

Quantum querying based on multicontrolled Toffoli gates for causal Feynman loop configurations and directed acyclic graphs

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Quantum algorithms are a promising framework for unfolding the causal configurations of multiloop Feynman diagrams, which is equivalent to querying the directed acyclic graph (DAG) configurations of undirected graphs in graph theory. In this paper, we present a quantum algorithm for querying in both types of applications, using a systematic and sparing logic in the design of an oracle operator. The construction of the quantum oracle is based exclusively on multicontrolled Toffoli (MCX) gates and quantum NOT (Pauli- X) gates. The efficiency of the algorithm is evaluated by comparison with a quantum algorithm based on binary clauses. Furthermore, we analyze the impact of transpilation and introduce an appropriate metric to assess the complexity of the algorithm, the quantum circuit area. We explicitly analyze three-, four- and five-loop topologies, which have not previously been explored due to their higher complexity and the current limitations of quantum simulators.

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I. INTRODUCTION

Quantum computing [1] is currently an appealing approach with great potential to tackle complex problems in many fields where exploiting the quantum principles of superposition and entanglement could suppose an advantage. In the context of high-energy physics [2,3] recent applications of quantum algorithms include lattice gauge theories [4–7], track reconstruction [8–10], jet clustering algorithms [11–14], analyzing the formation of jets in a medium [15–17], simulation of parton showers [18–21], determination of parton densities [22,23], helicity amplitudes [20] and the color algebra [24] of elementary processes, heavy-ion collisions [25], quantum machine learning [26–28], and quantum integrators [29–32], including their application to loop Feynman integrals and decay rates at next-to-leading order [33,34]. In this work, we delve into the quantum determination of the causal structure of multiloop Feynman diagrams previously analyzed in [35,36].

Improving the accuracy of theoretical predictions for high-energy colliders is crucial because of the high demands this field will face [37], in particular during the current Run 3 of the CERN's Large Hadron Collider (LHC), the planned

high-luminosity LHC stage [38], and future collider projects [39–42]. As far as perturbative quantum field theory is concerned, one of the main needs is the study and appropriate treatment of the quantum fluctuations associated to multiloop Feynman diagrams. In accordance with this need, there has been a remarkable effort in the field to provide powerful frameworks to meet this challenge [43].

Aiming for improving the efficiency of multiloop-level computations with a proper treatment of singularities, we work in the framework of the loop-tree duality (LTD) [44–64]. The emergence of noncausal singularities in the customary Feynman representation of loop integrals implies considerable numerical instabilities, whereas in the LTD representation, noncausal singularities are explicitly absent, providing the advantage of significantly more stable integrands [65,66]. In particular, the latest achievements in LTD are based on its most distinctive feature: the existence of a manifestly causal representation and its connection with directed acyclic graph (DAG) configurations in graph theory [65–76]. A comprehensive review of classical algorithms in graph theory is presented in Ref. [77].

The fact that a Feynman propagator has two on-shell states, which are therefore naturally encoded in a qubit, makes quantum computing a potentially efficient way of dealing with some aspects of multiloop Feynman integrals. In Ref. [35], an amplitude amplification or Grover's based [78,79] quantum algorithm was proposed to unfold the causal configurations of multiloop Feynman diagrams. A similar study based on a variational quantum

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eigensolver (VQE) approach was presented in Ref. [36]. The quantum algorithm of Ref. [35] is more expensive in terms of the total number of qubits, theoretical quantum depth (defined in Sec. III) and transpiled quantum depth, compared to the VQE approach [36]. However, the VQE approach requires longer runs than the algorithm described in Ref. [35].

In this paper, we present an enhanced quantum algorithm for querying causality of multiloop Feynman diagrams through a more systematic and comprehensible implementation of the causal conditions for identifying DAG configurations [80]. These causal conditions are encoded by identifying each cycle with a multicontrolled Toffoli gate, which significantly simplifies the design of the oracle operator and thus the implementation of complex loop topologies. Also, we propose a metric called the quantum circuit area to properly evaluate the performance of the algorithm. The quantum circuit area is defined as the product of the transpiled quantum circuit depth and the number of qubits required in the transpilation. The proposed quantum algorithm achieves a significant reduction in qubit requirements and quantum circuit area. This reduction in the number of required qubits allows us to explore multiloop topologies of higher complexity that were previously inaccessible due to the current limitations of quantum simulators. In addition, the main practical advantage of the proposed algorithm is a significant reduction in the RAM usage and computational cost for classically simulating the corresponding circuits.

II. CAUSALITY FROM THE LOOP-TREE DUALITY

Generic loop integrals and scattering amplitudes, with n propagators and P external legs are defined in the Feynman representation as integrals in the Minkowski space of L loop momenta

$$\mathcal{A}_F^{(L)} = \int_{\ell_1 \dots \ell_L} \mathcal{N}(\{\ell_s\}_L, \{p_j\}_P) \prod_{i=1}^n G_F(q_i), \quad (1)$$

where the momenta of the Feynman propagators, q_i^μ , are linear combinations of the loop and external momenta, and the numerator $\mathcal{N}$ is given by the specific theory. The integration measure in dimensional regularization [81,82] reads $\int_{\ell_s} = -i\mu^{4-d} \int d^d \ell_s / (2\pi)^d$, with d the number of spacetime dimensions and μ an arbitrary energy scale. Feynman propagators are conveniently written as

$$G_F(q_i) = \frac{1}{(q_{i,0} - q_{i,0}^{(+)})(q_{i,0} + q_{i,0}^{(+)}),} \quad (2)$$

where $q_{i,0}^{(+)} = \sqrt{\mathbf{q}_i^2 + m_i^2 - i0}$ are the on-shell energies, with $q_{i,0}$ and $\mathbf{q}_i$ the temporal and spacial components of q_i ,

respectively, and m_i the mass of the propagating particle. The infinitesimal factor $i0$ is the usual complex prescription of a Feynman propagator.

Singularities in the integrand of Eq. (1) arise when Feynman propagators are set on shell, explicitly, when the energy component $q_{i,0}$ takes one of the values $\pm q_{i,0}^{(+)}$ in Eq. (2). An important fact to take into account is that not all potential singular configurations of the integrand in Eq. (1) lead to physical singularities of the integral. In the case of the Feynman representation of loop integrals, noncausal singularities are unavoidable. Regarding the LTD framework, its more relevant feature is the existence of a manifestly causal representation, where noncausal singularities are absent. The direct LTD representation of Eq. (1) is computed by applying the Cauchy's residue theorem through the evaluation of nested residues [67]. To obtain the LTD causal representation we sum over all the nested residues, explicitly canceling all the noncausal contributions. Although summing over all nested residues cancels out these nonphysical singularities, this cancellation becomes increasingly complex for more involved loop topologies, requiring extensive algebraic manipulations. Furthermore, the LTD causal representation is found to be reinterpreted in terms of entangled causal thresholds [65,66]. The analytical causal reconstruction is achieved by matching all combinations of $n - L$ threshold configurations that are causally compatible to each other, leading to the LTD causal representation,

$$\mathcal{A}_D^{(L)} = \int_{\ell_1 \dots \ell_L} \frac{1}{x_n} \sum_{\sigma \in \Sigma} \frac{\mathcal{N}_{\sigma(i_1, \dots, i_{n-L})}}{\lambda_{\sigma(i_1)}^{h_{\sigma(i_1)}} \dots \lambda_{\sigma(i_{n-L})}^{h_{\sigma(i_{n-L})}}} + (\lambda_p^+ \leftrightarrow \lambda_p^-), \quad (3)$$

with $x_n = \prod_{i=1}^n 2q_{i,0}^{(+)}$ and $h_{\sigma(i)} = \pm$. The Feynman propagators from Eq. (1) are substituted in Eq. (3) by causal propagators of the form $1/\lambda_p^\pm$, with

$$\lambda_p^\pm = \sum_{i \in p} q_{i,0}^{(+)} \pm k_{p,0}, \quad (4)$$

where p is a partition of the on-shell energies, and $k_{p,0}$ is a linear combination of the external-momenta energy components. Given the sign of $k_{p,0}$, either λ_p^- or λ_p^+ becomes singular after all propagators in the partition p are set on shell. The combinations of entangled causal propagators represent causal threshold configurations that can occur simultaneously which are collected in the set Σ . Canceling the nonphysical singularities may be straightforward in simple cases, whereas in more complex cases rearranging the resulting expression into the form of Eq. (3) remains a nontrivial combinatorial task, as it requires identifying all the causal compatible configurations with the LTD constraints for a given multiloop topology. While this step may not constitute the sole computational bottleneck in LTD applications, it is a necessary prerequisite for the analytic simplification and numerical integration, in particular using

quantum methods [31–34,76], and its combinatorial complexity scales rapidly with the number of loops. The quantum algorithm presented here targets this specific step as a first contribution toward a broader quantum-assisted LTD framework.

A first step in the procedure for obtaining theoretical predictions in LTD is to derive the causal representation shown in Eq. (3), which requires identifying all compatible configurations among causal thresholds (causal singular configurations). This process can be viewed as querying multiple solutions over an unstructured database [78,79]. In the quantum setting, the algorithm starts from a uniform superposition over all possible configurations. Therefore, the search can be considered as unstructured because all elements of the database are initially indistinguishable. We note that while the initial quantum state is an unstructured uniform superposition, the question of whether the underlying graph admits classical algorithms with sublinear scaling remains open. We therefore treat the problem as unstructured for the purposes of implementing amplitude amplification, without attempting quantum speedup over classical approaches.

This exercise is equivalent to select all the DAG configurations of an undirected graph in graph theory. In the following section we present a systematic and efficient quantum algorithm to address the identification of causal configurations of multiloop Feynman diagrams and DAGs in graphs theory.

III. QUANTUM CAUSAL QUERYING

The proposed algorithm recovers the central ideas from Ref. [35] on amplitude amplification or Grover's quantum algorithm and considers a generalized description of multiloop topologies by treating them as directed graphs made of edges and eloops [70,71]. An edge is defined as the union of multiple Feynman propagators connecting two

interaction vertices. Once propagators are substituted by edges, the remaining loops of the graph define the number of eloops, which is smaller than the number of loops of the original Feynman diagram. The convenience of working with eloops in a causality scenario is given by the fact that the only feasible causal configurations are those for which the momentum flows of all propagators belonging to each edge are aligned in the same direction.

