# **Open-Shop Scheduling With Hard Constraints**

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Encoding hard constrained optimization problems into a variational quantum algorithm often turns out to be a challenging task. In this work, we provide a solution for the class of open-shop scheduling problems (OSSP), which we achieve by rigorously employing the symmetries of the classical problem.

An established approach for encoding the hard constraints of the closely related traveling salesperson problem (TSP) into mixer Hamiltonians was recently given by Hadfield et al.'s Quantum Alternating Operator Ansatz (QAOA). For OSSP, which contains TSP as a special case, we show that desired properties of similarly constructed mixers can be directly linked to a purely classical object: the group of feasibility-preserving bit value permutations. We also outline a generic way to construct QAOA-like-mixers for these problems. We further propose a new variational quantum algorithm that incorporates the underlying group structure more naturally, and implement our new algorithm for a small OSSP instance on an IBM Q System One. Unlike the QAOA, our algorithm allows bounding the amount and the domain of parameters necessary to reach every feasible solution from above: If J jobs should be distributed, we need at most  $J(J-1)^2/2$  parameters.

# I. INTRODUCTION

Logistic and scheduling tasks are a major branch within the collection of hard optimization problems for relevant industrial applications. A prominent representative of those is the *open-shop scheduling problem* OSSP(M, T, J) which we consider in this work: Given M machines with T time slots each, one has to distribute J jobs such that every job gets performed precisely once and no position is filled with more than one job. Not only is OSSP at the mathematical core of many real world problems, it also prominently incorporates the well-known *traveling salesperson problem* (TSP) as a subclass, i.e. we have TSP = OSSP(1, T, T).

Its practical relevance as well as the fact that solving an instance of OSSP can easily turn out to be a hard task for classical computers, make OSSP an interesting target for the application of quantum algorithms. Confronted with the restricted capabilities of available quantum computer architectures, the class of variational quantum algorithms<sup>1-5</sup> (VQAs) is here receiving a particular amount of attention, since it promises to yield tools for tackling computational challenges within the NISQ<sup>6,7</sup> era.

There are, however, certain hurdles to overcome. The basic input for applying a VQA to an optimization problem is an encoding of an objective function f into a multiqubit objective Hamiltonian  $H_f$  such that - in case of a minimization problem - optimal solutions correspond to the smallest expectation value attainable by a quantum state<sup>8</sup>. In contrast to other popular problems, like MAX-CUT or 3-Sat, the OSSP additionally demands us to not only consider the encoding of an objective function, but also the encoding of further constraints. As a consequence, a VQA ideally has to perform its optimization only on a subset of 'allowed/feasible' quantum states, i.e. those that respect constraints. The major contribution of this work is a systematic analysis of symmetry structures in OSSP which will enable us to design a class of VQA algorithms that will, by construction, only optimize over feasible states.

In general, there are two strategies for handling constrained optimization problems:

- softcoded constraints. Any assignment is considered feasible, but the constraints enter the objective function as additional terms and penalize assignments that were originally infeasible. The modified objective function results in a more complex objective Hamiltonian. In exchange, the ground state search can be conducted in the entire qubit space without the necessity of preserving feasibility throughout the routine. A comprehensible introduction and case study using Qiskit and IBM quantum computers will be published soon<sup>9</sup>.
- hardcoded constraints. The objective function (and thus the objective Hamiltonian) is left unmodified, while the ground state search is restricted to the subspace corresponding to feasible solutions. Preservation of feasibility is typically ensured by additional gates representing the classical constraints.

Most VQAs such as the variational quantum eigensolver<sup>3</sup> or the quantum approximate optimization algorithm<sup>10</sup> are originally formulated for unconstrained problems and thus are merely applicable to softcoded instances. However, several case studies indicate that softcoding the constraints often either leads to suboptimal

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optimization landscapes or issues with feasibility<sup>11–13</sup>. This is why quantum algorithms with built-in possibilities for hardcoding constraints received increasing interest. Most notably, Hadfield et al.<sup>14</sup> extended the quantum approximate optimization algorithm to the quantum alternating operator ansatz (QAOA) which can also be applied to hardcoded constrained optimization problems. Unlike its predecessor, the QAOA is formulated with a problem-dependent mixer and is therefore sensitive to different feasibility structures.

Albeit there is a massive catalogue<sup>15</sup> of classical constraint analysis available for these problems, concrete instances were mainly heuristically constructed. However, the underlying feasibility structure was not completely exploited. One particular interesting construction for scheduling-type problems is the *constraint graph*  $model^{16,17}$ . Here the bit strings are identified with vertices, joint by edges corresponding to the constraints. This allows investigating the feasibility structure with well-known results from graph theory. Most notably, one can identify graph automorphisms with feasibilitypreserving bit permutations. With this work, we incorporate the whole structure into a more refined view on the QAOA and also come up with a new VQA design for OSSP-instances.

In Section III we apply the constraint graph model to the general OSSP. We first embed the notions of solutions and solution-preserving functions into the graphtheoretical language. Utilizing this additional point of view, we fully characterize the group F of feasibilitypreserving bit permutations. Furthermore, we uncover block structures within the OSSP-constraints. This ultimately reveals that F acts transitively on the set of all solutions.

In Section IV we then draw the connection between the classical description of F and specific VQA designs. Firstly, we review how the QAOA works in general and proceed with a discussion of its main ingredients. We give refined definitions for 'phase separator' and 'mixer' gates and detail a general construction for suitable mixers from elements of F. In particular, the transitive action of F is directly translated into substantial mixing properties. Second, we introduce a new VQA suitable for OSSP-instances. It is fundamentally based on decomposing bit value permutations into products of transpositions. In contrast to the QAOA, we can bound the number of parameters necessary to reach every possible solutions: While the number of OSSP-solutions is O(J!), only  $O(J^3)$  parameters are necessary.

We simulate our new VQA on an OSSP(2,2,4)-instance without noise. In addition, for an OSSP(1,3,3)-instance, we implement our VQA on an IBM Q System One and compare the results with the ones from a noiseless simulator. The results are presented in Section V. We observe a strong sampling of optimal solution states, but also residual sampling of 'nearby' states. That is, for computational basis states with small Hamming distance from the optimal state. However, we explain this behavior in context of our method.

