Asymptotically Improved Grover’s Algorithm in any Dimensional Quantum System with Novel Decomposed \( n \)-qudit Toffoli Gate

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Abstract

As the development of Quantum computers becomes reality, the implementation of quantum algorithms is accelerating in a great pace. Grover’s algorithm in a binary quantum system is one such quantum algorithm which solves search problems with numeric speed-ups than the conventional classical computers. Further, Grover’s algorithm is extended to a \( d \)-ary quantum system for utilizing the advantage of larger state space. In qudit or \( d \)-ary quantum system \( n \)-qudit Toffoli gate plays a significant role in the accurate implementation of Grover’s algorithm. In this paper, a generalized \( n \)-qudit Toffoli gate has been realized using qudits to attain a logarithmic depth decomposition without ancilla qudit. Further, the circuit for Grover’s algorithm has been designed for any \( d \)-ary quantum system, where \( d \geq 2 \), with the proposed \( n \)-qudit Toffoli gate so as to get optimized depth as compared to state-of-the-art approaches. This technique for decomposing an \( n \)-qudit Toffoli gate requires access to higher energy levels, making the design susceptible to leakage error. Therefore, the performance of this decomposition for the unitary and erasure models of leakage noise has been studied as well.

1 Introduction

The proliferation of quantum algorithms is gradually grabbing the eye of researchers. Quantum computers are available for physical implementation, hence researchers are more interested towards working on it. Computationally hard problems can be promisingly deciphered using quantum algorithms [1]. Grover’s algorithm [2] is a good case in point in quantum algorithms. It is a searching algorithm to search data from an unstructured database, which gives quadratic speed-ups as compared to the classical counterparts.

Classical computers are designed on transistors, which deals with binary bits at the physical level. For this, quantum computers are also designed to deal with qubit technology for its simplicity. Albeit, the fundamental physics behind the quantum system is not inherently binary, on the contrary, quantum system can have an infinite arity of discrete energy levels. In reality, the limitation lies in the fact that we need to control the system as per our needs. Hence, including additional discrete energy levels will help us realize the qudit technology quite comprehensively, which makes the system more flexible with data storage and helps in faster processing of quantum information.

In this work, we extend Grover’s algorithm to any dimension, hence comes the concept of qudit. Qudit technology is that quantum technology, which deals with \( d \)-ary quantum system, where \( d \geq 2 \) [3]. For providing larger state space, simultaneous multiple control operations, we graduate to qudits which eventually reduce the circuit complexity and aggrandize the efficiency of quantum algorithms [4] [5] [6]. For example, \( N \) qubits can be expressed as \( \sum_{i=0}^{N} i \) qudits, which straightway ushers to \( \log_{d} d \)-factor in run-times [7] [8]. However, this decomposition technique requires the system to occasionally access states outside the computational space. This is an engineering challenge, and makes the system particularly susceptible to leakage error [9] [10]. We have, therefore, shown the effect of erasure and unitary leakage model on this decomposition. The \( d \)-ary quantum computing system can be effectuated on various physical technologies, for instance continuous, spin systems [11] [12], nuclear magnetic resonance [13] [14], photonic systems [15], ion trap [16], topological quantum system [17] [18] [19] and molecular magnets [20].
In this paper, we have designed an efficient quantum circuit for Grover’s algorithm using the proposed novel decomposed \( n \)-qudit Toffoli gate \[21\]. For physical implementation of \( n \)-qudit Toffoli gate, it is of utmost importance to decompose it into one-qudit and/or two-qudit gates. In \[22\], authors have proposed a qubit-qurit approach to decompose generalized Toffoli gate, which we have extended for \( n \)-qudit Toffoli decomposition with the use of \(|d\rangle\) and \(|d+1\rangle\) quantum state as temporary storage, which is a novel approach as optimized depth has been achieved. Simply by adding a discrete energy level, we can easily have the higher dimension quantum state for temporary use, as these are present only in intermediate states in \( d \)-ary quantum system or qudit system. However, input and output states are qudits, only in the intermediate operations, we introduce the \(|d\rangle\) and \(|d+1\rangle\) quantum state of \( d+2 \)-ary quantum system without hampering the operation of initialization and measurement on physical devices. By introducing this \( d+2 \)-ary quantum system, the constraint of arity specific Toffoli decomposition can be avoided. To the best of our knowledge, it is a first of its kind approach. Our novelty lies in the fact that:

- We propose a novel technique to decompose generalized \( n \)-qudit Toffoli gate with logarithmic depth with no-ancilla qudit.
- As an example, we show 8-qubit Toffoli (\( C_7^{\text{NOT}} \)) gate realization and a comparative study depicts that our approach is better than the existing approaches in terms of a constant factor of gate cost reduction.
- We also design a circuit for Grover’s algorithm for any \( d \)-ary quantum system using proposed decomposed \( n \)-qudit Toffoli gate so that we can reduce the logarithmic factor in time complexity of Grover’s algorithm.
- We have studied the performance of this decomposition technique for the erasure and unitary model of leakage error. However, any probable noise mitigation techniques are postponed for future work.