The distinguishing idea introduced in this paper is a change of logic in the construction of the oracle operator. The tagging of the unidirectional cycles representing eloops is done through the application of multicontrolled Toffoli (MCX) gates and NOT (Pauli-X) gates, having as a core difference with Ref. [35] the absence of binary clauses comparing adjacent edges. This logical procedure significantly simplifies the design and encoding of the corresponding quantum circuits. To evaluate the efficiency of the proposal, we focus on the number of qubits required for the algorithm implementation, on the quantum circuit depth and on the quantum circuit area. Before describing the algorithm, we review some relevant concepts for a better understanding of the work developed.

Regarding the efficiency of the amplitude amplification, it is important to note the relevance of the mixing angle, defined as $\theta = \arcsin \sqrt{r/N}$, that measures the ratio of the r winning states over the total number of states in the search space, $N = 2^n$, and the optimal number t of the algorithm iterations. If $r \sim N/4$, then $\theta \sim \pi/6$, and one iteration is sufficient because $\sin^2 \theta_t \sim 1$ with $\theta_t = (2t + 1)\theta$. It has been shown from classical [65,66] and quantum [35] analysis of the multiloop topologies depicted in Fig. 1 that the number of causal configurations is typically about one half of the total number of possible states. This implies $\theta \sim \pi/4$, which does not lead to any reasonable amplitude amplification. However, given a causal solution of a loop Feynman diagram, the mirror state with all the momentum

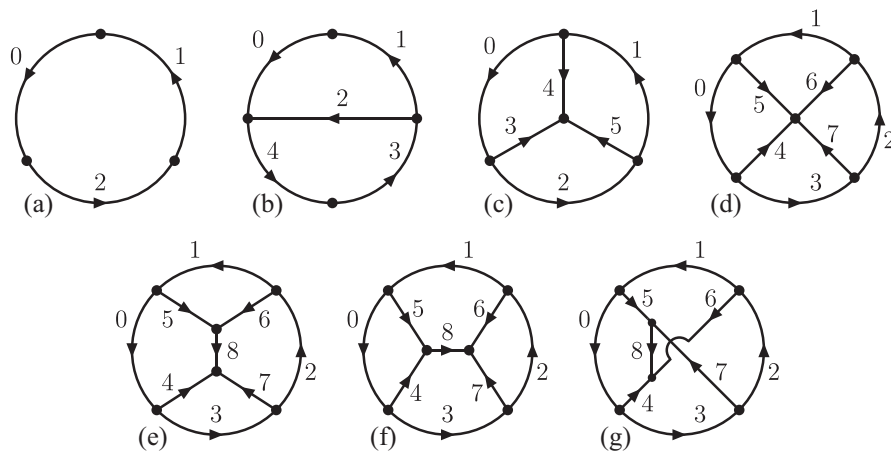


FIG. 1. From left to right and top to bottom: one eloop with three vertices, two eloops with four vertices, three eloops with four vertices, four eloop with a four-point contact interaction, and four eloops t -, s - and u -channels. The direction of the arrows corresponds to the $|1\rangle$ states. External momenta are attached to the interaction vertices.

flows reversed is also a causal solution. Therefore, for one of the qubits representing an edge, we tag only one of its states so that the number of winning states is $r \sim N/4$, which is the optimal value for amplitude amplification in a single iteration. The total set of causal solutions is then obtained by reversing the momentum flows of all the causal states tagged. In the case that halving the number of solutions is not enough to adjust the ratio r/N in the required range, then we introduce an ancillary qubit [83] to increase the number of total states without increasing the number of solutions.

The implementation of the quantum algorithm requires three registers, $|e\rangle$, $|a\rangle$ and $|\text{out}\rangle$. The first register, $|e\rangle$, encodes the states of the edges. For each edge, $|0\rangle$ represents propagation in one direction, and $|1\rangle$ in the opposite direction. We define the boolean functions

$$s_j \equiv \bigwedge_{i \in s_j} e_i, \quad \bar{s}_j \equiv \bigwedge_{i \in s_j} \bar{e}_i, \quad (5)$$

where s_j labels the edge set e_i depending on the same linear combination of loop momenta. The bar in $\bar{s}_j$ denotes that the qubit states in this set are inverted with NOT gates, $|\bar{e}_i\rangle = X|e_i\rangle$. The number of edges in the set s_j is denoted by n_{s_j} and the total number of edges describing the corresponding multiloop topology is $n = \sum_j n_{s_j}$, which is the size of the register $|e\rangle$. The second required register is $|a\rangle$. It collects the causal conditions in eloop clauses, and its size is m , corresponding to the number of subloops that need to be tested. The last register, $|\text{out}\rangle$, stores the validation of the causal solutions in what is known as the oracle's marker. The algorithm takes as a first step the initialization of all the quantum registers. The register encoding the edges' states, $|e\rangle$, is initialized in a uniform superposition by applying Hadamard gates to each of its n qubits, $|e\rangle = H^{\otimes n}|0\rangle$. For the eloop clauses, the m qubits in the register $|a\rangle$ are initialized to $|1\rangle$ by applying NOT gates, $|a\rangle = X^{\otimes m}|0\rangle$. The oracle's marker qubit, $|\text{out}\rangle$, is initialized to one of the Bell states by applying $|\text{out}\rangle = H(X|0\rangle) = H|1\rangle \equiv |-\rangle$.

Following to the construction of the oracle operator, it is important to recall that causal configurations are identified as DAG configurations, therefore, the eloop clauses are established to suppress directed cyclic configurations. The eloop clauses are implemented through the application of multicontrolled Toffoli gates and NOT gates that validate whether a configuration is cyclic or acyclic. To provide a convenient notation, we define the multicontrolled Toffoli operation based on boolean clauses by

$$t(S_j) = \bigwedge_{k \in S_j} s_k, \quad \bar{t}(S_j) = \bigwedge_{k \in S_j} \bar{s}_k, \quad (6)$$

and

$$T(S_j) = t(S_j) \vee \bar{t}(S_j), \quad (7)$$

where the capital S_j contains the edge set generating the cyclic configuration involving the subloop j . Both conditions in Eq. (6) select the same subloop but with opposite edge directions. The composite condition in Eq. (7) embraces both directions of the given subloop associated to S_j . Let us recall that the eloop clause register $|a\rangle$ is initialized to $|1\rangle$, therefore, applying one of the conditions in Eqs. (6) and (7) unmarks a noncausal configuration from $|a\rangle$.

An important aspect to consider relating eloop clauses is whether or not the set S_j involves a fixed qubit, that is, a qubit tagged in a definite state $|0\rangle$ or $|1\rangle$. If the eloop clause condition does not involve a fixed qubit, we apply Eq. (7), which considers two multicontrolled Toffoli gates to validate both directions. The validation of both directions is stored in a single qubit $|a_i\rangle$, due to the fact that both configurations are mutually exclusive, i.e., applying one multicontrolled Toffoli gate does not overlap over the second one. In the case where the eloop clause involves a fixed qubit, the condition to probe involves only one direction, explicitly, only one of the two boolean conditions given in Eq. (6) is tested.

After the initialization of the registers and setting all the eloop clauses, the oracle operator is given by

$$U_w|e\rangle|a\rangle|\text{out}\rangle = (-1)^{f(a,e)}|e\rangle|a\rangle|\text{out}\rangle, \quad (8)$$

where $f(a,e) = (\bigwedge_i a_i) \wedge e_0$, and e_0 is the edge whose state is fixed. The procedure continues by performing the oracle operations in inverse order to restore every qubit but $|\text{out}\rangle$ to its initial state. The oracle operator tags the causal configurations according to Eq. (8) but does not alter the probabilities of these states. Then, a diffusion operator, U_s , amplifies the amplitude of the tagged states, increasing their probability in a measurement of the qubits. In particular, if $|w\rangle$ represents a uniform superposition of the tagged or winning states, and $|e_\perp\rangle$ is the orthogonal state, then

$$U_s(U_w|e\rangle) = \cos(3\theta)|e_\perp\rangle + \sin(3\theta)|w\rangle. \quad (9)$$

The probabilities of the orthogonal and winning states are $\cos^2(3\theta)$ and $\sin^2(3\theta)$, respectively. If $\sin^2(3\theta) \sim 1$, the probability of the orthogonal states is very suppressed and the measurement of the qubits in the register $|e\rangle$ selects the desired states with higher probabilities. The diffusion operator implemented in the quantum circuit is shown in Fig. 2 and is based on the diffusion operator described in the IBM Qiskit website.¹

The quantum algorithm presented in this paper has the advantage that the quantum circuit depth depends just on the number of eloop clauses and not on the number of edges per set, whereas the quantum circuit depth of the quantum

¹<http://qiskit.org/>

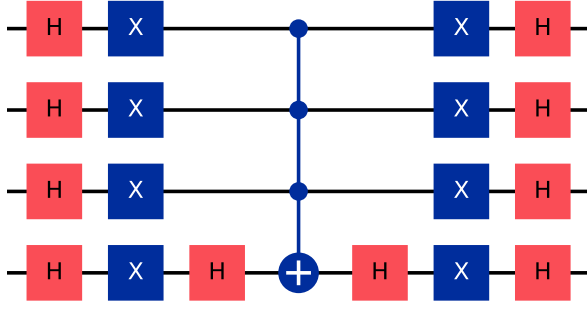


FIG. 2. Diffusion operator for four qubits.

algorithm using binary clauses [35] increases when additional edges per set are considered.

Let us recall that the quantum circuit depth [84] is defined as the integer number of gates that need to be executed along the longest path of the circuit from input to output, moving forward in time along qubit wires. The input is understood as the preparation of the qubits and the output as the measurement gate. An important feature of the quantum circuit depth is the impact of quantum gates acting on no common qubits, allowing to perform them at the same time step. On the other hand, if the gates act on at least one common qubit they have to be applied in different time steps, increasing by one unit the quantum circuit depth. The quantum circuit depth can be computed through the Qiskit routine, `QuantumCircuit.depth()`.²

As a consequence, the theoretical quantum depth reported here should be understood as a rough lower bound on circuit complexity, not as a physically meaningful measure. Transpiled depth, discussed in Sec. IV, provides a more realistic estimate.