# **II. PRELIMINARIES**

For the readers convenience we will review the basic notion of combinatorial optimization problems (COPs), especially the open-shop scheduling problem. We also briefly introduce the constraint graph model and cover the very basics of problem encoding onto quantum computers. Throughout this work, we will use the shorthand  $[N] \coloneqq \{1, \ldots, N\}$  where N is any natural number.

# 1. Constrained Combinatorial Optimization

In the following, we restrict to minimization problems, as maximization tasks may be considered analogously. Then a generic COP of *size* N with A constraints is of the form

$$\min_{\mathbf{z}\in Z(N)} f(\mathbf{z}) \quad \text{s.t. } c_a(\mathbf{z}) = 1, \quad a \in [A], \tag{1}$$

where

-  $Z(N) \coloneqq \{0,1\}^N$  is the bit strings of length N,

-  $f: Z(N) \to \mathbb{R}$  is the *objective function*, and

-  $c_a: Z(N) \to \{0, 1\}$  are the constraints.

Accordingly, a bit string z is said to fulfill a constraint  $c_a$  iff  $c_a(z) = 1$ . We will refer to COPs formally as triples  $(N, f, \{c_a\})$ . For a given COP C, we define its *solution* set as the set of all bit strings, fulfilling every constraint:

$$S(\mathcal{C}) \coloneqq \{ \boldsymbol{z} \in Z(N) : c_a(\boldsymbol{z}) = 1, \quad a \in [A] \}.$$
(2)

Furthermore, the *optimal solution set* is the set of all solution bit strings minimizing f, i.e.,

$$S_{\min}(\mathcal{C}) \coloneqq \left\{ \boldsymbol{z} \in S(\mathcal{C}) : f(\boldsymbol{z}) = \min_{\boldsymbol{z}' \in S(\mathcal{C})} f(\boldsymbol{z}') \right\} \subseteq S(\mathcal{C}).$$
(3)

We now examine particular types of constraints: For two bit strings  $z, z' \in Z(N)$  the bit-wise and operation produces a new bit string  $z \wedge z' \in Z(N)$ . |z| denotes the Hamming weight of z. For a subset  $I \subseteq [N]$  let  $z_I \in Z(N)$  with  $z_n = 1$  iff  $n \in I$ . The one-hot constraint and the at-most-one constraint associated with the index set I are

$$\hat{\zeta}_{I}(\boldsymbol{z}) \coloneqq \begin{cases} 1, & \text{if } |\boldsymbol{z} \wedge \boldsymbol{z}_{I}| = 1\\ 0, & \text{otherwise} \end{cases} \quad \text{and} \quad (4)$$

$$\eta_I(\boldsymbol{z}) \coloneqq \begin{cases} 1, & \text{if } |\boldsymbol{z} \wedge \boldsymbol{z}_I| \le 1\\ 0, & \text{otherwise.} \end{cases}$$
(5)

# 2. Open-Shop Scheduling

Let us formally introduce the OSSP, depending on the three parameters

- M: number of machines,
- T: number of time slots per machine, and
- J: number of jobs.

The J jobs should be distributed to the MT available positions such that

- J: every job gets performed precisely once
- **P**: no position is filled with more than one job.

Note that OSSP(T, 1, T) has the exact same structure as the *T*-city TSP.

In order to bring OSSP := OSSP(J, M, T) into the form (1), we introduce N = MTJ bits, identify  $[N] \cong [M] \times [T] \times [J]$ , and set

$$z_{mtj} \coloneqq \begin{cases} 1, & \text{if job } j \text{ runs on machine } m \text{ at time } t, \\ 0, & \text{otherwise.} \end{cases}$$
(6)

The job assignment constraints  $\mathbf{J}$  and the position assignment constraints  $\mathbf{P}$  then read

$$\mathbf{J}: \sum_{m=1}^{M} \sum_{t=1}^{T} z_{mtj} = 1, \quad j \in [J] \text{ and } (7)$$

$$\mathbf{P}: \sum_{j=1}^{J} z_{mtj} \le 1, \quad (m,t) \in [M] \times [T].$$
(8)

Thus  $\mathbf{J}$  and  $\mathbf{P}$  are one-hot and at-most-one constraints, respectively. Namely, we have

$$\mathbf{J}: c_j \coloneqq \zeta_{\Delta_{(j)}}, \ j \in [J] \quad \text{and} \tag{9}$$

$$\mathbf{P}: c_{m,t} \coloneqq \eta_{\Delta_{(m,t)}}, \ (m,t) \in [M] \times [T]$$
(10)

with job blocks  $\Delta_{(j)} := [M] \times [T] \times \{j\}$  and position blocks  $\Delta_{(m,t)} := \{m\} \times \{t\} \times [J]$ . The constraints are equivalently captured in the coordinate relation

$$(m,t,j) \sim (m',t',j') :\iff (m=m' \land t=t') \lor j=j'.$$
(11)

Note that ' $\sim$ ' is reflexive and symmetric, but not transitive. Since we are mainly interested in the constraints, we leave the objective function f unspecified.

Lastly, the OSSP solution set (expressed as a coordinate set) is explicitly given by

$$\bigcup \Big\{ \{ (m_j, t_j, j) : j \in [J] \} \\
: (m_1, t_1) \neq \cdots \neq (m_J, t_J) \in [M] \times [T] \Big\}.$$
(12)

Therefore, it possesses

$$\frac{(MT)!}{(MT-J)!} \tag{13}$$

solutions.

### 3. Constraint Graph Model

The solution set of a COP  $C = (N, f, \{c_a\})$  can be further studied by introducing the so-called *constraint* graph<sup>16,17</sup>. First we identify [N] with a vertex set V = $\{v_1, \ldots, v_N\}$ . Moreover, the bit string  $\mathbf{z}_I$ , associated to the subset  $I \subseteq [N]$ , is identified with the subset of vertices  $V_I \coloneqq \{v_n : n \in I\} \subseteq V$ .

