I. ABSTRACT

This paper introduces the use of special variational forms for variational quantum eigensolvers that have properties of representing certain constraints on the search domain of a linear constrained quadratic binary optimization problem solution. Four constraints that usually appear in several optimization problems are modeled. The main advantage of the proposed methodology is that the number of parameters on the variational form remain constant and depend on the number of variables that appear on the constraints. Moreover, this variational form always produces feasible solutions for the represented constraints differing from penalization techniques commonly used to translate constrained problems into unconstrained one. The methodology is implemented for two known optimization problems: the Facility Location Problem and the Set Packing Problem. The results obtained for this two problems with VQE using 2-Local variational form and a general QAOA implementation are compared, and indicate that less quantum gates and parameters were used, leading to a faster convergence.

II. INTRODUCTION

Binary quadratic optimization problems are among the main and well-studied combinatorial problems. The term binary means that the variables can assume only two possible values, which are usually 0 or 1. In Ising models, these variables could be -1 or 1. In this paper the following formulation is used for a Linear Constrained Quadratic Binary Optimization Problem (LCQBO):

\[
\begin{align*}
\min_x & \quad x^T Q x \\
\text{s.t.} & \quad Ax = b \\
& \quad Bx \leq c \\
& \quad x \in \{0, 1\}
\end{align*}
\]

Classically, one of the global optimization techniques to solve this problem is by using Branch and Bound, which is not efficient when the number of variables increase, since the search tree could grow exponentially. As an alternative, some heuristics with lower guaranty are used.

Heuristics based on quantum computing have recently been developed to solve the unconstrained version of the LCQBO, called Quadratic Unconstrained Binary Optimization (QUBO). Some of these heuristics are the Variational Quantum Eigensolver (VQE) and its special form called Quantum Approximation Algorithm (QAOA). The VQE was initially applied on quantum chemistry problems, such as the problem of searching for molecular ground states (minimum energy of the system). Once QUBO problems can be mapped as an Ising formulation, which is one of the formulations for the Hamiltonian calculation, it is possible to solve the QUBO with VQE and to approximate the solution of an LCQBO by using penalisation techniques, reducing it to QUBO.

Another approach for solving the QUBO is to use quantum computation based on the quantum adiabatic theorem. This approach allows ground states calculations but it has limitations when solving QUBO problems.

The use of variational forms for expressing Ansatzes solutions for the VQE algorithm had an important contribution on the development of an efficient VQE solver. Despite that, there is still a challenge in using the classical solver part of VQE, which is to ensure the expression of every solution in the search domain that is parameterized by means of rotation angles and cnot gates.

For quantum chemistry problems there are tailored strategies for representing Ansatzes as an Unitary Coupled Cluster (UCC) and its Singles and Doubles Excitation Variational Form (UCCSD). For these strategies the Ansatz only contains single and double excitation operators, which potentially decrease the number of parameters for representing states. Some of these Ansatzes are particularly developed to work efficiently with hardware, even though they still have the limitation of over-sampling the Hilbert space. There is also the dynamic creation of Ansatzes, where an operator is added to the Ansatz at every step, from a pre-defined set of operators, this technique is called Adaptive Derivative Assembled Pseudo-Trotter (ADAPT-VQE). In this paper we compare our solution with 2-Local circuits as Ansatzes, which is an heuristic circuit to map the Hilbert space that assumes that qubits have almost 2 local qubits, and then they can be circularly entangled to represent the system.

Taking this into account, this paper aims to address...
this difficulty when VQE is formulated for LCQBO with the construction of special variational forms in a way that the search domain attain specific constraints. In [10] is presented a methodology to prepare different types of constraints from those proposed in this paper.

This paper is organized as follows, In Section III A the development of the variational forms in order to attain certain constraints for the search space domain is explained. Next, Section III B shows the use of the variational forms in two different optimization problems: the Facility Location Problem (FLC) and the Linear Assignment Problem (LAP). In Section IV we discuss the findings are summarized and some future work are outlined. Finally, Section V A presents a review of the VQE in order to understand the position of our contribution on the development of an efficient VQE solver for LCQBO problems, and circuit cost criteria to compare other Ansatzes.