The direct use of `QuantumCircuit.depth()` assigns a quantum depth of 1 to any Toffoli gate, regardless of the number of control qubits. Therefore, the theoretical quantum depth reported should be understood as a rough lower bound on the quantum circuit's complexity. A more comprehensive and realistic analysis requires including *transpilation* in the evaluation of the quantum circuit depth, which will be discussed in Sec. IV. We refer to the depth obtained from the untranspiled quantum circuit as the theoretical quantum depth, and to the depth after transpilation as the transpiled quantum depth; the latter is, however, backend dependent.

The output of the quantum algorithm after a measurement is the selection of a single configuration. In order to identify all the solutions it is required to prepare and measure a certain number of times (shots), having as an output a frequency histogram. An estimation of the minimal number of shots required to distinguish all causal from noncausal configurations with 50% chance that the search succeeds in a quantum simulator, in the sense that none of the r winning

states is missed, is given by³

$$N_{\text{shots}} \approx r \log(r) (1 + \mathcal{O}(\cos^2(\theta_t))), \quad (10)$$

assuming an efficient amplification of the causal states, i.e. $\cos(\theta_t) \sim 0$. At this stage, we emphasize that although the required number of shots for applications in particle physics may diminish the expected Grover's quadratic speed-up, the main challenge lies in the design and implementation of the oracle operator, which is greatly simplified and systematized by the algorithm presented in this work. For applications in which one or a few acyclic states need to be identified, the quadratic speed-up is expected to be preserved.

To illustrate the algorithm implementation, let us start with the two-loop topology with three sets of edges depicted in the top left of Fig. 3. We consider two edges per set to include three additional vertices representing external particles. Concretely, we have $n = 6$, $s_0 = 0 \wedge 1$, $s_1 = 2 \wedge 3$ and $s_2 = 4 \wedge 5$, using the short-hand notation $i \equiv e_i$. As previously stated, we start by preparing the three registers: the $|e\rangle$ register in a uniform superposition $H^{\otimes n}|e_i\rangle$, the register $|a\rangle$ initialized in the state $|1\rangle$ and the oracle's marker in the state $|-\rangle$, as shown in the first time step of the quantum circuit of Fig. 3 (top right). The loop clauses are given by

$$\begin{aligned} a_0^{(2)} &= t(s_0 \wedge s_2), \\ a_1^{(2)} &= t(s_0 \wedge \bar{s}_1), \\ a_2^{(2)} &= T(s_1 \wedge s_2), \end{aligned} \quad (11)$$

where $S_0 = s_0 \wedge s_2$, $S_1 = s_0 \wedge \bar{s}_1$ and $S_2 = s_1 \wedge s_2$. The loops clauses in Eq. (11) are implemented by multiccontrolled Toffoli gates taking as control the qubits in the set S_j and as target the qubit $|a_j\rangle$ with $j = 0, 1, 2$. Explicitly, $a_0^{(2)}$ and $a_1^{(2)}$ are implemented by a single multiccontrolled Toffoli gate, whereas $a_2^{(2)}$ is implemented by two multiccontrolled Toffoli gates.

For the oracle's marker, another multiccontrolled Toffoli gate is used. The initial mixing angle is $\theta = 36.8^\circ$ (see Table I) by fixing the qubit $|e_0\rangle$. The multiccontrolled Toffoli gate implementing the oracle's marker takes as control the qubits in the register $|a\rangle$ and the qubit $|e_0\rangle$, and as target the qubit $|out\rangle$. After applying the oracle operations in reverse order, we apply the diffusion operator to the register $|e\rangle$. Table I shows the results of the two quantum circuits in Fig. 3, going from 16 to 10 total number of qubits for implementation, and from 22 to 14 quantum circuit depth. Figure 4 shows the output of the quantum circuit in Fig. 3 (top-right).

In the following sections we explore in detail the performance of the proposed quantum algorithm by analyzing

²<https://qiskit-test.readthedocs.io>

³The success chance raises to 99% for $N_{\text{shots}} \approx 1.3r \log(r)$. We thank the referee for suggesting this scaling formula that is more accurate than our initial estimate [35].

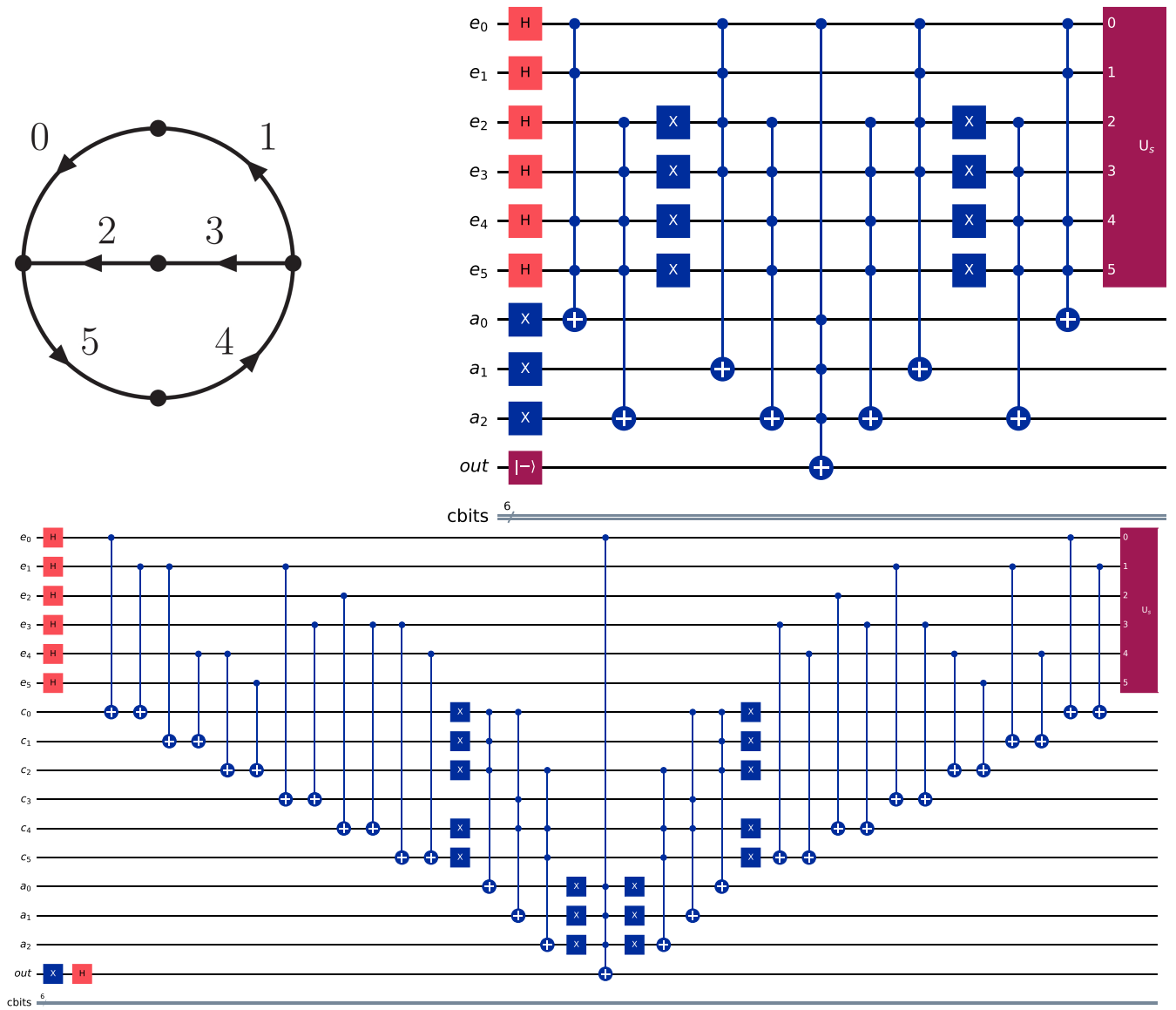


FIG. 3. Top left: two-loop topology with two edges per edge set. Top right: quantum circuit with an oracle operator based on multicontrolled Toffoli gates and NOT gates. Bottom: implementation of the quantum algorithm presented in Ref. [35] using CNOT gates for the binary clauses and multicontrolled Toffoli gates for the registers $|a\rangle$ and $|out\rangle$.

the number of qubits needed for the implementation and the corresponding theoretical quantum circuit depth.

IV. EFFICIENCY ASSESSMENT

In this section we assess the efficiency of the proposed quantum algorithm by comparing the implementation results with the quantum algorithm and the multiloop topologies analyzed in Ref. [35]. These multiloop topologies are depicted in Fig. 1 considering one edge in each edge set s_i . The results are summarized in Table II which displays the number of qubits required for the implementation, the theoretical quantum circuit depth, the related mixing angle and the number of causal configurations.

The columns of total number of qubits and quantum circuit depth have two numbers: the first one gives the data on the current approach and, the second one the information of the quantum algorithm using binary clauses. The remaining columns are: the initial mixing angle, an indicator for the appropriate selection of the iteration number and the number of causal states. From Table II, we observe that in all cases the initial mixing angle is close to $\pi/6$, suggesting the application of only one iteration; from the fifth column we have that the value of the mixing angle after the first iteration approaches $\pi/2$, leading to the optimal probability amplification, $\sin^2(\theta_t) \sim 1$ with $t = 1$.