The constraints enter as edges of the graph: Two vertices  $v_m$  and  $v_n$  are joint by an edge iff there is a constraint that prohibits the two bits  $z_m$  and  $z_n$  from taking the value 1 at the same time. Since this construction is symmetric, the constraint graph G = (V, E) is undirected. Thus, the edges are unordered pairs of vertices and we may address an edge  $e \in E$  with its end points. Assuming that we have defined a coordinate relation '~' similar to (11), we can express the set of edges simply as

$$E = \{ (v_m, v_n) : m \sim n \}.$$
(14)

For one-hot and at-most-one constraints we can be more concrete: If  $\zeta_I \in \{c_a\}$  or  $\eta_I \in \{c_a\}$  all vertices  $v_n$  with  $n \in I$  are mutually connected, i.e., they form a clique in the constraint graph. Figure 1 shows the constraint graph of an OSSP(2, 2, 4)-instance.

A solution to  $\mathcal{C}$  does not violate any constraint. Thus it corresponds to an independent set (or coclique) in the associated constraint graph  $G(\mathcal{C})$ . If  $\mathcal{C}$  incorporates Jone-hot constraints and some additional at-most-one constraints (such as the OSSP), every solution has Hamming weight J. Accordingly, we call any vertex subset  $W \subseteq V$ a solution to  $\mathcal{C}$  iff

- (i) |W| = J,
- (ii) W is an independent set.

Moreover, we say that a permutation  $\rho: V \to V$  preserves feasibility iff  $\rho(W)$  is again a solution whenever  $W \subseteq V$  is a solution. We denote with F the set of all feasibility-preserving permutations. As the composition of two feasibility-preserving permutations preserves feasibility again and the identity also preserves feasibility, one readily deduces that F is a subgroup of Sym(V). Via the identification of bit strings with vertex subsets, F can also be interpreted as acting on the solution set  $S(\mathcal{C})$ , i.e., on a set of bit strings. However, the notions of solutions and of F can also be considered independently of any underlying COP.

We remark that we could alternatively have declared the complement graph of  $G(\mathcal{C})$  as the actual constraint graph. Then, solutions would correspond to cliques instead of cocliques, but the underlying structure would not change since a graph and its complement have the same automorphism group (see Section III). This equivalent point of view is noteworthy since many results in graph theory are formulated in terms of cliques. However, we proceed with our original definition.



FIG. 1: OSSP(2,2,4) constraint graph. In the above graph, the vertices are labeled using the coordinate system (m,t,j). In addition, the three job blocks  $\Delta_{(j)}, j \in [4]$ , are depicted.

### 4. Encoding on Quantum Computers

Consider a COP  $C = (N, f, \{c_a\})$ . The standard encoding procedure identifies each bit string z with a computational basis state  $|z\rangle$  of the *N*-qubit space  $\mathcal{H} := \mathbb{C}^{2^N}$ . This induces a representation of functions over Z(N) as linear operators on  $\mathcal{H}$ . Namely, the classical objective function f is mapped to an objective Hamiltonian, diagonal in the computational basis

$$f \mapsto C \coloneqq \sum_{\boldsymbol{z} \in Z(N)} f(\boldsymbol{z}) |\boldsymbol{z}\rangle \langle \boldsymbol{z} |.$$
 (15)

For unconstrained problems the minimization task is then equivalent to finding a computational basis state which is a ground state of C. However, in the constrained case, the ground state search has to be restricted to the *solution space* 

$$\mathcal{S} \coloneqq \operatorname{span}\{|\boldsymbol{z}\rangle : \boldsymbol{z} \in S(\mathcal{C})\} \subsetneq \mathcal{H}.$$
 (16)

The optimal solution space

$$S_{\min} \coloneqq \operatorname{span}\{|\boldsymbol{z}\rangle : \boldsymbol{z} \in S_{\min}(\mathcal{C})\}$$
 (17)

then is a subspace of S and is the eigenspace of  $C|_{S}$ , corresponding to its smallest eigenvalue. Unlike  $\mathcal{H}$ , S does not admit any favorable tensor product structure in general. This is precisely what makes constrained optimization more challenging on a quantum computer.

# III. FEASIBILITY STRUCTURE OF OPEN-SHOP SCHEDULING

In this chapter we investigate the constraint graph of an OSSP instance. Our focus lies on determining the feasibility-preserving subgroup F and its properties. For brevity, we will not distinguish between the COP and its constraint graph in what follows.

# 1. Feasibility-Preserving Graph Automorphisms

Let G = (V, E) be a graph. Recall that a graph automorphism is a bijection  $\varphi : V \to V$  such that  $\varphi$  as well as  $\varphi^{-1}$  preserve adjacency. One can actually prove that any bijective graph homomorphism between G and itself is already a graph automorphism. We start with the general observation that graph automorphisms are always feasibility-preserving.

**Proposition 1** ([18]). Let G = (V, E) be a graph with solution set S. It holds that  $Aut(G) \subseteq F$ .

**Proof.** Let  $\varphi \in \operatorname{Aut}(G)$  and let  $W \in S$  be arbitrary. Since  $\varphi : V \to V$  is bijective, it holds that  $|\varphi(W)| = |W| = J$ . Let  $\varphi(v), \varphi(w) \in \varphi(W)$ . Since W is an independent set, it holds that  $vw \notin E$ . With the isomorphism property of  $\varphi^{-1}$ , it follows that  $\varphi(v)\varphi(w) \notin E$ ; hence  $\varphi(W)$  is again an independent set. This shows that  $\operatorname{Aut}(G) \subseteq F$ .  $\Box$ 

For general graphs G, F will be a strict superset of Aut(G). In case of the OSSP graph, however, equality

holds. In order to prove this we utilize a simple auxiliary result.

**Proposition 2** ([18]). Let G = (V, E) be a graph with solution set S. If for all non-adjacent  $v, w \in V$  there exists  $W \in S$  such that  $v, w \in W$ , then Aut(G) = F.

*Proof.* By Proposition 1 it suffices to show that  $F \subseteq$  Aut(G). Let  $\rho \in F$  and  $v, w \in V$  with  $\rho(v)\rho(w) \notin E$ . Then, there exists  $W \in S$  so that  $\rho(v), \rho(w) \in W$ . Since F is a group,  $\rho^{-1}$  is also feasibility-preserving, hence  $v, w \in \rho^{-1}(W) \in S$  are non-adjacent. Thus the bijective map  $\rho$  fulfills ( $\rho(v)\rho(w) \notin E \implies vw \notin E$ ) which is an equivalent characterization of a graph automorphism. □

Consider again the OSSP solution set (12). Note that any pair (m, t, j), (m', t', j') corresponding to nonadjacent vertices, i.e.,  $(m, t) \neq (m', t')$  and  $j \neq j'$ , can be augmented to form a solution to OSSP. Therefore, we can apply Proposition 2 and conclude that Aut(OSSP) = F.