III. RESULTS

A. Tailored Variational Forms (TVF)

In this section we will create parameterized circuits for variational forms for representing specific constraints. For the starting point we will choose \(|\psi\rangle_0 = |0\rangle^N\), where \(N\) is the number of qubits, and apply a quantum circuit represented by the gate \(U_c\) for obtaining only feasible solutions for our binary problems.

1. Binary comparison constraints

The main idea is to model the behavior of a binary comparison sequence of constraints, such as:

\[ x_i \leq x_{i+1} \forall i = 0 \ldots N \]  

with \(x_0 = 0\). The possible solutions for the variables \(x_i\) and \(x_{i+1}\) are shown in Table I.

| \(x_i\) | \(x_{i+1}\) | Possible |
|---|---|---|
| 0 | 0 | yes |
| 0 | 1 | yes |
| 1 | 0 | no |
| 1 | 1 | yes |

Table I. Possible solutions for constraint [8].

Therefore, it is possible to code the variables \(x_i\) on \(N\) qubits states as in equation [10].

\[ |x_1 \ldots x_i \ldots x_N\rangle \]  

If all qubits states from Table I were generalized, then only the states with the following sequence would be obtained.

\[ |0\ldots00\rangle, |0\ldots01\rangle, |0\ldots11\rangle, \ldots, |1\ldots11\rangle \]  

As an alternative, it is possible to use the following non-conventional qubit representation with integers on ket notation, as shown in equation [8].

\[ |0\rangle, |2^{N-1}\rangle, |2^{N-1} + 2^{N-2}\rangle, \ldots, \left| \sum_{j=N-i}^{N-1} 2^j \right\rangle \]  

If the variational form in Figure I were applied to a \(|0\rangle\), the result would be the desired superposition of states shown in [8], with the amplitude probabilities parameterized on angles \(\theta_i\).

\[ x_1 : |0\rangle \circ R_y(\frac{\pi}{2}) \circ R_x(\frac{\pi}{2}) \]
\[ x_2 : |0\rangle \circ R_y(\frac{\pi}{4}) \circ R_x(\frac{\pi}{4}) \]
\[ x_3 : |0\rangle \circ R_y(\frac{\pi}{8}) \circ R_x(\frac{\pi}{8}) \]
\[ \vdots \]
\[ x_N : |0\rangle \circ R_y(\frac{\pi}{2^{N-1}}) \circ R_x(\frac{\pi}{2^{N-1}}) \]

Figure 1. Variational form with \(\theta_i\) parameters to represent all possible \(x_i\) states.

Where \(R_y\) is a single-qubit rotation through \(\theta\) angle in radians around the y-axis.

To illustrate how this circuit only gets answers as in [8], with probabilities depending on \(\theta_i\) angles, let us apply the circuit for the first 2 qubits and observe the sequence formed. The states initialize in \(|0\rangle^N\), then \(R_y(\theta_i)\) is applied for every qubit and the following is obtained.

\[
\left( \cos \frac{\theta_1}{2} |0\rangle + \sin \frac{\theta_1}{2} |1\rangle \right) \otimes \left( \cos \frac{\theta_2}{4} |0\rangle + \sin \frac{\theta_2}{4} |1\rangle \right) \\
\rightarrow \left( \cos \frac{\theta_1}{2} \cos \frac{\theta_2}{4} |00\rangle + \cos \frac{\theta_1}{2} \sin \frac{\theta_2}{4} |01\rangle \\
+ \sin \frac{\theta_1}{2} \cos \frac{\theta_2}{4} |10\rangle + \sin \frac{\theta_1}{2} \sin \frac{\theta_2}{4} |11\rangle \right) \otimes \ldots
\]  

Now, applying the cnot gate with qubit 1 as a control
and qubit 2 as a target:

\[
\left( \cos \frac{\theta_1}{2} |0\rangle + \sin \frac{\theta_1}{2} |1\rangle \right) \otimes \\
\left( \cos \frac{\theta_2}{4} |0\rangle + \sin \frac{\theta_2}{4} |1\rangle \right)
\]