Counting the number of qubits needed, the proposed quantum algorithm lowers significantly the total number of

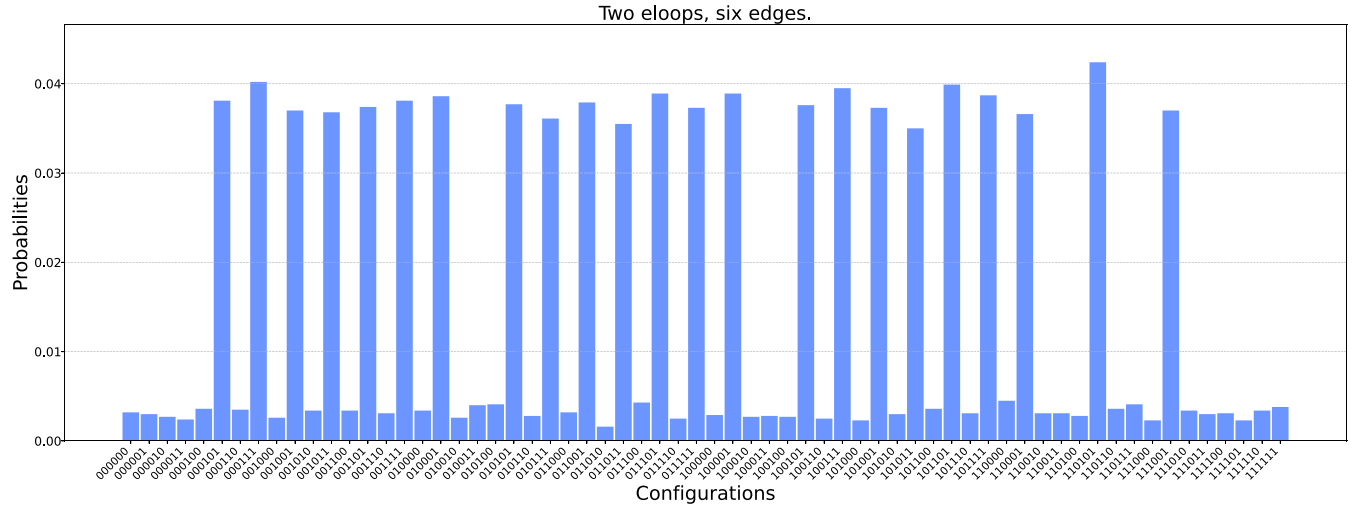


FIG. 4. Output for the algorithm implementation of the two-loop topology with six edges. The total number of causal configurations is 23 out of 64.

qubits required for the implementation with respect to a binary-clause algorithm, going from a reduction of two qubits in the case of one loop with three vertices, to a reduction of fourteen qubits in the u -channel at four loops. Regarding the theoretical quantum circuit depth, we notice that the new approach yields smaller values for all multiloop topologies, with the only exception of the four-loop u -channel, which is a nonplanar diagram. It is important to note that the values shown in Table II correspond to multiloop configurations with one edge per edge set. For these configurations it is sufficient to

satisfy the boolean clauses in Eq. (6) for subloops involving a small number of edge sets, while longer strings of edge sets need to be checked when multiple edges in the edge sets are considered. However, the number of loop clauses reaches a maximum that depends on the multiloop topology and does not scale with the number of edges (see Table IV), while the number of binary clauses scales with the number of edges. In Sec. V, we study multiloop topologies with multiple edges in each edge set, which require testing the maximum number of loop clauses.

TABLE I. Quantum circuit requirements of the quantum algorithms used to analyze the two-loop topology in Fig. 3. The first number in the second and third columns is from the quantum algorithm proposed in this work, whereas the second number corresponds to the binary-clause algorithm [35]. The columns with a single entry have the same value for both algorithms. The numbers in the last two columns are the number of causal configurations and the total number of states, respectively.

Fig.	loops (edges)	Qubits	Quantum depth	θ	$\sin^2(\theta_t)$	Causal states	Total states
3	Two (6)	10 16	14 22	36.8°	0.87	23	64

TABLE II. Quantum resources required and quantum circuit depth of the quantum algorithms used to analyze the multiloop topologies in Fig. 1. The first number in the third and fourth columns is from the quantum algorithm proposed in this work, whereas the second number corresponds to Ref. [35]. The columns with a single entry have the same value for both algorithms. The numbers in the last two columns are the number of causal configurations and the total number of states, respectively.

Figs.	loops (edges)	Qubits	Quantum depth	θ	$\sin^2(\theta_t)$	Causal states	Total states
1(a)	One (3)	5 7	6 18	37.7°	0.84	3	8
1(b)	Two (5)	9 14	12 21	32.0°	0.99	9	32
1(c)	Three (6)	11 19	18 24	25.7°	0.95	12	64
1(d)	four ^(c) (8)	14 25	16 23	33.5°	0.97	39	256
1(e), 1(f)	four ^(t,s) (9)	15 28	20 25	26.5°	0.97	102	512
1(g)	four ^(u) (9)	19 33	32 28	28.3°	0.99	115	512

Continuing with the analysis of the quantum circuit depth, we observe in Table II that the quantum circuit depth for the three-loop diagram [Fig. 1(c)] is greater than the quantum circuit depth for the four-loop diagram with one four-particle interaction vertex (Fig. 1(d), also called N³MLT in Ref. [66]). To better understand this behavior, we compare the loop clauses needed to implement the two topologies, and analyze the presence of multicontrolled Toffoli gates acting on noncommon qubits along the circuits. The loop clauses required for the three-loop topology are

$$\begin{aligned} a_0^{(3)} &= t(s_0 \wedge s_1 \wedge s_2), & a_1^{(3)} &= t(s_0 \wedge s_3 \wedge \bar{s}_4), \\ a_2^{(3)} &= T(s_1 \wedge s_4 \wedge \bar{s}_5), & a_3^{(3)} &= T(s_2 \wedge \bar{s}_3 \wedge s_5), \end{aligned} \quad (12)$$

and for the four-loop topology are

$$\begin{aligned} a_0^{(4)} &= t(s_0 \wedge s_1 \wedge s_2 \wedge s_3), & a_1^{(4)} &= T(s_2 \wedge s_6 \wedge \bar{s}_7), \\ a_2^{(4)} &= t(s_0 \wedge s_4 \wedge \bar{s}_5), & a_3^{(4)} &= T(\bar{s}_1 \wedge \bar{s}_5 \wedge s_6), \\ a_4^{(4)} &= T(\bar{s}_3 \wedge s_4 \wedge \bar{s}_7). \end{aligned} \quad (13)$$

In the three-loop topology, Fig. 1(c), the loop clauses in Eq. (12) are implemented in the quantum circuit using six multicontrolled Toffoli gates. The clauses $a_0^{(3)}$ and $a_1^{(3)}$ validate only one direction of the corresponding subloops, requiring a single multicontrolled Toffoli gate, while $a_2^{(3)}$ and $a_3^{(3)}$ test the subloops in both directions, requiring two multicontrolled Toffoli gates each. In addition, the oracle

operator needs seven NOT gates. In this case, given that the Toffoli gates act in at least one common edge, they must be executed in different time steps to avoid interference. Note that the final number of multicontrolled Toffoli gates and X gates is doubled to return the $|a\rangle$ register to its initial state, and an extra multicontrolled Toffoli gate is required that includes the oracle marker. The initialization of the $|a\rangle$ and $|out\rangle$ registers also needs additional NOT gates. The quantum circuit for the three-loop topology 1(c) is shown in Fig. 5.

In the analysis of the four-loop scenario, Fig. 1(d), the loop clauses specified in Eq. (13) are implemented into the quantum circuit with eight multicontrolled Toffoli gates: a single multicontrolled Toffoli gate for $a_0^{(4)}$ and $a_2^{(4)}$, and two multicontrolled Toffoli gates for $a_1^{(4)}$, $a_3^{(4)}$, and $a_4^{(4)}$. In addition, the oracle operator requires ten NOT gates, as shown in Fig. 6. As for the three-loop case, these oracle operations are also applied in reversed order. The edge configuration of this topology allows several multicontrolled Toffoli gates to act on distinct qubits. This arrangement enables the simultaneous execution of certain operations within the same time step, which explains the lower quantum circuit depth.

An important feature of multicontrolled Toffoli gates to be discussed is transpilation. The transpilation process consists of compiling a given quantum circuit to match the specific topology and native gate set of a particular quantum device hardware, as well as its optimization in order to run on noisy intermediate scale quantum (NISQ) era computers. In the quantum circuit model, high-level quantum circuits are constructed using unitary operators that are implemented

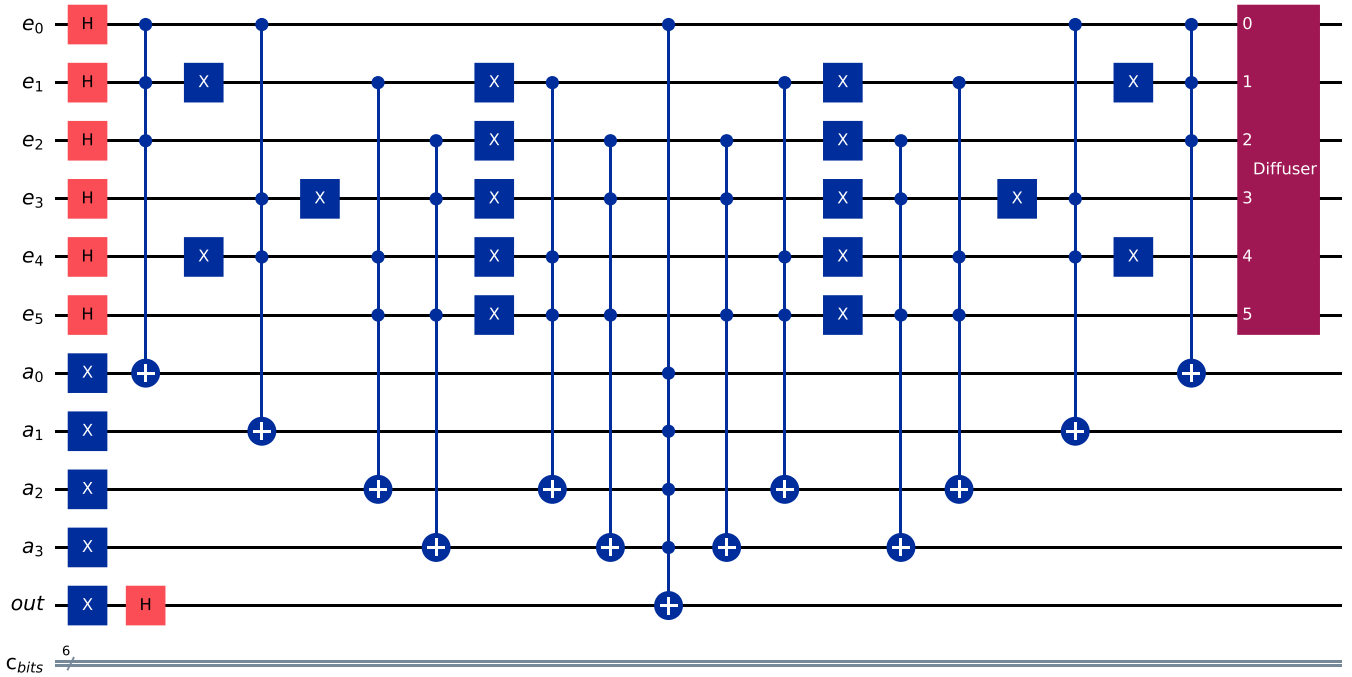


FIG. 5. Quantum circuit for the three-loop topology with six edges [Fig. 1(c)]. The output is 12 causal configurations out of 64 states.