### 2. Determining F

Since the relation (11) is divided in two logically disjoint parts, one concludes that the constraint graph is given by the cartesian product<sup>19</sup> of the two graphs  $K^P$ and  $K^J$  for P := MT, where  $K^n$  is the complete graph with *n* vertices. With some effort one can show the following theorem.<sup>20</sup>

**Theorem 3.** Let G be a graph and  $H_1, \ldots, H_k$  be representatives of the isomorphism types of indecomposable components<sup>19</sup> of G.

Let  $m_i$  be the number of indecomposable components of G which are isomorphic to  $H_i$ . Then, it holds

Theorem 3 states that knowing the indecomposable components of a graph reduces the problem of determining its automorphism group to the symmetries of the indecomposable components. In the situation of OSSP we are mostly done since it is not difficult to show that complete graphs are indecomposable. The automorphism group of complete graphs simply is the whole symmetric group over its vertex set because all vertex permutations are graph automorphisms. Therefore, the automorphism group of OSSP is given by

$$F = \operatorname{Aut}(OSSP) \cong \begin{cases} (S_J \times S_J) \rtimes S_2 & P = J, \\ S_P \times S_J & P > J. \end{cases}$$
(18)

We observe that the *busy* case (P = J) differs structurally from the *non-busy* case (P > J). For the latter case we simply obtain an automorphism group that is the direct product of *position permutations* and *job permutations*. However, in the busy case, we obtain a *wreath*  $product^{21}$  structure. There is an additional non-trivial automorphism which interchanges between position and jobs. In our subsequent analysis, however, we will consider the subgroup

$$F' := S_J \times S_J \le (S_J \times S_J) \rtimes S_2 \tag{19}$$

in order to treat both cases similarly. The concrete action of an element  $(\sigma, \tau) \in S_P \times S_J$  on a coordinate tuple (m, t, j) is given by

$$^{(\sigma,\tau)}(m,t,j) = (\sigma(m,t),\tau(j)).$$
 (20)

We now argue that  $S_P \times {\text{id}} \leq F$  acts transitively on the solution set (12). Let  $s, s' \subset [M] \times [T] \times [J]$  be two solutions, hence there exist  $m_1, \ldots, m_J, m'_1, \ldots, m'_J \in [M]$ and  $t_1, \ldots, t_J, t'_1, \ldots, t'_J \in [T]$  such that

$$s = \{(m_1, t_1, 1), \dots, (m_J, t_J, J)\} \text{ and } s' = \{(m'_1, t'_1, 1), \dots, (m'_J, t'_J, J)\}.$$

Since  $S_P$  acts *P*-transitively on  $[M] \times [T]$  and  $P \geq J$ , there exists  $\sigma \in S_P$  such that

$$^{\sigma}(m_j, t_j) = (m'_j, t'_j)$$

holds for all  $j \in [J]$ , i.e.  ${}^{(\sigma, \mathrm{id})}s = s'$ . Thus we have just concluded

**Theorem 4** ([18, 22]). The action of F on the solution set S is transitive for the OSSP.

### 3. Block Structure

We further characterize the group action of F (resp. F') via block systems. Given a group G acting on some set X, a subset  $\Delta \subset X$  with  $1 < |\Delta| < |X|$  is called a  $block^{23}$  of G iff

$$\forall g \in G : \ ^g \Delta = \Delta \ \lor \ ^g \Delta \cap \Delta = \emptyset.$$

A partition of X into blocks of G is then called a *block* system.

It is immediately clear that the collection of job blocks  $\Delta_{(j)}$  and of position blocks  $\Delta_{(m,t)}$  each form a block system of F (resp. F'). Furthermore, one readily verifies that F (resp. F') acts transitively on  $[M] \times [T] \times [J]$ . Recall that the job and position blocks result from onehot and at-most-one constraints and are therefore cliques in the constraint graph. That is, all vertices in a block are adjacent, which implies that a solution is a subset  $s \subset [M] \times [T] \times [J]$  such that each element in s belongs to exactly one block in each of the two partitions into position blocks and job blocks. In both cases this yields a bijection between elements in s and the job blocks. In the busy case there is an additional bijection between elements in s and the non-busy



FIG. 2: OSSP(2,2,4) constraint graph with feasible solution. The colored vertices are a maximally independent set and thus constitute a feasible solution.

case s only occupies a subset of all position blocks. Since each element of a solution exactly corresponds to one position and to one job block, we can capture the action of F (resp. F') on the solution set S equivalently as its action on the blocks. Here, [23, Proposition 1.37] states that if the blocks are maximal with respect to inclusion (which they are here), then the block-wise action of F is primitive, i.e., it does not possess blocks on its own.

We lastly focus on the busy case. Since the normal action of  $S_J$  on J elements is *sharply transitive*, for every two blocks there is exactly one element in  $S_J$  which maps between them. The solutions are now precisely the J! permutations of these blocks. Furthermore, each of the two copies of  $S_J$  is a stabilizer for one of the block structures and is also a normal subgroup of F'. Therefore we can identify the solutions with one of those subgroups and get a  $regular^{23}$  group action. Note that for the non-busy case the unique identification of solutions with elements of  $S_P$  or  $S_J$  is not possible as one has

$$|S_J| = J! < \frac{P!}{(P-J)!} < P! = |S_P|.$$
(21)

We leave it as an open problem to find and characterize subgroups of  $S_P$  that are in bijection with the solution set.

# IV. DESIGNS FOR VARIATIONAL QUANTUM ALGORITHMS

In this chapter, we utilize our knowledge about feasibility-preserving permutations to study VQAs. The underlying connection is due to the fact that 'classical' operations on bit strings may be considered as 'quantum' permutation operators acting on the associated qubit space  $\mathcal{H}$ .

Consider a COP C. Any group G that acts on Z(N) (resp. on S(C)) also acts on the computational basis (resp. on the feasible computational basis states) via

$${}^{g}|\boldsymbol{z}\rangle \coloneqq |{}^{g}\boldsymbol{z}\rangle, \quad g \in G.$$
 (22)

By linearity, we can extend this action to the whole space  $\mathcal{H}$  (resp.  $\mathcal{S}$ ), yielding linear operators  $\rho(g) \in \mathcal{L}(\mathcal{H})$  (resp.