(11)

\[
\rightarrow \left( \cos \frac{\theta_1}{2} \cos \frac{\theta_2}{4} |00\rangle + \cos \frac{\theta_1}{2} \sin \frac{\theta_2}{4} |01\rangle \\
+ \sin \frac{\theta_1}{2} \cos \frac{\theta_2}{4} |11\rangle + \sin \frac{\theta_1}{2} \sin \frac{\theta_2}{4} |10\rangle \right) \otimes \ldots 
\]

(12)

Then, let us apply \( R_y(\theta/2) \) gate to the second qubit:

\[
\rightarrow \left( \cos \frac{\theta_1}{2} \cos \frac{\theta_2}{2} |0\rangle + \cos \frac{\theta_1}{2} \sin \frac{\theta_2}{2} |0\rangle \\
+ \sin \frac{\theta_1}{2} |1\rangle \right) \otimes \ldots 
\]

(13)

By induction from equations (10) and (13), one can observe that if the operation is performed for \( N \) qubits then equation (14) is obtained.

\[
|\psi(\theta)\rangle = \sum_{i=0}^{N} \left( \prod_{k=i+1}^{N} \cos \frac{\theta_k}{2} \right) \sin \frac{\theta_{N-i+1}}{2} \left( \sum_{j=N-i}^{N-1} 2^j \right)
\]

(14)

with \( \theta_{N+1} = \pi \). As can be seen in (14), \( N \) parameters \( \theta \), \( 2N-1 \) gates \( R_y \) and \( N-1 \) cnots gates are needed to represent \( N+1 \) states in \( |\psi\rangle \).

2. Sum less than one constraints

Similarly as in Section III A.1 the variational form for representing constraints (15) for a set of variables will be deduced as follows.

\[
\sum_{i=1}^{N} x_i \leq 1
\]

(15)

The possible solutions that variables \( x_i \) and \( x_{i+1} \) can obtain are presented in Table II.

| \( x_i \) | \( x_{i+1} \) | Possible |
|---|---|---|
| 0 | 0 | yes |
| 0 | 1 | yes |
| 1 | 0 | yes |
| 1 | 1 | no |

Table II. Possible answers for constraints (15).

The same representation as in (10) is used. Then, in a similar way if the states from Table I were generalised, we want to obtain only states with the following sequence:

\[
|00\ldots0\rangle, |10\ldots0\rangle, |01\ldots0\rangle, \ldots, |01\ldots1\rangle
\]

(16)

Or using the following non conventional qubit representation:

\[
|0\rangle, |2^0\rangle, |2^1\rangle, \ldots, |2^{i-1}\rangle
\]

(17)

If variational form in Fig 2 were used, it would give us the desired states (16) with the amplitude probabilities depending on \( \theta \) angles.

![Figure 2. Variational form with \( \theta \) parameters to represent all possible \( x_i \) states for equation (15).](image)

Next, by applying gates to the \( |0\rangle \) initial state and perform similar analysis as in (9) and (13) we obtain:

\[
|\psi(\theta)\rangle = \sum_{i=1}^{N+1} \left( \prod_{k=1}^{i-1} \sin \frac{\theta_k + 1_{(k=1)} \pi}{2} \right) \\
\cdot \cos \frac{1_{(i=1)} \pi - \theta_i}{2} \left( 1_{(N>i)} 2^{i-1} \right)
\]

(18)

where: \( \theta_{N+1} = 0 \) and \( 1_{(N>i)} \) is an indicator function such that \( 1_{(N>i)} = 1 \) if \( N > i \) and 0 otherwise.

3. Other types of constraints

Mapping the possible solutions of a constraint and expressing it in a circuit can give us the idea that other constraints can be constructed in a similar way. In 16 circuits are implemented for the following equality constraints:

\[
\sum_{i=1}^{N} x_i = 1
\]

(19)

\[
(1-x)(1-y) = 0
\]

(20)
Another type of constraints that can be represented are \([21]\). It could be done by mixing the circuits from Figure 1 and from Figure 2.

\[
\sum_{i=1}^{N-1} x_i \leq x_N \quad (21)
\]

Also the constrained version of (21):

\[
\sum_{i=1}^{N-1} x_i = x_N \quad (22)
\]

Table III. Penalization techniques to model some inequality constraints \([3]\).

| Constraint | Equivalent Penalty |
|------------|---------------------|
| \(x \leq y\) | \(\lambda (x - xy)\) |
| \(\sum_i x_i \leq 1\) | \(\lambda \left( \sum_i \sum_j x_i x_j \right)\) |

In the next section, the test problems used to validate TVF are described in details.