The structure of this paper is as follows. Section 2 describes the universal qudit gates. Section 3 defines Grover’s algorithm in \( d \)-ary quantum system. Section 4 illustrates the decomposition of the proposed \( n \)-qudit Toffoli gate and the comparative analysis. The performance of this decomposition under leakage noise has been studied in Section 5. Section 6 describes our conclusions.

2 Generalized Qudit Gates

A qudit is the unit of quantum information for \( d \)-ary quantum system \[23, 24\]. Qudit states can be expressed by a vector in the \( d \) dimensional Hilbert space \( \mathcal{H}_d \) \[7, 25\]. The vector space is the span of orthonormal basis vectors \( \{|0\rangle, |1\rangle, |2\rangle, \ldots, |d-1\rangle\} \). The general form of qudit state can be described as

\[
|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle + \alpha_2 |2\rangle + \cdots + \alpha_{d-1} |d-1\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_{d-1} \end{pmatrix}
\]

where \( |\alpha_0|^2 + |\alpha_1|^2 + |\alpha_2|^2 + \cdots + |\alpha_{d-1}|^2 = 1 \) and \( \alpha_0, \alpha_1, \ldots, \alpha_{d-1} \in \mathbb{C}^d \). An overview of generalized qudit gates is presented in this section. This generalisation can be defined as discrete quantum states of any arity \[26\]. Unitary qudit gates \[27, 28\] usually need to be applied on qudits to modify the quantum state of a quantum algorithm \[29\]. To synthesize Grover’s algorithm in \( d \)-ary quantum system, one needs to consider one-qudit generalized gates such as NOT gate (\( X_d \)), phase-shift gate (\( Z_d \)), Hadamard gate (\( F_d \)), two-qudit generalized CNOT gate (\( C_\times,d \)) and Generalized \( n \)-qudit Toffoli gate(\( C_n^X,d \)) as basic requirements. All the mentioned gates are described as follows:

2.1 Generalized NOT Gate

\( X_d \) is the generalized NOT or increment gate of binary NOT gate in a \( d \)-ary quantum system \[30\]. The \((d \times d)\) matrix representation of \( X_d \) is as follows:
\[
X_d = \begin{pmatrix}
0 & 0 & \ldots & 0 & 1 \\
1 & 0 & \ldots & 0 & 0 \\
0 & 1 & \ldots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & 1 & 0
\end{pmatrix}
\]

### 2.2 Generalized Phase-Shift Gate

\( Z_d \) is the generalized phase-shift gate of binary phase-shift gate \( Z \) in a \( d \)-ary quantum system [30]. The \((d \times d)\) matrix representation of \( Z_d \) is as follows:

\[
Z_d = \begin{pmatrix}
1 & 0 & 0 & \ldots & 0 \\
0 & \omega & 0 & \ldots & 0 \\
0 & 0 & \omega^2 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & \omega^{d-1}
\end{pmatrix}
\]

### 2.3 Generalized Hadamard Gate

\( F_d \) is the generalized quantum Fourier transform or generalized Hadamard gate of binary Hadamard gate [6, 31] in \( d \)-ary quantum system, which helps in preparing superposition of input basis states in Grover’s algorithm. The \((d \times d)\) matrix representation of \( F_d \) is as follows:

\[
F_d = \begin{pmatrix}
1 & 1 & 1 & \ldots & 1 \\
1 & \omega & \omega^2 & \ldots & \omega^{d-1} \\
1 & \omega^2 & \omega^4 & \ldots & \omega^{2(d-1)} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & \omega^{d-1} & \omega^{2(d-1)} & \ldots & \omega^{(d-1)(d-1)}
\end{pmatrix}
\]