 $\rho_{\mathcal{S}}(g) \in \mathcal{L}(\mathcal{S})$  which are simply permutation matrices in the computational basis. In group representation theory this construction is known as the *permutation representation*<sup>24</sup>.

### 1. Relation to the QAOA

Consider a COP with encoded objective Hamiltonian C, solution space  $S \subseteq \mathcal{H}$ , and optimal solution space  $S_{\min} \subseteq S$ . Starting from a *feasible* initial state  $|\iota\rangle \in S$ , we alternately apply parametrized 'phase separator' gates  $U_{\mathrm{P}}(\gamma)$  and 'mixer' gates  $U_{\mathrm{M}}(\beta) p$  times, where p is the circuit depth. This yields a parametrized trial state

$$|\vec{\beta}, \vec{\gamma}\rangle \coloneqq \left(\prod_{o=1}^{p} U_{\mathrm{M}}(\beta_{o}) U_{\mathrm{P}}(\gamma_{o})\right) |\iota\rangle.$$
 (23)

After preparing  $|\vec{\beta}, \vec{\gamma}\rangle$ , we evaluate

$$F_p(\vec{\beta}, \vec{\gamma}) \coloneqq \langle \vec{\beta}, \vec{\gamma} | C | \vec{\beta}, \vec{\gamma} \rangle \tag{24}$$

on the quantum computer and pass this quantity to a classical optimizer which updates the parameters  $\vec{\beta}$ ,  $\vec{\gamma}$  in order to minimize  $F_p(\vec{\beta}, \vec{\gamma})$ .

# Phase Separator

The unitary phase separator is supposed to render the classical objective function's behavior but is technically merely required to be diagonal in the computational basis. We want to be more precise and suggest the following definition.

**Definition 5.** A Hamiltonian *H* is called a *phase separator Hamiltonian* iff it fulfills the following two conditions:

- (i) H is diagonal in the computational basis.
- (ii) The eigenspace of  $H|_{\mathcal{S}}$  corresponding to its smallest eigenvalue is  $\mathcal{S}_{\min}$ .

Then

$$U_{\rm P}(H,\gamma) \coloneqq e^{-i\gamma H} \tag{25}$$

is the corresponding (parametrized) phase separator.

The canonical choice for a phase separator Hamiltonian is the objective Hamiltonian C. However, there might be decent approximations of C which are easier to implement and still preserve the optimal solution space. Since the phase separator is itself diagonal in the computational basis it trivially leaves the solution space Sinvariant!

### Mixer

The unitary mixer is supposed to 'preserve' and 'explore' the solution space S. Preservation of S simply means that  $U_{\mathrm{M}}(\beta)(S) \subseteq S$  should hold for all  $\beta \in \mathbb{R}$ . The exploring condition is defined as follows: For all  $z, z' \in S$ , there should exist a power  $r \in \mathbb{N}$  and a parameter value  $\beta \in \mathbb{R}$  so that  $\langle z | U_{\mathrm{M}}^r(\beta) | z' \rangle \neq 0$ .

Our aim for a refined definition is now to mimic the two properties of the original QAOA mixer Hamiltonian

$$B = \sum_{n=1}^{N} \sigma_x^{(n)} \tag{26}$$

for unconstrained problems, but tailored to the constrained case. B, considered as a matrix in the computational basis, is component-wise non-negative and irreducible. Irreducibility means that the matrix B does not leave any non-trivial *coordinate subspace* invariant. That is, the only two subspaces of  $\mathcal{H}$  which are a linear span of computational basis states and are left invariant under B are  $\{0\}$  and  $\mathcal{H}$ . For brevity, we will address every linear span of computational basis states as a *coordinate subspace*. Our crucial observation is that the concept of irreducibility is indeed a fundamental mixing property which should be preserved in the constrained case<sup>25</sup>.

In order to establish also 'sequential' mixers<sup>14</sup>, we utilize the following result which can be proved by considering each Hamiltonian as the adjacency matrix of a graph.<sup>26</sup>

**Proposition 6.** Let  $\{H_i\}_{i \in I} \subset \mathcal{L}(\mathcal{H}), 0 < |I| < \infty$ , be a family of Hamiltonians, component-wise non-negative in the computational basis, such that  $H_i(S) \subseteq S$  holds for all  $i \in I$ . Then the following two statements are equivalent:

- (i) Any coordinate subspace  $X \subseteq S$  that is left invariant under every  $H_i|_S$ , is trivial.
- (ii)  $\left(\sum_{i \in I} H_i\right)|_{\mathcal{S}} \in \mathcal{L}(\mathcal{S})$  is irreducible in the computational basis.

**Definition 7.** A family of Hamiltonians  $H = \{H_i\}_{i \in I} \subset \mathcal{L}(\mathcal{H})$  fulfilling the conditions in Proposition 6 is called a

mixing family. The corresponding (parametrized) simultaneous mixer is defined as

$$U_{\mathrm{M},0}(\mathsf{H},\beta) \coloneqq e^{-i\beta\sum_{i\in I}H_i}.$$
(27)

Specifying a permutation  $\sigma \in S(I)$ , the corresponding (*parametrized*) sequential mixer is defined as

$$U_{\mathrm{M},\sigma}(\mathsf{H},\beta) \coloneqq \prod_{i \in I} e^{-i\beta H_{\sigma(i)}}.$$
 (28)

We present here a general method for schedulingtype problems for obtaining suitable mixers from the feasibility-preserving subgroup F. Following the permutation representation, we identify each  $g \in F$  via its action on Z(N) with a linear operator  $\rho(g) \in \mathcal{L}(\mathcal{H})$ , and via its restricted action on  $S(\mathcal{C})$  with a linear operator  $\rho_{\mathcal{S}}(g) \in \mathcal{L}(\mathcal{S})$ . Both representations yield permutation matrices in the computational basis. In the same way we have identified  $S(\mathcal{C})$  with  $\mathcal{S}$ , we may also identify every subset of solutions with coordinate subspaces of  $\mathcal{S}$ . Then it readily follows that F acts transitively on  $S(\mathcal{C})$  iff the only coordinate subspaces of  $\mathcal{S}$  that are left invariant by every  $\rho_{\mathcal{S}}(g), g \in F$ , are  $\{0\}$  and  $\mathcal{S}$ .