1. Facility Location Problem

The Facility Location Problem (FLP) consists of deciding which facilities should be opened from a set of \(n\) possible facilities. In various situations, the facilities location decision and the assignment of clients to the facilities are made simultaneously \([19]\). This problem can be applied to a numerous types of real problems, such as deciding the location of distribution centers, airports, schools, hospitals, police stations, and others.

To formulate the FLP, let us define \(f_i\) as the fixed cost of opening facility \(i\), for \(i = 1, ..., n\), and \(c_{ij}\) as the cost of serving customer \(j\) by the facility \(i\), for \(j = 1, ..., m\) and \(i = 1, ..., n\).

The variables of the FLP are the following:

\[
y_i = \begin{cases} 
1 & \text{if facility } i \text{ is opened}, \\
0 & \text{otherwise}.
\end{cases}
\]

\[
x_{ij} = \begin{cases} 
1 & \text{if facility } i \text{ serves customer } j, \\
0 & \text{otherwise}.
\end{cases}
\]

Then, the FLP can be formulated as presented in equations (23) to (25).

B. Applications

All numerical experiments were implemented using the IBM quantum computing suite named Qiskit 0.19.2 \([17]\) with Python 3.7.5. As a backend we use qasm simulator with noise modeling. For the classical optimization algorithm we choose COBYLA \([18]\), this solver performed better than others state of the art solvers for our test cases. All calculations of the expected value of the objective function took 1024 circuit executions for the three methodologies tested. For the initial set of parameters random numbers on the interval \([-\pi, \pi]\) were used, as is usually done when the VQE is initialized.

For comparison purposes, two algorithms are used: QAOA and one algorithm based on VQE using 2-Local variational forms. Our criteria to set parameters on 2-Local and QAOA are based on the similarity with the number of parameters and single-gates and double-gates on its correspondent TVF. For the 2-Local, we choose a depth of 1 with \(R_y\) and cnots as rotation and entanglement blocks. For the QAOA, we choose \(p = 2\) in order to get 4 parameters in total, which are similar to the number of parameters using TVF. As it can be seen, one important decision in the process of implementing the 2-Local and QAOA Ansatzes is the necessity to estimate meta-parameters without a clear criteria.

To model the constraints of our test problems using the 2-Local and the QAOA algorithms, penalization techniques were used as indicated in \([3]\), and are shown in Table III where \(\lambda\) is a penalization factor.
The objective function \( \min_{x,y} \sum_{i=1}^{n} f_i y_i + \sum_{i=1}^{n} \sum_{j=1}^{m} c_{ij} x_{ij} \) (23) minimizes the total cost of assigning customers to facilities. Constraints \( \sum_{i=1}^{n} x_{ij} = 1 \) \( j = 1, \ldots, m \) (24) guarantee that each customer \( j \) is served by exactly one facility, and constraints \( x_{ij} \leq y_i \) \( i = 1, \ldots, n \) \( j = 1, \ldots, m \) (25) guarantee that each customer \( j \) can only be assigned to a facility \( i \) if that facility \( i \) is open. For a more detailed review on the FLP and solution techniques, see [20].

It is possible to model constraints (24) by adding the penalization function \( \lambda \sum_{j=1}^{m} (1 - \sum_{i=1}^{n} x_{ij})^2 \) to the objective function. Observe that the variable \( y_i \) appears in various constraints (25) with the variable \( x_{i,j} \), so the circuit presented in Figure 1 can’t be used, since is not possible to put constraints (24) and (25) at the same time. As an alternative, it is possible to use a circuit that inverts the order of the qubit inequality and that allows the first qubit to control more than 1 qubit as is detailed in Figure 5. Note that Figure 5 is not equivalent to Figure 1.

![Figure 5](image_url)

Figure 5. Reformulated variational form to fit the FLP characteristics.