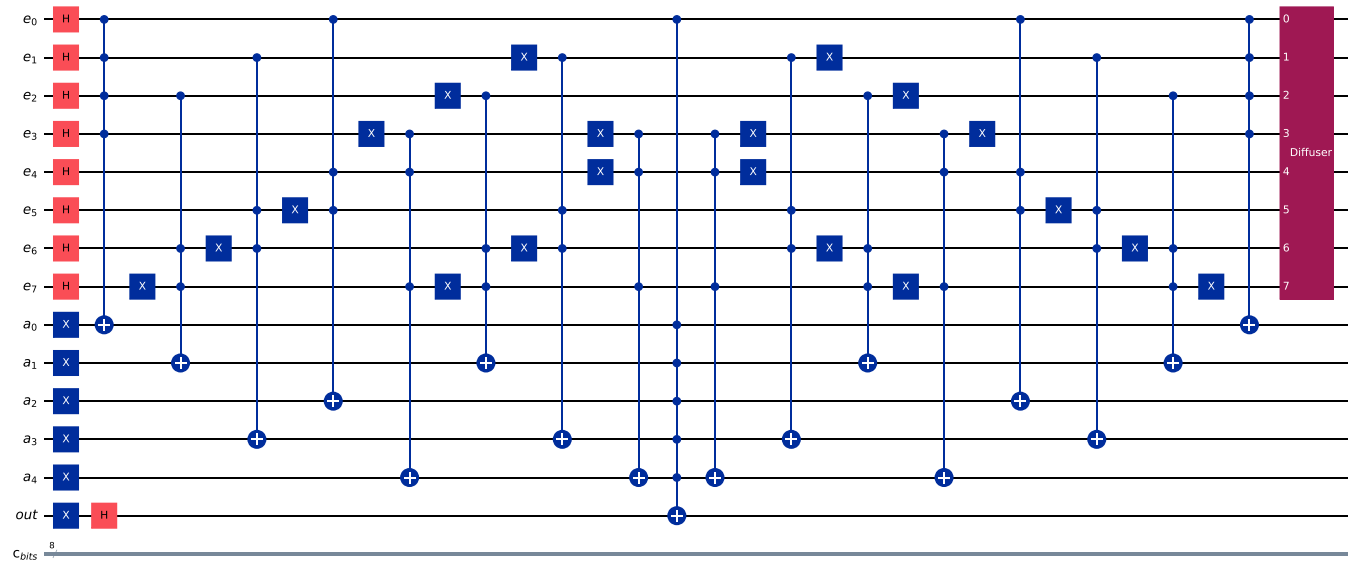


FIG. 6. Quantum circuit for the four-loop topology with eight edges [Fig. 1(d)]. The output is 39 causal configurations out of 256 states.

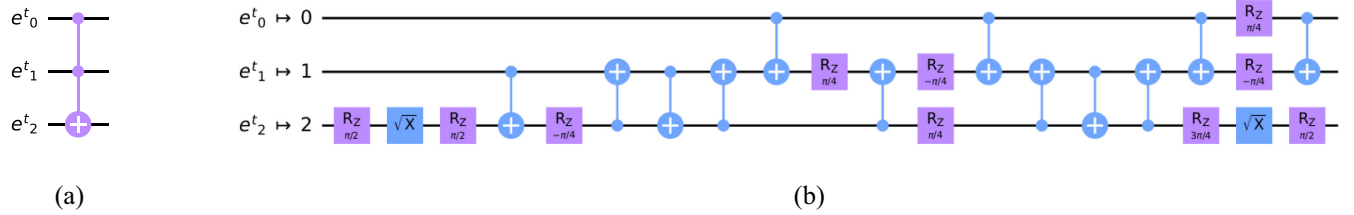


FIG. 7. (a) Quantum circuit representation for the Toffoli gate. (b) Equivalent quantum circuit of the Toffoli gate transpiled to the `ibmq_belem` device from IBMQ.

as quantum gates. When deploying these circuits on actual quantum hardware, however, they must undergo a decomposition of the unitary quantum gates into the native gate set of the target quantum device. Additionally, optimization processes are employed to minimize the noise effects and enhance the accuracy of the output results.

The impact of transpilation for a Toffoli gate on the quantum circuit depth is illustrated in Fig. 7. The Toffoli gate in Fig. 7 operates on three qubits: two control qubits and one target qubit. For our analysis, we employed the 5-qubit quantum processor `ibmq_belem` (which is now retired⁴; however, a simulated fake backend⁵ remains accessible). This quantum processor contains a native gate set consisting on I , R_Z , SX , X , $CNOT$ and reset gates. The theoretical quantum circuit depth of the Toffoli gate shown in Fig. 7(a) is one, however its transpilation for the quantum hardware results in a quantum circuit depth of nineteen as illustrated in Fig. 7(b). The transpilation of each Toffoli

gate increases the quantum circuit depth and therefore has an impact on quantum noise and gate errors.

To analyze the impact of transpilation, we focus on the four-loop topology of Fig. 1(d). We study the transpiled quantum circuit depth for relevant metrics in different quantum backends, both simulated and real quantum hardware, as shown in Table III. The transpiled quantum circuit depth is quite backend-dependent, and is larger for the multiccontrolled Toffoli algorithm than for the binary-clause algorithm. The former also requires more two-qubit gates. However, for classical simulators of quantum backends with a limited number of available qubits, only the multiccontrolled Toffoli algorithm is capable of handling complex graph topologies. Whether this advantage extends to physical quantum hardware, including platforms where multiqubit controlled gates may be natively supported [85–87] remains an open question beyond the scope of this work.

It is important to highlight that transpilation may involve more qubits than formally required in the design of the quantum circuit. To address this concern we propose a new quantum metric, the quantum circuit area, which provides a better understanding of algorithmic efficiency in both

⁴<https://docs.quantum.ibm.com/guides/retired-qpus>

⁵https://docs.quantum.ibm.com/api/qiskit-ibm-runtime/fake_provider

TABLE III. Key metrics for the transpilation of the quantum circuit corresponding to the four-eloop topology of Fig. 1(d) in different quantum devices for the binary-clause (BC) and multicontrolled Toffoli (MCX) algorithms.

Quantum device (qubits)	Four-eloop topology of Fig. 1(d)			
	Transpiled quantum circuit depth		Two-qubit gates	
	BC	MCX	BC	MCX
FakeMelbourneV2 (14)	Not enough qubits	1909	Not enough qubits	1562
FakeMumbaiV2 (27)	1495	2163	1484	1762
ibm_brisbane (127)	4188	5695	1558	1748
ibm_kyoto (127)	4726	5969	1558	1748
ibm_osaka (127)	4672	5043	1558	1748
ibm_sherbrooke (127)	4411	5334	1558	1748

quantum simulators and quantum hardware. The quantum circuit area is defined as the product of the quantum circuit depth and the number of qubits required in the transpilation. This metric provides a more comprehensive evaluation depending in both requirements, the quantum depth of the circuit and its qubit usage, yielding a more complete measure of the computational complexity of the quantum circuit.

Continuing the analysis of the four-eloop topology shown in Fig. 1(d), we present in Fig. 8 the transpiled quantum circuit depth and the transpiled quantum circuit area as a function of the optimization levels on different quantum hardware for both algorithms. The results show a similar evolution in terms of the optimization levels. Despite the fact that the quantum circuit depth in Fig. 8 is higher for the multicontrolled Toffoli algorithm, the quantum circuit area is much smaller compared to the binary-clause algorithm. Therefore, the proposed algorithm achieves a reduction in qubit count and quantum circuit area compared to the binary-clause algorithm, as summarized in Table II and Fig. 8, manifesting a more efficient use of quantum resources in the design of the oracle operator.

V. MULTILoop TOPOLOGIES WITH MULTIPLE NUMBER OF EDGES IN EACH EDGE SET

In the previous section, we have shown a significant reduction in the total number of qubits required to implement the quantum algorithm proposed in this work. This achievement allows us to explore more complex topologies than those affordable with the algorithm presented in Ref. [35], due to the limitations of the current quantum simulators in terms of the number of qubits. In this section, we inquire into the implementation of the proposed algorithm to involved three-, four- and five-eloop topologies; the number of qubits required for an arbitrary number of edges per edge set is shown in Table IV. The lower limits on the number of qubits in the $|a\rangle$ register correspond to multiloop topologies with only one edge per set. The maximum numbers are saturated when all edges contain at least two edges. The particular cases to explore

are illustrated in Fig. 9. The Table V shows the total number of qubits and quantum circuit depth comparing the algorithm proposed in this work with the one in Ref. [35]. This table also provides the mixing angle and the probability of the causal states. Additionally, Table VI compiles the details for the algorithm implementation, number of edges, loop clauses to test in the oracle operator, and Toffoli and NOT gates required for the oracle operator. It is important to remark that from the multiloop topologies depicted in Fig. 9, only the three-eloop topology with nine edges and the simplest five-eloop are formally reachable with the algorithm in Ref. [35] in the Qiskit quantum simulator.

A. Three loops with nine and twelve edges

At three loops, we work with the selected multiloop topologies shown in Figs. 9(a) and 9(b). The first three-eloop topology [Fig. 9(a)] considers two edges in the external sets of edges and one edge in the internal sets of edges, and the boolean functions are given by,

$$\begin{aligned} s_i &= 2i \wedge (2i + 1), & i \in \{0, 1, 2\} \quad \text{and} \\ s_i &= 3 + i, & i \in \{3, 4, 5\}. \end{aligned} \quad (14)$$

Regarding the loop clauses, it requires the four loop clauses in Eq. (12).