As we have shown in Section III, the action of F on S(OSSP) is indeed transitive. In addition, F consists of bit (value) permutations. Thus, the operator analogs  $\rho(F)$  respect the tensor product structure of the qubit space  $\mathcal{H}$ , namely

$$\rho(g)\bigotimes_{n=1}^{N}|\psi_{n}\rangle =\bigotimes_{n=1}^{N}|\psi_{g(n)}\rangle.$$
(29)

Starting from the unitary operators  $\rho(F) = \{W_g\}_{g \in F}$ , we construct a family of Hamiltonians by taking suitable matrix logarithms  $\{iL(W_g)\}_{g \in F}$ .<sup>27</sup> A direct calculation yields that  $A \subseteq \mathcal{H}$  is a *W*-invariant subspace iff *A* is an L(W)-invariant subspace. Thus, the constructed family  $\{iL(W_g)\}_{g \in F}$  admits the just introduced mixing property and can therefore be used to build simultaneous and sequential mixers.

#### 2. A Quantum Group Optimization Algorithm

We propose a VQA tailored to busy OSSP-instances<sup>22</sup>, thus conceptually considering the TSP. Namely, given a complete graph G = (V, E) (not the constraint graph!) with |V| = J vertices, we consider the quadratic objective function

$$f: Z(J^2) \to \mathbb{R}$$
$$\boldsymbol{z} \mapsto \sum_{\{u,v\} \in E} d_{uv} \sum_{j=1}^J (z_{u,j} z_{v,j+1} + z_{v,j} z_{u,j+1}),$$
(30)

where  $d_{uv}$  is the distance between city u and v (i.e., the weight of the edge incident with u and v). Then  $z_{u,j} = 1$ 

means that city v is visited at time  $j^{28}$ . Our method above gives now a way to describe the whole solution set S of this problem with a bit-to-qubit mapping. Namely, the set of all solutions is identified with the symmetric group  $S_J$ . Fixing one solution  $s \in S$ , we can consider the problem of optimizing f equivalently as optimizing

$$\hat{f}: S_J \to \mathbb{R}; \quad g \mapsto f({}^g s).$$
 (31)

Thus the TSP and, more generally, any generic busy OSSP-instance are, in fact, optimization problems over symmetric groups. The underlying group structure can be exploited in the following way: Consider an arbitrary  $\sigma \in S_J$ . There is a well-known representation as a product of at most  $\frac{J(J-1)}{2}$  transpositions<sup>29</sup>. We can further write every transposition as a product of some of the J-1 specific transpositions  $\tau_1 = (1, 2), \ldots, \tau_{J-1} = (J - 1, J)$  in  $S_J$ . In summary, we find for  $\sigma \in S_J$  a binary vector  $r^{(\sigma)} \in \{0, 1\}^{\frac{J(J-1)^2}{2}}$  such that

$$\sigma = \prod_{k=1}^{\frac{J(J-1)}{2}} (\tau_1^{r_{k_1}^{(\sigma)}} \cdots \tau_{J-1}^{r_{k_{J-1}}^{(\sigma)}}).$$
(32)

Recall that the elements of  $S_J$  simultaneously act on multiple vertices, namely those lying in different position blocks, but having the same job coordinate. The representation of a transposition  $\tau_i$  as elements in  $\mathcal{L}(\mathcal{H})$ thus yields a sum of disjoint SWAP gates, each SWAP gate corresponding to one position block:

$$\tau_i \stackrel{\frown}{=} \sum_{p=1}^{P} \mathrm{SWAP}_{(i,i+1)}^{(p)} \eqqcolon B_i$$

Here, SWAP<sup>(p)</sup><sub>(*i*,*i'*)</sub> interchanges the *i*-th and the *i'*-th qubit in the *p*-th position block. Since all SWAP gates are also hermitian, the operator  $B_i$  is again hermitian. Introducing  $\frac{J(J-1)^2}{2}$  parameters and exponentiating each transposition operator  $B_i$  then yields the following implementation of  $\sigma$  as a parameterized quantum circuit:

$$U(\vec{\beta}) = \prod_{k=1}^{\frac{J(J-1)}{2}} e^{i\beta_{k_1}B_1} \cdots e^{i\beta_{k_{J-1}}B_{J-1}}.$$
 (33)

Due to the fact that  $e^{i\gamma \text{SWAP}}$  is equal to SWAP with a global phase *i* for  $\gamma = \frac{\pi}{2}$  and 1 for  $\gamma = 0$ , we can directly transfer Theorem 4 to the gate implementation of permutations in  $S_J$  to conclude that every solution is reachable with a circuit  $U(\vec{\beta})$  for appropriate  $\vec{\beta} \in [0, \frac{\pi}{2}]^{\frac{J(J-1)^2}{2}}$ . Therefore, the number of gates (not decomposed) is within  $O(J^3)$ .

The resulting VQA consists out of the following steps:

- 1. Start in a solution state  $|\iota\rangle \in \mathcal{S}$ .
- 2. Apply the parameterized quantum circuit (33).

- 3. Variationally optimize  $\vec{\beta} \in [0, \frac{\pi}{2}]^{\frac{J(J-1)^2}{2}}$  using a classical optimization rule.
- 4. Measure the final outcome state in the computational basis.

Furthermore, the parameter space is always the same and especially compact, regardless of the objective function f. This has to be seen in contrast to general QAOAmixers for which no comparable restriction of the necessary parameter space is possible. Thus, in our case, sampling methods for parameter adaptation like the sampled gradient descent (compare Section V 2) are particularly powerful since they eventually grant access to the whole compact parameter space.

The identification of the set of feasible solutions with  $S_J$  further suggests a dynamic programming<sup>30</sup> ansatz: Iteratively optimize over subgroup series of the form

$$1 = \langle \tau_i : i \in I_0 \rangle \le \ldots \le \langle \tau_i : i \in I_n \rangle = S_J, \qquad (34)$$

with ascending index sets  $I_0 \subset \ldots \subset I_n$ , by restricting to the set of corresponding mixers  $B_i$  with  $i \in I_k$ ,  $k \in [n]$ .