Then, it is possible to represent constraints (26) by creating a circuit according to Algorithm 1 that generalizes the circuit in Figure 5.

**Algorithm 1 Facility location problem circuit construction**

Require: Number of clients \( m \) and facilities \( n \).

Require: label first \( m \) qubits as \( x_{i,j} \) \( i = 1 \ldots n ; j = 1 \ldots m \)

Require: label following \( n \) qubits as \( y_i \) \( i = 1 \ldots n \)

1: set all qubits with state 0.
2: for \( i = 1 \ldots n \) do
3: apply \( R_y(\theta_{y_i}) \) on \( y_i \)
4: for \( j = 1 \ldots m \) do
5: apply \( R_y(\theta_{x_{i,j}}) \) on \( x_{i,j} \)
6: apply \( H \) on \( x_{i,j} \)
7: apply \( CX \) with \( y_i \) as a control and \( x_{i,j} \) as target
8: apply \( H \) on \( x_{i,j} \)
9: apply \( R_y(\theta_{x_{i,j}}) \) on \( x_{i,j} \)
10: end for
11: end for

As a test, the FLP instance presented in equations (26) to (29) was implemented using our methodology.

\[
\begin{align*}
\min_{x,y} & \quad 5y_1 + 10y_2 + 3x_{1,1} + 2x_{2,1} \\
\text{s.t.} & \quad x_{1,1} + x_{2,1} = 1 \\
& \quad x_{1,1} \leq y_1 \\
& \quad x_{2,1} \leq y_2
\end{align*}
\]

(26) (27) (28) (29)

This instance includes two facilities and one client, with their respective costs, and it is implemented with 4 qubits \( q_1 \leftarrow x_{1,1}, q_2 \leftarrow x_{2,1}, q_3 \leftarrow y_1, q_4 \leftarrow y_2 \). A penalty factor of \( \lambda = 100 \) is used.

In Figure 6 the most probable solution that corresponds to the state \(|1010\rangle\) can be seen. This solution means that the facility 1 is open and it delivers to the only client. Observe that at Figure 7 the optimal circuit with set of final parameters \( \theta = (1.51, -3.44, 2.97, -0.0688) \).

![Figure 6](image_url)

Figure 6. Comparison histogram solution for the FLP instance (eqs. (26) to (29)), using TVF, 2-Local and QAOA.

![Figure 7](image_url)

Figure 7. Optimal circuit for the FLP instance (eqs. (26) to (29)), using proposed methodology.

COBYLA took 45 iterations to get to the final objective function value of 8.0. In Figure 8 the evolution of the Energy state for the different approaches is illustrated. Observe that since less penalization functions were used for representing equality constraints while using the proposed methodology, the energy state starts in small values compared with the other approaches, facilitating the convergence of the objective function. Another important part of the validation of our methodology is the verification of the cost of the Ansatz implementation using all
methodologies tests, as we observe the proposed has less cost compared with the others, we can warranty that for larger instances of the FLP problem since 2-Local Anzat increases the number of cnots with the number of qubits. In contrast, the number of parameters are certainly less than other methodologies, facilitating the convergence of the classical optimization part.

## Table IV. Number of cnots and SU(2) gates and parameters for tested circuits of TVF, 2-Local, and QAOA to solve FLP instance (26) to (29).

| Var. Form | # SU(2) | # cnots | # param. | Cost |
|-----------|---------|---------|----------|------|
| TVF       | 10      | 2       | 4        | 30   |
| 2-Local   | 14      | 3       | 8        | 44   |
| QAOA      | 26      | 12      | 4        | 146  |

Figure 8. Comparison of evolution of the expected objective function for the FLP instance (eqs. (26) to (29)), using TVF, 2-Local and QAOA.

### 2. Linear Assignment Problem

The Multi-dimensional Assignment Problem (MAP) is a classical NP-Hard combinatorial optimization problem [21], so for sake of simplicity and as a demonstrative example on how to use Tailored variational forms, the Linear Assignment Problem (LAP) will be used here.

The LAP consists of assigning a set of workers to perform a set of jobs, while minimizing the total cost of the assignment. More specifically, given a set of $n_1$ jobs and $n_2$ workers, with more workers than jobs to be executed, the cost for a worker $j$ to execute a job $i$ is $c_{i,j}$. The premise of this assignment is that every job will be done by a worker, considering that every worker can do only one job.