For the second three-eloop topology [Fig. 9(b)], we take two edges in all the sets of edges, and the boolean functions are given by,

$$s_i = 2i \wedge (2i + 1), \quad i \in \{0, \dots, 5\}. \quad (15)$$

It requires, in addition to the loop clauses in Eq. (12), the following loop clauses to test acyclicity over four sets of edges

$$\begin{aligned} a_4^{(3)} &= \mathbf{t}(s_0 \wedge s_1 \wedge s_3 \wedge \bar{s}_5), \\ a_5^{(3)} &= \mathbf{T}(s_1 \wedge s_2 \wedge \bar{s}_3 \wedge s_4), \\ a_6^{(3)} &= \mathbf{t}(s_0 \wedge s_2 \wedge \bar{s}_4 \wedge s_5). \end{aligned} \quad (16)$$

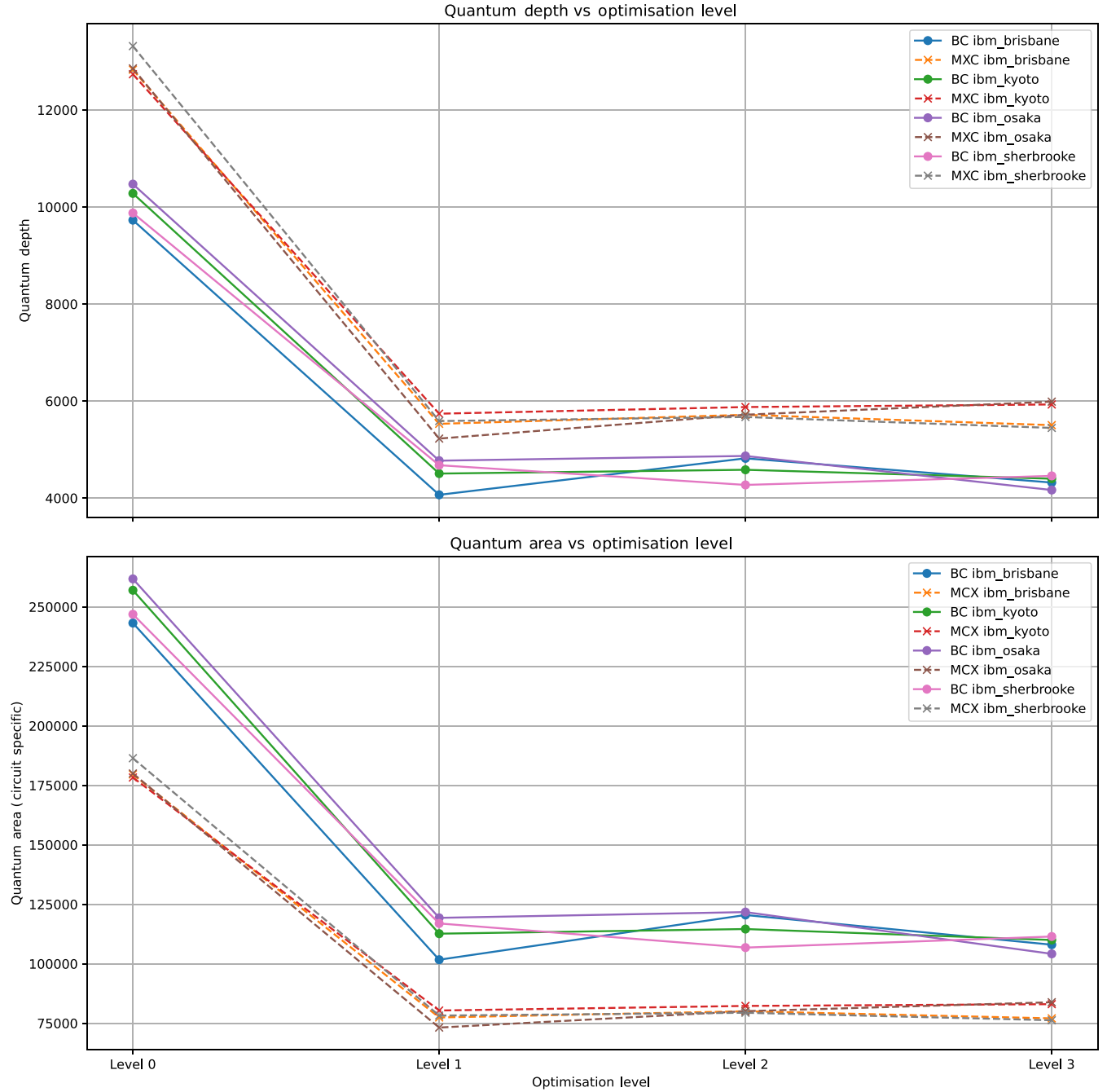


FIG. 8. Quantum circuit depth (upper plot) and quantum circuit area (bottom plot) for the four-loop topology of Fig. 1(d) using the binary-clause (BC) and the multicontrolled Toffoli (MCX) algorithms for various optimization levels on currently available quantum hardware backends.

The total number of qubits required to implement the configurations in Eq. (14) and Eq. (15) is fourteen and twenty-one respectively, and the quantum circuit depth results in eighteen and thirty-two, respectively. In the binary-clause approach these configurations require twenty-five and thirty-six qubits, and the quantum circuit depths would be twenty-seven and thirty-three, respectively; the latter exceeding the number of qubits available on the Qiskit simulator.

TABLE IV. Number of qubits required for an arbitrary three-, four- and five-loop configuration in Fig. 9. The total number of qubits includes the oracle's marker.

loops	$ e\rangle$	$ a\rangle$	Total qubits
Three	n or $n + 1$	4–7	$n + (5 \text{ to } 9)$
four ^(c,t,s,u)	n or $n + 1$	5–13	$n + (6 \text{ to } 15)$
five ^(c)	n or $n + 1$	6–21	$n + (6 \text{ to } 22)$

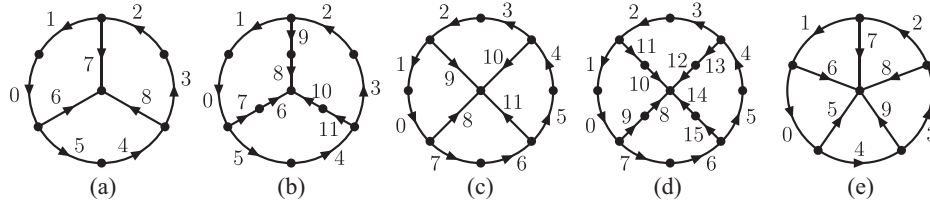


FIG. 9. From left to right: three loops with six and nine vertices, four loops with a four-point interaction and twelve or sixteen vertices, and five loops with a five-point interaction. External momenta are attached to the interaction vertices.

The quantum circuit implemented for the configuration in Eq. (15) is shown in Fig. 10.

Regarding the number of loop clauses, any three-loop topology with multiple edges located exclusively in the external sets of edges do not enlarge the minimum number of clauses to be tested, whereas including two or more edges in every edge set requires to test the maximum number of loops clauses. In fact, thirty-two is the maximum quantum circuit depth that a three-loop topology can have due to the fact that the quantum circuit depth of the proposed quantum algorithm increases with the number of loop clauses but it does not scale with additional edges.

B. Four loops with twelve and sixteen edges

The four-loop examples to analyze are those depicted in Figs. 9(c) and 9(d). The first loop topology [Fig. 9(c)]

considers two edges in the external sets of edges and one edge in the internal sets of edges, and are given by

$$\begin{aligned} s_i &= 2i \wedge (2i + 1), & i \in \{0, 1, 2, 3\} \quad \text{and} \\ s_i &= 3 + i, & i \in \{4, 5, 6, 7\}. \end{aligned} \quad (17)$$

The second loop topology [Fig. 9(d)], consists in two edges in every edge set,

$$s_i = 2i \wedge (2i + 1), \quad i \in \{0, \dots, 7\}. \quad (18)$$

The complete set of loop clauses for the four-loop topology of Fig. 9(d), together with the loop clauses from Eq. (13) are given by

$$\begin{aligned} a_5^{(4)} &= \mathbf{t}(s_0 \wedge s_1 \wedge s_4 \wedge \bar{s}_6), & a_6^{(4)} &= \mathbf{T}(s_1 \wedge s_2 \wedge s_5 \wedge \bar{s}_7), \\ a_7^{(4)} &= \mathbf{T}(s_2 \wedge s_3 \wedge \bar{s}_4 \wedge s_6), & a_8^{(4)} &= \mathbf{t}(s_0 \wedge s_3 \wedge \bar{s}_5 \wedge s_7), \\ a_9^{(4)} &= \mathbf{t}(s_0 \wedge s_1 \wedge s_2 \wedge s_4 \wedge \bar{s}_7), & a_{10}^{(4)} &= \mathbf{T}(s_1 \wedge s_2 \wedge s_3 \wedge \bar{s}_4 \wedge s_5), \\ a_{11}^{(4)} &= \mathbf{t}(s_0 \wedge s_2 \wedge s_3 \wedge \bar{s}_5 \wedge s_6), & a_{12}^{(4)} &= \mathbf{t}(s_0 \wedge s_1 \wedge s_3 \wedge \bar{s}_6 \wedge s_7). \end{aligned} \quad (19)$$

The implementation of the algorithm for these two cases requires a total number of eighteen and thirty-three qubits, respectively, compared to thirty-three and fifty for the binary-clause approach. In terms of the quantum circuit depth, it is sixteen for Fig. 9(c) and forty-six for Fig. 9(d), hence a maximum quantum circuit depth of forty-six for any four-loop topology independently of the number of

edges. Similar to the previous cases of three loops, the four-loop topology associated to Eq. (17) does not need to test additional loop clauses besides the minimum requirement. The quantum circuit for Fig. 9(c) is shown in Fig. 11.

For the four-loop topology configuration in Fig. 9(d) with two edges in all the sets of edges, it is necessary to check additional loop clauses, considering those associated with

TABLE V. Quantum resources required and quantum circuit depth for the quantum algorithm implementation of the multiloop topologies in Fig. 9. The first and second numbers in the third and fourth columns correspond to the algorithm proposed in this work and to the algorithm in Ref. [35], respectively. The mixing angle and the probability of the causal states after amplitude amplification are the same for both algorithms.

Figs.	loops (edges)	Total qubits	Quantum depth	θ	$\sin^2(\theta_t)$
9(a)	Three (9)	14 25	18 27	35.2°	0.93
9(b)	Three (12)	21 36	32 33	28.0°	0.99
9(c)	four ^(c) (12)	18 33	16 31	32.8°	0.98
9(d)	four ^(c) (16)	31 50	46 53	27.7°	0.98
9(e)	five ^(c) (10)	17 31	24 25	28.9°	0.99

TABLE VI. Number of qubits required in the $|e\rangle$ and $|a\rangle$ registers for the algorithm implementation of the multiloop topologies depicted in Fig. 9, number of Toffoli and X gates, number of causal states and total number of states.

