). The tail-assignment problem with the minimum number of selected routes can now be formulated as

$$\min \sum_{i=1}^{|R|} c_{r_i} x_{r_i}, \quad (A8)$$

$$\min \sum_{i=1}^{|R|} x_{r_i}, \quad (A9)$$

$$\max \sum_{i=1}^{|R|} \omega_{r_i} x_{r_i}, \quad (A10)$$

$$s.t. \quad x_{r_i} + x_{r_j} \leq 1, r_i \cap r_j \neq \emptyset, \quad (A11)$$

$$x_{r_i}, x_{r_j} \in \{0, 1\}. \quad (A12)$$

The objective Eq. (A8) is to minimize the total cost of the selected routes, and the objective Eq. (A9) is to minimize the total number of the selected routes, and the objective Eq. (A10) is to maximize the sum of the weights of each

route, subject to constraints Eq. (A11) ensuring that two routes with $r_i \cap r_j \neq \emptyset$ cannot be selected simultaneously. According to the importance of the objective function, it is arranged as Eq. (A10), Eq. (A9), and Eq. (A8) in descending order.

The tail-assignment problem with the minimum number of selected routes is transformed into a single objective constrained optimization problem

$$\max \quad \lambda_1 \sum_{i=1}^{|R|} \omega_{r_i} x_{r_i} - \lambda_2 \sum_{i=1}^{|R|} x_{r_i} - \lambda_3 \sum_{i=1}^{|R|} c_{r_i} x_{r_i}, \quad (\text{A13})$$

$$\text{s.t.} \quad x_{r_i} + x_{r_j} \leq 1, r_i \cap r_j \neq \emptyset, \quad (\text{A14})$$

$$x_{r_i}, x_{r_j} \in \{0, 1\}, \quad (\text{A15})$$

where $\lambda_1 > \lambda_2 > \lambda_3 > 0$, and their values can be determined according to experience. The corresponding phase separation Hamiltonian is obtained by replacing x_{r_i} with $\frac{1 - \sigma_i^Z}{2}$

$$H_P = \lambda_1 \sum_{i=1}^{|R|} \omega_{r_i} \frac{1 - \sigma_i^Z}{2} - \lambda_2 \sum_{i=1}^{|R|} \frac{1 - \sigma_i^Z}{2} - \lambda_3 \sum_{i=1}^{|R|} c_{r_i} \frac{1 - \sigma_i^Z}{2}. \quad (\text{A16})$$

We study instances for three different problem sizes of tail-assignment problem with the minimum number of selected routes given in Table II, corresponding to 6, 8, and 10 routes, respectively.

TABLE II. Information about the tail-assignment problem with the minimum number of selected routes instances.

$ F $	$ R $	Number of instances	Number of solutions
12	6	1	1
16	8	1	1
20	10	1	1

We conducted numerical simulations for the examples in the table shown in Fig. 8. In Fig. 8, the mean success probability as a function of level p for the three different problem sizes is plotted with random initialization method. The numerical result shows that the mean success probability of 10 route instance is higher than that of 8 route instance for $p \leq 6$. This fact can seem counterintuitive, as one could naively think that larger instances correspond to harder problems. In addition, we note that the mean success probability of the 10 route instance shows a downward trend for $7 \leq p \leq 8$. For the counterintuitive phenomena shown in Fig. 8, we will study them in future work.

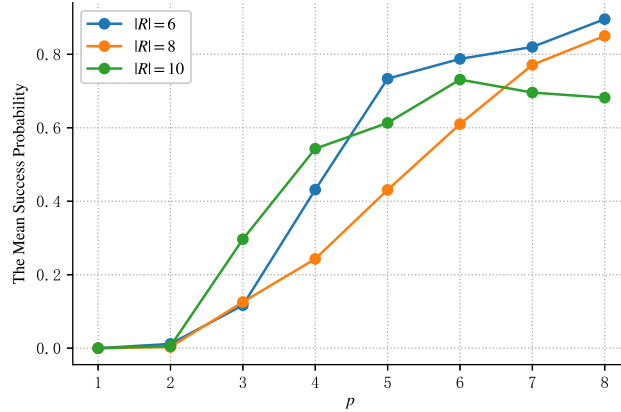


FIG. 8. Success probability for solving the tail-assignment problem with the minimum number of selected routes.