The LAP can be formulated as presented in equations (30) to (33).

$$\max_x \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} c_{i,j} x_{i,j}$$  \hspace{1cm} (30)

subject to:

$$\sum_{j=1}^{n_2} x_{i,j} = 1 \quad i = 1, \ldots, n_1$$ \hspace{1cm} (31)

$$\sum_{i=1}^{n_1} x_{i,j} \leq 1 \quad j = 1, \ldots, n_2$$ \hspace{1cm} (32)

$$x_{i,j} \in \{0,1\} \quad i = 1, \ldots, n_1; j = 1, \ldots, n_2$$  \hspace{1cm} (33)

Where variable $x_{i,j}$ is 1 if job $i$ is done by worker $j$, and 0 otherwise.

All $x_{i,j}$ variables of the LAP with the same $i$ index in constraint (32) can directly use the possible solutions presented in Figure 2 since $x_{i,j}$ variable only appears in one constraint, which is one limitation on this methodology. To represent constraint (31), a penalization is used, as in the FLP presented previously. Thereby, it is possible to formulate the Algorithm 2 to construct the Ansatz for LAP problem.

**Algorithm 2 Linear assignment problem circuit construction**

**Require**: number of jobs $n_1$ and workers $n_2$

**Require**: Costs $c_{i,j}$ of a job $i$ done by worker $j$

1. set all qubits with state 0.
2. for $j = 1, \ldots, n_2$ do
3. for $i = 1, \ldots, n_1$ do
4. set qubit label $x_{i,j}$
5. apply $R_y(\theta_{x_{i,j}})$ on $x_{i,j}$
6. if $i > 1$ then
7. apply $CZ$ with $x_{i-1,j}$ as a control and $x_{i,j}$ as target
8. apply $Z(\theta_{x_{i,j}})$
9. end if
10. end for
11. for $i = n_1, \ldots, 2$ do
12. apply $CZ$ with $x_{i-1,j}$ as a control and $x_{i,j}$ as target
13. end for
14. apply $X$ on $y_i$
15. end for

To test the proposed methodology for the LAP, the following instance is proposed.

$$\max_x 5x_{1,1} + 8x_{1,2} + 7x_{2,13} + 11x_{2,2}$$  \hspace{1cm} (34)

subject to:

$$x_{1,1} + x_{1,2} = 1$$ \hspace{1cm} (35)

$$x_{2,1} + x_{2,2} = 1$$ \hspace{1cm} (36)

$$x_{1,1} + x_{2,1} \leq 1$$ \hspace{1cm} (37)

$$x_{1,2} + x_{2,2} \leq 1$$ \hspace{1cm} (38)

This instance of the FLP is implemented with 4 qubits ($q_1 \leftarrow x_{1,1}, q_2 \leftarrow x_{1,2}, q_3 \leftarrow x_{2,1}, q_4 \leftarrow x_{2,2}$).

In Figure 9 the most probable solution that correspond to the state $|01110\rangle$ can be observed. This solution means that job 1 will be done by worker 2, and
job 2 will be done by worker 1. Figure 10 presents the optimal circuit with set of final parameters $\theta = (0.01, -3.22, -1.68, 3.42)$.

Figure 9. Comparison histogram solution for the LAP instance (eqs. (34) to (38)), using TVF, 2-Local and QAOA.

\[
\begin{align*}
    x_{1,1} : |0\rangle & \xrightarrow{R_y(0.01)} |0\rangle \\
    x_{1,2} : |0\rangle & \xrightarrow{R_y(-3.22)} |1\rangle \\
    x_{2,1} : |0\rangle & \xrightarrow{R_y(-1.68)} |1\rangle \\
    x_{2,2} : |0\rangle & \xrightarrow{R_y(3.42)} |0\rangle
\end{align*}
\]

Figure 10. Optimal circuit for the set LAP instance (eqs. (34) to (38)), using TVF.