# V. NUMERICAL RESULTS

### 1. Noiseless Implementation

First, we demonstrate our just introduced VQA without noise on an OSSP(2,2,4)-instance. Figure 1 displays its constraint graph. The group of job permutations is thus given by  $S_J = S_4$ .

After assigning a bit to each of the 16 elements in  $[2] \times [2] \times [4]$  via

$$(m, t, j) \mapsto 4(m-1) + 2(t-1) + j,$$
 (35)

we explicitly generate  $S_J$  with  $\tau_1$ ,  $\tau_2$ , and  $\tau_3$ :

$$S_J = \langle (1,2)(5,6)(9,10)(13,14), (2,3)(6,7)(10,11)(14,15), (3,4)(7,8)(11,12)(15,16) \rangle.$$
(36)

Consequently, we have to implement three distinct mixer Hamiltonians  $B_1$ ,  $B_2$ ,  $B_3$ . As a concrete example, consider the permutation

which corresponds to the Hamiltonian

$$B_{1} = \sum_{p=1}^{4} \text{SWAP}_{(1,2)}^{(p)}$$
  
= SWAP\_{(1,2)} + SWAP\_{(5,6)}  
+ SWAP\_{(9,10)} + SWAP\_{(13,14)}.

bit string	valu
0010000110000100	5
0010000101001000	5
0010010000011000	7
0100000100101000	7
0010100000010100	7
0100001000011000	8
0100000110000010	8
0010100001000001	8
0010010010000001	8
1000000100100100	8
0001001010000100	9
0001001001001000	9
1000001000010100	9
1000000101000010	9
0100001010000001	9
0100100000100001	10
0100100000010010	10
0001010000101000	10
0001100000100100	10
1000001001000001	10
1000010000100001	11
1000010000010010	11
0001100001000010	11
0001010010000010	11

TABLE I: Every solution bit strings to OSSP(2,2,4) is listed with its objective value under the objective function (37) with weights (38).

Using again the enumeration (35), we consider the following objective function

$$f: \{0,1\}^{16} \to \mathbb{R}, \quad \boldsymbol{z} \mapsto \sum_{m,t,j} \omega_{mtj} z_{mtj}.$$
 (37)

We collect the weights in two machine-specific  $weight\ matrices$ 

$$(\omega)_{1tj} = \begin{pmatrix} 3 & 2 & 2 & 3 \\ 2 & 2 & 3 & 0 \end{pmatrix}, \quad (\omega)_{2tj} = \begin{pmatrix} 2 & 2 & 4 & 2 \\ 1 & 1 & 4 & 2 \end{pmatrix}.$$
(38)

Table I displays the objective values for all feasible solutions of the OSSP(2,2,4).

In addition to the just constructed mixers, we also implement the QAOA-phase separator. Mixer and phase separator together result in the following parametrized quantum circuit

$$U(\vec{\beta}, \vec{\gamma}) = \underbrace{e^{i\beta_1 B_1} e^{i\beta_2 B_2} e^{i\beta_3 B_3} e^{i\gamma_1 C}}_{2} \cdot \cdot \cdot \underbrace{e^{i\beta_4 B_1} e^{i\beta_5 B_2} e^{i\beta_6 B_3} e^{i\gamma_2 C}}_{6} \cdot \cdot \cdot \underbrace{e^{i\beta_{16} B_1} e^{i\beta_{17} B_2} e^{i\beta_{18} B_3} e^{i\gamma_6 C}}_{6}.$$
(39)

Choosing an initial state  $z_0$ , the variational optimization



FIG. 3: Sampling amplitudes of bit strings. One of the optimal solutions dominates the sampling; all other computational basis states are suppressed.

task now reads

$$\min\{\langle \boldsymbol{z}_0 | U(\vec{\beta}, \vec{\gamma})^* \, C \, U(\vec{\beta}, \vec{\gamma}) | \boldsymbol{z}_0 \rangle : \vec{\beta} \in [0, \pi/2]^{18}, \vec{\gamma} \in \mathbb{R}^6\}$$

$$\tag{40}$$

As a concrete feasible initial state, we choose

$$|z_0\rangle = |1000010000100001\rangle$$

The whole quantum circuit is implemented in Qiskit. For the classical parameter adaptation we use the renowned COBYLA as a global optimization routine. Figure 3 and Table II display the numerical results<sup>22</sup>.

We observe a dominating sampling of one of the optimal solution states (791 out of 1024 counts), indicating a fast convergence behavior. Bit strings which have a small Hamming distance to it are also sampled, but with a significantly smaller amplitude. This is due to the fact that the construction of the optimal computational basis state is merely approximate. Any deviation from it is reflected in the measurement statistics because the projective measurements do not reliably give the correct bit values in this case. These byproducts are mostly infeasible states, which is a direct consequence of the underlying feasibility structure: Distinct solution bit strings differ in, at least, four positions since if one reassigns one job to a position occupied by another job, one also has to reassign the latter one. Obtaining distributions with some nonsolution bit strings in hardcoded instances is, however, very common as the final measurement is insensitive to any feasibility structure.

bit string	counts	Hamming distance	is solution?
0010000101001000	781	0	$\operatorname{true}$
0010000101000100	95	2	false
0010000110001000	74	2	false
0010000100101000	15	2	false
0010000110000100	12	4	$\operatorname{true}$
0100000101001000	10	2	false
0010010001001000	9	2	false
0010000101000010	7	2	false
1000000101001000	6	2	false
0010000100011000	6	2	false
0010010001000100	3	4	false
1000000110001000	1	4	false
0010010010001000	1	4	false
0010100001001000	1	2	false
0010000100100001	1	4	false
0010000110000010	1	4	false
0010000100010100	1	4	false

TABLE II: Measured bit strings with their respective counts. The total amount of counts is 1024. In addition, the Hamming distance to the most frequently sampled bit string 0010000101001000 is shown as well as whether a given bit string is feasible or not.

### 2. Implementation With Noise

Second, we consider an OSSP(1,3,3)-instance, i.e. a TSP instance with 3 cities, and demonstrate our VQA on a real (noisy) quantum hardware: the IBM Q System One. In addition, we simulate the application with a classical computer.