Figs.	eloops(edges)	$ e\rangle$	$ a\rangle$	Toffoli gates	NOT gates	Causal states	Total states
9(a)	Three (9)	9	4	14	45	170	512
9(b)	Three (12)	13	7	21	48	1804	8192
9(c)	four ^(c) (12)	12	5	17	66	1199	4096
9(d)	four ^(c) (16)	17	13	39	85	28343	131072
9(e)	five ^(c) (10)	10	6	25	37	240	1024

subloops generated with four and five edge sets, Eq. (19), giving a total of thirteen loop clauses for all the causal configurations.

C. Five eloops with ten edges

The last loop topology we implement has five eloops with a single edge per set s_i which is depicted in Fig. 9(e). The loop clauses to validate are composed by

$$\begin{aligned}
 a_0^{(5)} &= \mathsf{T}(s_0 \wedge s_1 \wedge s_2 \wedge s_3 \wedge s_4), & a_1^{(5)} &= \mathsf{T}(s_0 \wedge s_5 \wedge \bar{s}_6), \\
 a_2^{(5)} &= \mathsf{T}(s_1 \wedge s_6 \wedge \bar{s}_7), & a_3^{(5)} &= \mathsf{T}(s_2 \wedge s_7 \wedge \bar{s}_8), \\
 a_4^{(5)} &= \mathsf{T}(s_3 \wedge s_8 \wedge \bar{s}_9), & a_5^{(5)} &= \mathsf{T}(s_4 \wedge \bar{s}_5 \wedge s_9).
 \end{aligned} \quad (20)$$

The mixing angle is $\theta = 28.9^\circ$ without the need of fixing a qubit from the register $|e\rangle$. This means that the querying probability for finding the 240 causal states out of the 2^{10} total states is close to one, $\sin^2(\theta_t) = 0.99$, with a single iteration, $t = 1$.

In terms of quantum resources, the algorithm based on multiccontrolled Toffoli gates requires seventeen qubits to build the corresponding quantum circuit (Fig. 12) with a quantum circuit depth of twenty-three versus thirty-one qubits and a quantum circuit depth of twenty-five. Note that in this case the inclusion of additional edges in the five-loop topology would prevent the binary-clause algorithm from being implemented in the Qiskit quantum simulator, given its limited capacity of 32 qubits.

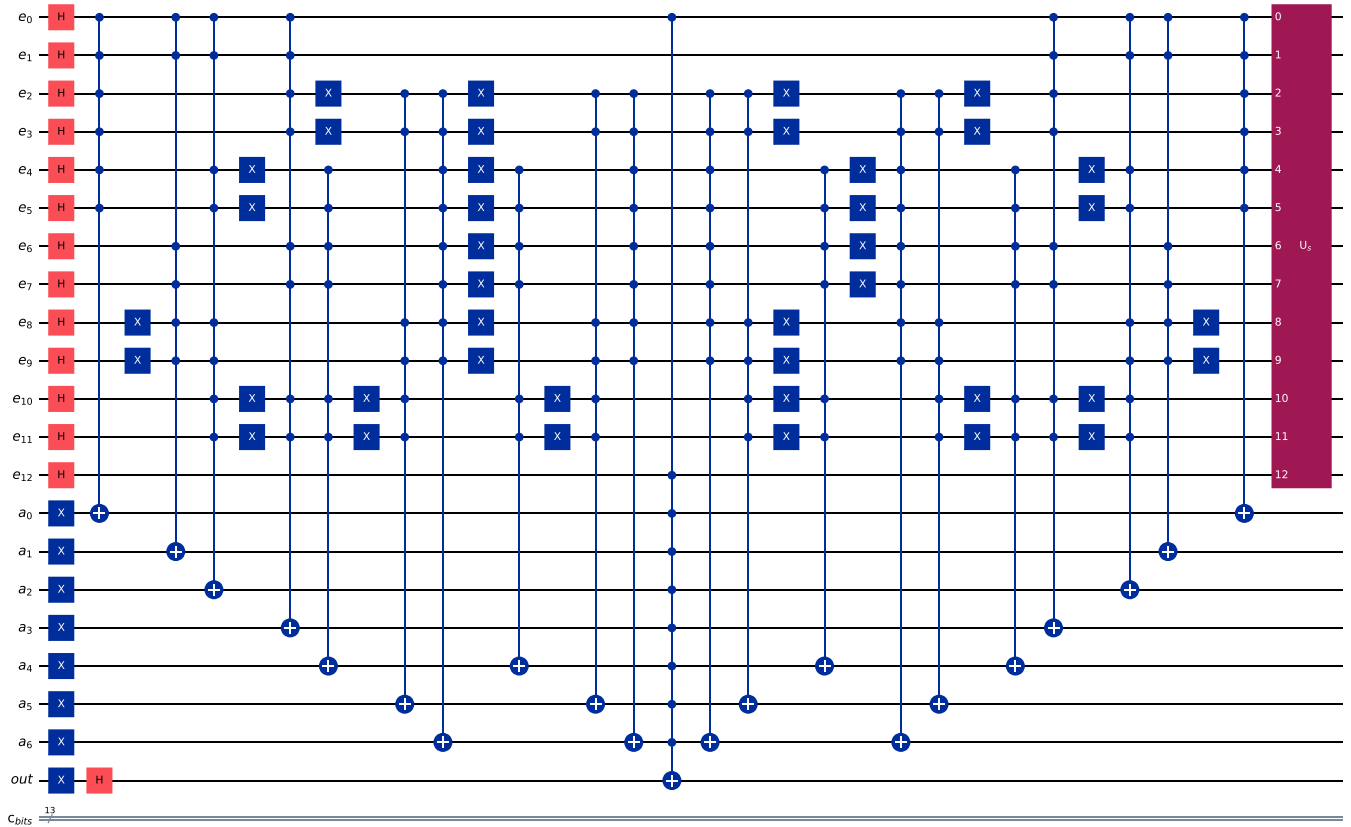


FIG. 10. Quantum circuit for the three-elooop topology with twelve edges [Fig. 9(b)]. The output is 1804 causal configurations out of 8192 states. The last qubit in the $|e\rangle$ register is an ancillary qubit used to adjust the initial mixing angle to the optimal value.

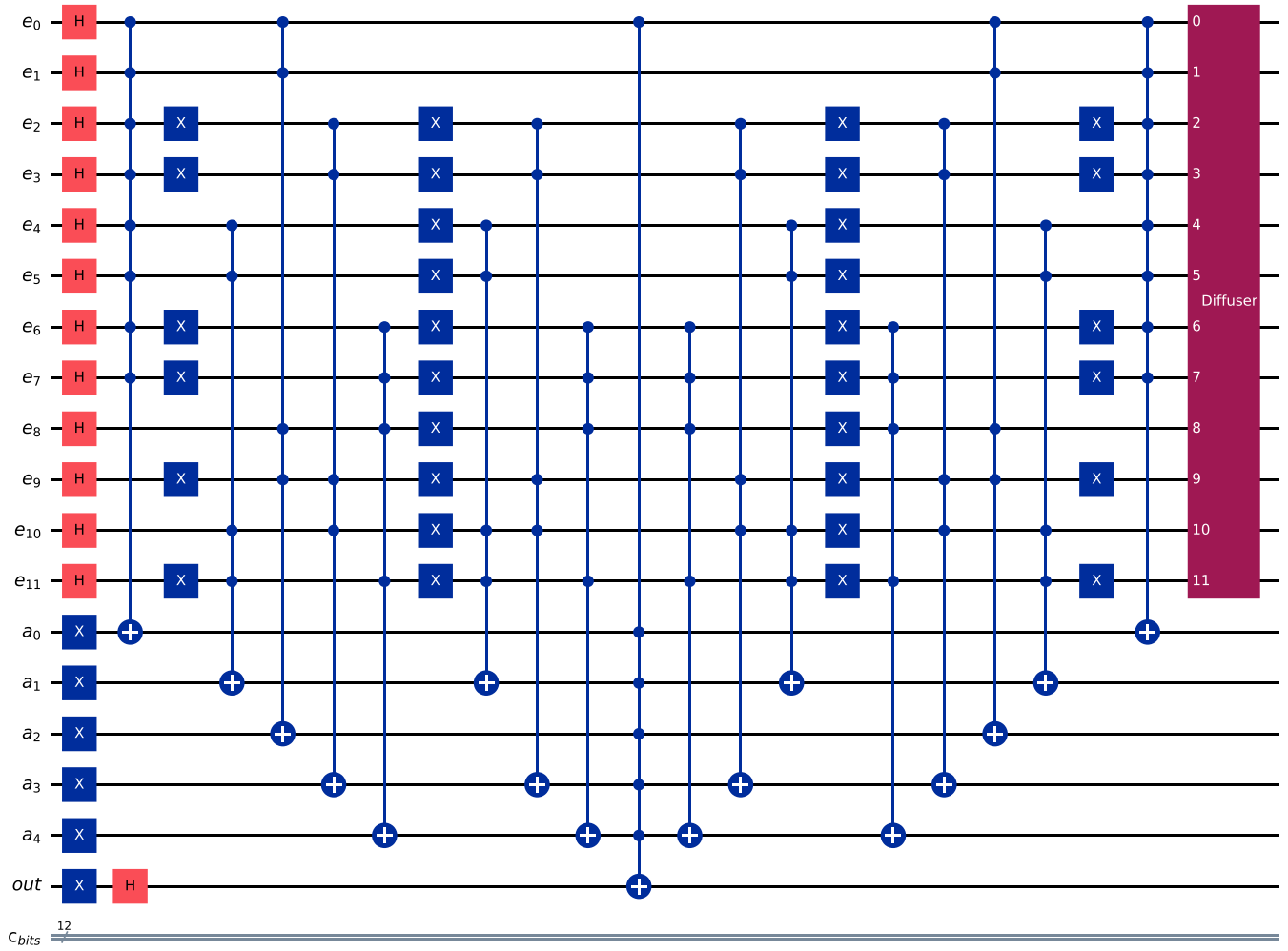


FIG. 11. Quantum circuit for the four-loop topology in Fig. 9(c). The output is 1199 causal configurations out of 4096 states.