For the LAP instance proposed, COBYLA took 45 iterations to get the final objective function of 15. As can be see in Figure 11, TVF needed less iterations to converge to the optimal solution, while the other converged to infeasible solutions, as is shown in Figure 9. In this case, the computational cost is slightly higher than the 2-Local Ansatz, as is presented in Table V.

| Var. Form | # $SU(2)$ | # cnots | # param. | Cost |
|-----------|-----------|---------|----------|------|
| TVF       | 6         | 4       | 4        | 46   |
| 2-Local   | 14        | 3       | 8        | 44   |
| QAOA      | 24        | 8       | 4        | 104  |

Table V. Number of cnots and $SU(2)$ gates and parameters for the tested circuits of TVF, 2-Local, and QAOA to solve LAP instance (eqs. (34) to (38)).

Figure 11. Comparison of the evolution of the expected objective function for the LAP instance (eqs. (34) to (38)), using TVF, 2-Local and QAOA.

Hilbert space is not explore, it only searches the set of points where the solutions are feasible, since exploring the entire Hilbert space could imply in more computational cost for the classical optimization part [12]. Another advantage is that, as observed, the construction of a TVF has a constant number of parameters for a given number of qubits. Additionally, to create a TVF there is no need to previously decide meta-parameters. In general, Variational forms as the 2-Local or the QAOA, those meta-parameters usually multiply the number of parameters of a block of rotation and entangler gates, and there is no clear procedure to define those meta-parameters, besides the empirical ones.

One limitation is that we do not have a general criteria to combine this TVFs in order to represent a variable that appears in more than one constraint on a LCQBO problem. As a future work, it is possible to approximate the TVFs by reducing it in circuits on blocks with a predefined depth, in order to use less cnots gates. Another possible development is that with expressions (14) and (18), the gradient with respect to the parameters $\theta$ can be calculated, and used in gradient-based methods.

V. METHODS

A. Variational Quantum Eigensolver

The VQE is a hybrid algorithm that has a quantum part and a classical part [22]. It is a type of near-term algorithm that uses noisy quantum computers to calculate expectation values of a minimum energy state. Originally, the VQE was used in quantum chemistry to approximate the minimum estate of energy of a quantum system represented by a Hamiltonian using the Varia-
tional theorem. Then, some class of classical optimization problems called QUBO problem could be mapped on like Hamiltonians. Next, Algorithm 3 presents the overall procedure for a generic VQE for solving QUBO problems.

**Algorithm 3 General variational quantum eigensolver**

Require: Set Number of shots $N_{\text{shots}}$

Require: Give initial state $|\psi_0\rangle$

Require: Map quadratic objective function $Q$ to Pauli gates $H_i$

1: while classical optimization condition do
2: Construct Ansatz $U(\theta_k)$
3: Apply Ansatz to the initial state: $|\psi(\theta_k)\rangle = U(\theta_k) |\psi_0\rangle$
4: Measure output $|\psi(\theta_k)\rangle$ $N_{\text{shots}}$ times
5: Calculate the expectation value of the objective function $E \approx \sum_i \langle \psi(\theta_k) | H_i | \psi(\theta_k) \rangle$
6: Classical optimization algorithm update $\theta_k$
7: end while
8: Optimal set of parameters $\theta^*$

In Algorithm 3 we observe that first it is needed to define the number of times that the Ansatz circuit will be executed at one iteration of the VQE. Then, it is necessary to inform an initial state $|\psi_0\rangle$. In quantum chemistry, this state usually is calculated with a classical procedure like the Hartree–Fock method [22]. To solve optimization problems there is no clear strategy to calculate this initial state, but as in quantum chemistry, this could be done by getting a solution of a fast classical heuristic or by a relaxation method that leads to a good quality feasible solution.

Since we are trying to minimize a classical QUBO problem we need to map the objective function to diagonal Hamiltonians $H_i$ represented by Pauli gates. First we use ising representations of QUBO problems [1]. One practical way to make this transformation is to replace every $x_i$ variable on the original classical problem by $(1 - Z_i)/2$, where $Z_i$ is a Pauli gate applied in qubit $i$ with $\pm 1$ eigenvalues on its matrix representation. Since we can translate quadratic objective functions to diagonalized Hamiltonian it is possible to use penalization strategy to convert a linear equality constraint as $Ax = b$ into $\lambda \|Ax - b\|_F$ on the objective function [1].