The group of job permutations is given by  $S_J = S_3$ . Since we only have one machine, we simply drop the machine coordinate and consider the enumeration

$$(t,j) \mapsto 3(t-1)+j.$$
 (41)

Thus, the generators  $\tau_1$  and  $\tau_2$  of  $S_J$  read

$$S_J = \langle (1,2)(4,5)(7,8), (2,3)(5,6)(8,9) \rangle.$$
(42)

We further consider the objective function

$$f: \{0,1\}^9 \to \mathbb{R}, \quad \boldsymbol{z} \mapsto \sum_{t,j} \omega_{tj} z_{tj}.$$
 (43)

with weight matrix

$$(\omega)_{tj} = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 2 & 3 \\ 1 & 2 & 2 \end{pmatrix}.$$
 (44)

Both mixer Hamiltonians  $B_1$  and  $B_2$  together with

bit string	value	
001010100	5	
001100010	6	
010001100	6	
010100001	7	
100001010	8	
100010001	8	

TABLE III: Every solution bit strings to OSSP(3,1,3) is listed with its objective value under the objective function (43) with weights (44).

the QAOA-phase separator constitute the parametrized quantum circuit

$$U(\vec{\beta}, \vec{\gamma}) = \underbrace{e^{i\beta_1 B_1} e^{i\beta_2 B_2} e^{i\gamma_1 C}}_{1} \underbrace{e^{i\beta_3 B_1} e^{i\beta_4 B_2} e^{i\gamma_2 C}}_{2} \times \underbrace{e^{i\beta_5 B_1} e^{i\beta_6 B_2} e^{i\gamma_3 C}}_{3}.$$
(45)

However, this circuit is yet too deep to be fully implemented on the quantum device. Therefore, we restrict our circuit to the first factor of (45). Choosing the feasible initial state

$$|\boldsymbol{z}_0\rangle = |100010001\rangle,$$

we can predict which feasible states are actually accessible in this setting. Restricting to one factor in (45) classically corresponds to having only access to four group elements: id,  $\tau_1$ ,  $\tau_2$ , and  $\tau_1\tau_2$ . Their application to  $z_0$  yields

<sup>id</sup>
$$\boldsymbol{z}_0 = \boldsymbol{z}_0, \ ^{\tau_1}\boldsymbol{z}_0 = 010100001,$$
  
 $^{\tau_2}\boldsymbol{z}_0 = 100001010, \ ^{\tau_1\tau_2}\boldsymbol{z}_0 = 010001100.$  (46)

According to Table III, the colored bit string is thus the optimal accessible feasible solution.

For the actual parameter adaptation we use sampled gradient descent:

- 1. Construct a ball  $\mathbb{B}_i \subset [0, \pi/2]^3$  around some parameter values  $\vec{\beta}_i$ .
- 2. Sample new parameter values uniformly from  $\mathbb{B}_i$ .
- 3. Apply the correspondingly parametrized circuit to the initial state and measure the expectation value of C.
- 4. Choose parameter values  $\vec{\beta}_{i+1}$  from the sample minimizing the expectation value and repeat step 1 with  $i \mapsto i+1$ .

The size of the constructed ball  $\mathbb{B}_i$  is adapted in each step *i*: The steeper the drop in expectation values, the smaller the radius becomes. For our numerical execution we choose random initial parameters and a sample size of 40 in each step.



FIG. 4: First iteration with sampled gradient descent. The initial state  $|z_0\rangle$ , corresponding to a maximum of the objective function, is already barely sampled.



FIG. 5: Second iteration with sampled gradient descent. The local optimum is now also sampled on the IBM Q System One, while its simulated amplitude is also increasing.

Figure 4-Figure 8 show the amplitudes obtained after each round of the sampled gradient descent. After five iterations we indeed observe a dominating sampling of the local optimum. There remains, however, a noisy background both in the simulation as well as on the IBM Q System One. We again observe increased amplitudes for



FIG. 6: Third iteration with sampled gradient descent.The amplitude of the local optimum further increases in both cases. Computational basis states with small Hamming distance are also more frequently sampled.

computational basis states which have small Hamming distance to the local optimum.

#### VI. OUTLOOK AND CONCLUSION

In this paper we presented a general approach for characterizing the feasibility structure of job-shop scheduling problems. We utilized the constraint graph model as a general interplay between graph and group theory for determining symmetries for certain problem instances. This additional perspective allowed us to find feasibilitypreserving mappings as graph automorphisms. For the open-shop case, we calculated the entire group of such feasibility-preserving functions and proved that it equals the automorphism group of the constraint graph. This is a very strong statement which unfortunately is not transferable to all other types of job-shop scheduling problems. For example, for a generic *flexible* job-shop instance, where each job is subdivided into an ordered sequence of operations, we can similarly construct a constraint graph and study its automorphism group. However, in this case, due to additional edges which break certain symmetries, the automorphism group is generally significantly smaller. In many cases, there is no possible identification between group elements and solutions anymore. The remaining symmetries can still be incorporated into QAOA-mixers but have to be supplemented with additional elements that do not correspond to classical bit permutations.

Let us emphasize one more time that the OSSP is



FIG. 7: Fourth iteration with sampled gradient descent. Both the simulated and the real amplitude of the local minimum start to dominate the histogram.



FIG. 8: Fifth iteration with sampled gradient descent. The simulated amplitude of the local optimum clearly dominates the histogram. On the real quantum device, its amplitude is also dominating, but with a more

intense noisy background.

equivalent to optimizing over a particular group (cf. (31)). We solved this type of problem by representing a symmetric group with exponentials of SWAP gates. The resulting algorithm has the advantage that the number of gates is polynomial in the problem size. The prior discussed transitive action of the group on the solution set guarantees that all possible solutions can be reached. In principle, we can generalize this procedure to an arbitrary (finite) group G, acting transitively on a given set of solutions S. Then, the permutation representation would still yield permutation operators on the qubit space which, however, will not correspond to actual qubit permutations. It would be interesting to characterize in the future the obtained operators and the performance of our algorithm for more exotic cases. However, operators that do not respect the tensor product structure of  $\mathcal{H}$  will be generally very difficult to implement.

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- <sup>26</sup>More precisely, in a first step, one can interpret the matrix representation of each Hamiltonian as the adjacency matrix of a weighted directed graph. However, since we are not interested in actual weights and all matrices are hermitian, it suffices to consider simply a graph. Furthermore, since all components are non-negative, no cancellation happens when summing up all the matrices<sup>18</sup>.
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