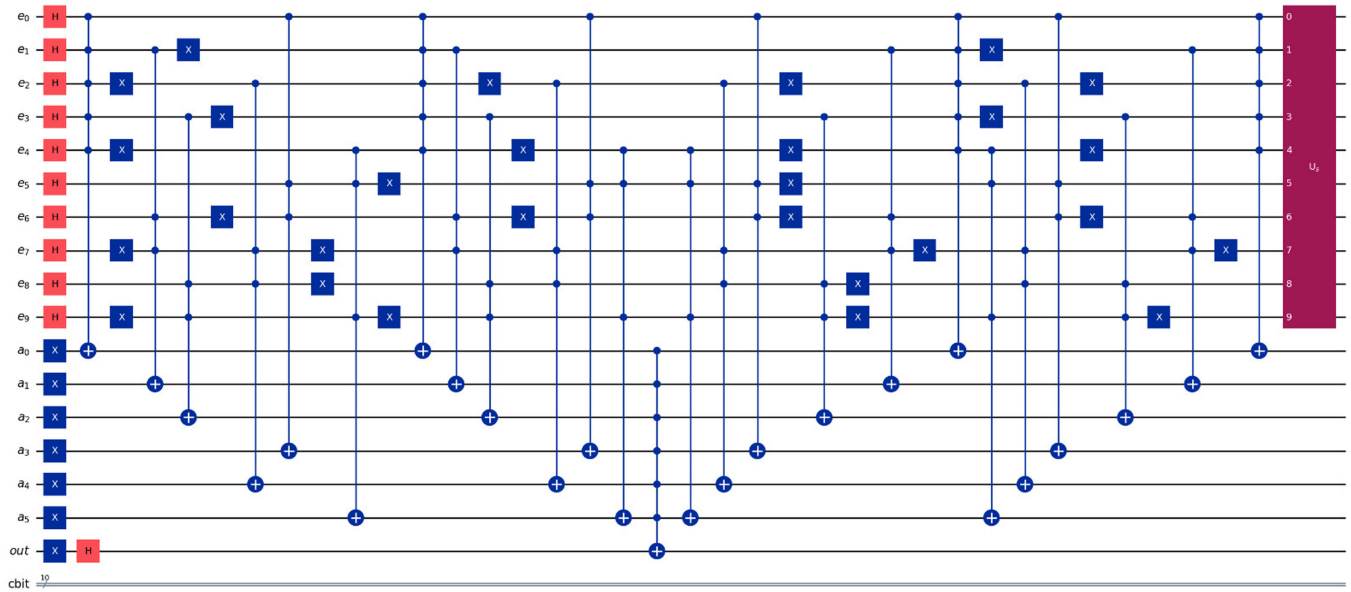


FIG. 12. Quantum circuit for the five-loop topology with one edge per line shown in Fig. 9(e). The output is 240 causal configurations out of 1024 states.

TABLE VII. Key metrics for the transpilation of the quantum circuit corresponding to the four-loop topology of Fig. 9(e) in different quantum devices for the binary-clause (BC) and multicontrolled Toffoli (MCX) algorithms.

Quantum device (qubits)	Five-loop topology, Fig. 9(e)			
	Transpiled quantum depth		Two-qubit gates	
	BC	MCX	BC	MCX
ibm_brisbane (127)	10745	13008	3629	4377
ibm_kyiv (127)	12410	13909	3629	4377
ibm_sherbrooke (127)	12485	13281	3629	4377

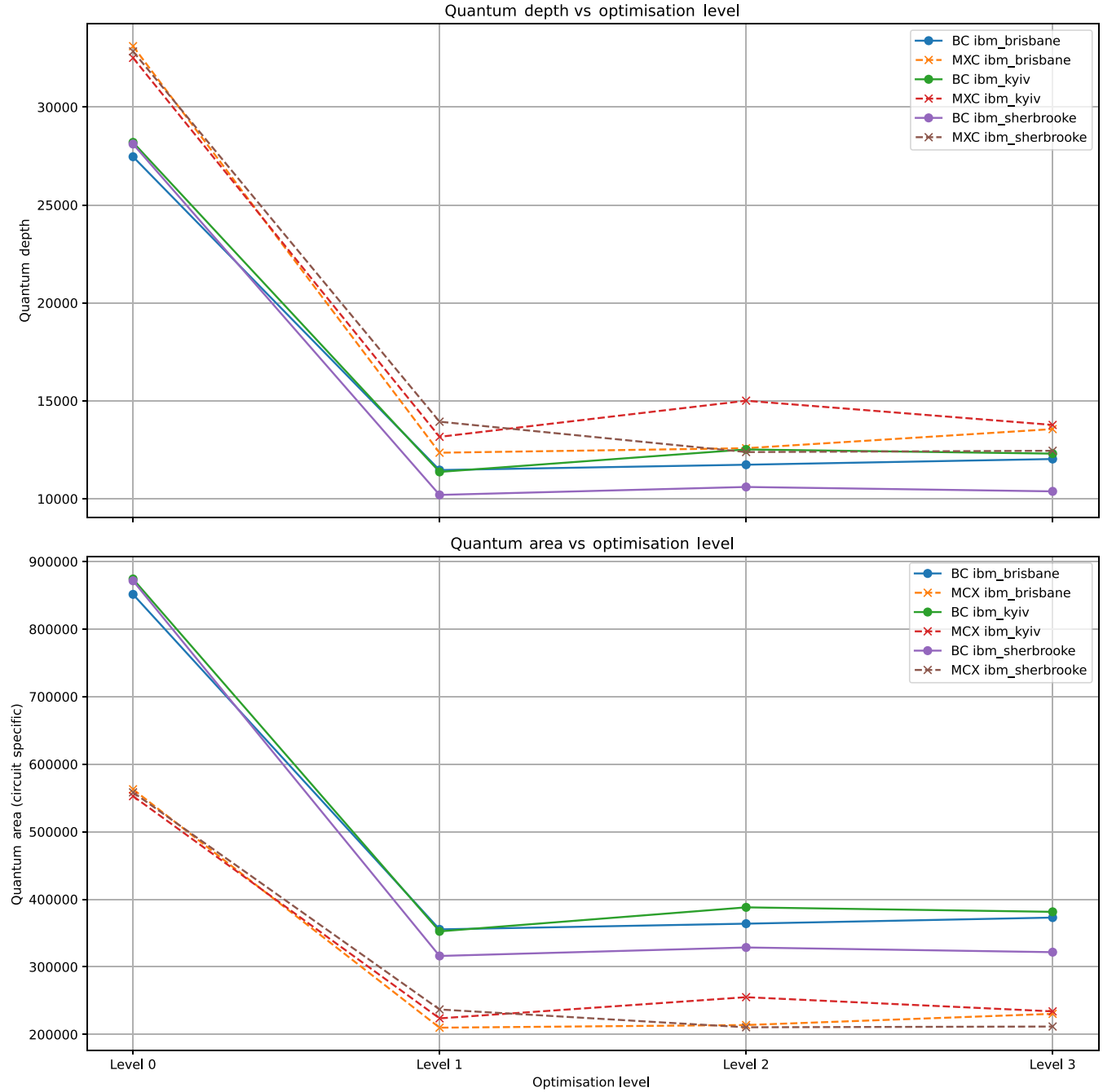


FIG. 13. Quantum circuit depth (upper plot) and quantum circuit area (bottom plot) for the five-loop topology of Fig. 9(e) in terms of optimization levels for the transpilation. The solid lines represent the transpilation of the BC quantum algorithm and the dashed lines represent the transpilation for the MCX.

Continuing the analysis of the five-loop topology we follow with the study of the transpiled quantum circuit depth for relevant metrics in different quantum backends, both simulated and real quantum hardware, as shown in Table VII. The transpiled quantum circuit depth is larger and requires more two-qubit gates for the multicontrolled Toffoli algorithm than for the binary-clause algorithm.

As mentioned in the previous section, to provide a more appropriate assessment of the complexity of the algorithm we use the quantum circuit area considering both, the transpiled quantum depth and qubit usage. In Fig. 13 we present the transpiled quantum circuit depth and the transpiled quantum circuit area as a function of the optimization levels on different quantum hardware, noting comparable results with the four-loop topology. It shows a similar evolution in terms of the optimization levels, and despite having a transpile quantum depth higher for the MCX algorithm, the quantum circuit area is smaller compared to the BC algorithm.

In addition, the simulations revealed a significant difference in execution time and resource consumption. The time taken in the ideal simulation in Qiskit (noiseless) was around 165 seconds for the BC algorithm and less than 0.1 seconds for the MCX algorithm. The BC algorithm simulation fully utilizes the computer processor (100% CPU load on an Intel i7 processor, running Qiskit local on a Linux operating system) and consumed $\sim 90\%$ of the available 64 GB RAM, pushing the limits of the quantum simulator. In contrast, the MCX algorithm simulation was executed with significantly fewer resources.

VI. CONCLUSIONS

We have presented an efficient and systematic quantum algorithm for identifying the causal configurations for multiloop Feynman diagrams, which is equivalent to querying DAG configurations of undirected graphs in graph theory. The approach presented in this paper defines an oracle operator using only multicontrolled Toffoli gates and NOT (Pauli- X) gates simplifying the design and encoding of the quantum circuits. Furthermore, it allows us to significantly reduce the total number of qubits required and the theoretical quantum circuit depth with respect to a binary-clause algorithm.

We have also analyzed the quantum complexity of the transpiled quantum circuits. In this case, the quantum circuit area is the most appropriate metric to assess the

complexity of the quantum algorithm due to the fact that jointly evaluates the number of qubits and the transpiled quantum depth. The quantum circuit area of the proposed algorithm is smaller than that of the BC algorithm, despite having a greater transpiled quantum circuit depth. The substantial reduction in qubit count and quantum circuit area directly translates into significantly lower RAM usage and computational cost required for classically simulating the quantum circuits, as explicitly showed for the five-loop topology in Sec. VC. The reduction in the required number of qubits has allowed us to explore complex multiloop topologies using the IBM Quantum platform that would otherwise be inaccessible; in particular, we have explicitly implemented three loops with six and nine vertices, four loops with twelve and sixteen vertices, and five loops with a five point interaction and ten edges, successfully identifying their causal configurations.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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