The following step is to determine the Ansatz that we will be used to sample the Hilbert space of solutions of our problem. Usually to do it, a parametric Ansatz $U(\theta)$ with wide potential to sample Hilbert space is created, while $\theta$ angles varies. One desirable characteristic of the Ansatz is to use less single and double qubit gates. This preference is because current quantum hardware has a limitation on the depth of the circuits that can be executed, and also a limited number of entanglement between qubits.

Then, the Ansatz is sampled a number of times for a fixed set parameters $\theta_k$. With this we can calculate an expectation value of the energy $\sum_i \langle \psi(\theta_k) | H_i | \psi(\theta_k) \rangle$. This expected value of the energy for state $|\theta_k\rangle$ represents an approximation for the objective function of the original classical optimization problem. This is based on the Variational method in quantum mechanics where the minimum energy and others energy states have a relation [39], and is equal only when the state $|\psi_g\rangle$ correspond to the ground state energy $E_g$.

$$E \geq \left( \sum_i \langle \psi(\theta_k) | H_i | \psi(\theta_k) \rangle \right) \geq E_g \quad (39)$$

The final component of the VQE algorithm is the classical optimization algorithm, where the parametric energy is minimized $\langle \psi(\theta) | H | \psi(\theta) \rangle$ with a classical solver by updating parameters $\theta$. In [24], many of the following solvers are explored and its effectiveness on considering or not noise on the objective function. Some of the most used solvers are: Simultaneous Perturbation Stochastic Approximation (SPSA) [25], the Nelder-Mead Simplex Method [26], Sequential Least Squares Programming (SLSQP) [27], and Adam [28]. One improved algorithm for objective functions with trigonometric functions is Nakanishi-Fujii-Todo algorithm (NFT) [29] solver, which is also robust against statistical error. One limitation of the parametric circuits in a classical optimization loop is that it creates extremely non-linear optimization problems where there exists plateaus around local minimum and also from where it is difficult to escape [12]. For our computational experiments we use Constrained Optimization by Linear Approximations (COBYLA) [13].

**B. Circuits costs**

All the variational forms proposed in this paper uses $R_y$ gates with parameters $\theta$. State of the art approaches for create an Ansatz variational form uses $R_y$ and $R_z$ rotations conjugated with cnot gates. Then it is repeated the Ansatz an empirical number of times, this is named the "depth" of the Ansatz [3]. When VQE is implemented and defined a depth, its created a set with polynomial number of parameters [2]. This set of parameters will be the search domain when is passed to the classical optimization problem part [15]. We need to use a metric to compare the cost of execute the Ansatzes that we use on section III B.

| Var. Form | $\#$ SU(2) | $\#$ cnots | $\#$ param. |
|-----------|-------------|-------------|--------------|
| Fig 1     | $2N - 1$    | $N - 1$     | $N$          |
| Fig 2     | $2N - 1$    | $2(N - 1)$  | $N$          |
| Fig 3     | $2N - 1$    | $4N - 6$    | $N$          |
| Fig 4     | $2N - 3$    | $3N - 5$    | $N - 1$      |

Table VI. Number of cnots, SU(2) gates and parameters to execute TVFs.

On table VI is shown the number of single-gates and
cnots to run tailored variational forms. This decomposition on basic gates is relevant since with the current Noisy Intermediate-Scale Quantum (NISQ) devices, noises impact more on the use of cnot gates, then an efficient quantum algorithm should avoid to use this gates when possible. It is possible to approximate it with a relation of that cnot gates takes 10 times more than a single-qubit gate as is showed in [30].

\[
\text{Total cost} = N_{CNOT} \times 10 + N_{SU(2)} \quad (40)
\]

VI. DATA AVAILABILITY

All data needed in the paper are present in the paper and/or the Supplementary Information.

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VIII. AUTHOR CONTRIBUTIONS

All authors initialized the project. M.P.Q. developed the theory, performed the experiments and analyzed the results. All authors contributed to designed the experimental setup, and writing the manuscript.

IX. COMPETING INTERESTS

The authors declare no competing interests.

X. ADDITIONAL INFORMATION

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