### 2.4 Generalized CNOT Gate

In a binary quantum system, quantum entanglement can be achieved by the use of a CNOT gate, which is a phenomenal property of quantum mechanics. For \( d \)-ary quantum systems, we need to generalise the binary 2-qubit controlled NOT gate to the \text{INCREMENT} gate: \text{INCREMENT} \ket{x} \ket{y} = \ket{x} \ket{(x + y) \mod d}, \text{iff } x = d - 1 [32]. In the next subsection, we extend this generalized CNOT or \text{INCREMENT} further to operate over \( n \) qubits as a generalized \( n \)-qubit Toffoli gate for generalising Grover’s algorithm in a \( d \)-ary quantum system. The \((d^2 \times d^2)\) matrix representation of the generalized CNOT gate is as follows:

\[
C_{X,d} = \begin{pmatrix}
I_d & 0_d & 0_d & \ldots & 0_d \\
0_d & I_d & 0_d & \ldots & 0_d \\
0_d & 0_d & I_d & \ldots & 0_d \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0_d & 0_d & 0_d & \ldots & X_d
\end{pmatrix}
\]

where \( I_d \) and \( 0_d \) are both \( d \times d \) matrices as shown below:

\[
I_d = \begin{pmatrix}
1 & 0 & 0 & \ldots & 0 \\
0 & 1 & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 1 & \ldots & 0 \\
0 & 0 & 0 & \ldots & 1
\end{pmatrix}
\]
2.5 Generalized $n$-qudit Toffoli Gate

A generalized $n$-qudit Toffoli gate $[21]$ is a generalisation of the generalized CNOT gate. Let us consider $n$-qudit Toffoli gate as $C_{X,d}^n$, such that the target qudit is incremented by 1 (mod $d$) only when all $n-1$ control qudits have value $d-1$. The $(d^n \times d^n)$ matrix representation of generalized $n$-qudit Toffoli gate is as follows:

$$C_{X,d}^n = \begin{pmatrix}
I_d & 0_d & 0_d & \ldots & 0_d \\
0_d & I_d & 0_d & \ldots & 0_d \\
0_d & 0_d & I_d & \ldots & 0_d \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0_d & 0_d & 0_d & \ldots & X_d
\end{pmatrix}$$

Due to technology constraints, a multi-controlled Toffoli gate can be replaced by an equivalent circuit comprising one-qudit and/or two-qudit gates, albeit at first, this has to be decomposed into a set of Toffoli gates for any dimensional quantum system $[33]$. In Figure 1, we have shown an example of the state-of-the-art approach of decomposition of an 8-qubit Toffoli gate with the help of an intermediate qutrit state $[34]$. Their equivalent circuit temporarily stores information directly in the qutrit $|2\rangle$ state of the controls. For circuit representation, we have used a circle to represent the control and rectangle to represent the target. As shown in Figure 1 for a Toffoli gate, we have used ‘1’ in the control circle to represent two qubit controls and '+' in the target box to represent the increment operator. This decomposed circuit can be treated as a binary tree of gates which establishes the logarithmic depth for a multi-controlled Toffoli gate. It has the property that the intermediate qubit of each sub-tree as well as the root can only be upraised to $|2\rangle$ if all of its seven control leaves are $|1\rangle$. To verify this property, we perceive that the qubit $q_4$ can only become $|2\rangle$ if and only if it was originally $|1\rangle$ and $q_2$ and $q_6$ qubits were previously $|2\rangle$. At the following level of the tree, we see qubit $q_2$ could have only been $|2\rangle$ if it was previously $|1\rangle$ and both $q_1$ and $q_3$s were $|1\rangle$ before and qubit $q_6$ could have only been $|2\rangle$ if it was previously $|1\rangle$ and both $q_5$ and $q_7$ qubits were $|1\rangle$ before. If any of the controls were not $|1\rangle$, the $|2\rangle$ state would fail to move to the root of the tree. Hence, the CNOT gate toggles the target qubit only if all controls are $|1\rangle$. The right half of the circuit is the mirror circuit to restore the control qubits to their original states. They have further decomposed their ternary Toffoli into 13 1-qutrit and 2-qutrit gates for physical implementation $[32]$.

![Figure 1: Decomposition of 8-qubit Toffoli $|34|)](image-url)
The limitation of this work is that it is restricted to binary quantum systems as they have mentioned the use of qutrits only. In our proposed approach we have generalized the decomposition for any dimensional quantum system.

3 Generalized Grover’s Algorithm in \(d\)-ary Quantum System

We address generalized Grover’s algorithm in \(d\)-ary quantum system in detail in this Section. The algorithm has two sub-parts: Oracle and diffusion \([2]\). Grover’s algorithm is a searching method for solving the unstructured database search problem, which can be defined as follows: given a collection of unstructured database elements \(x = 1, 2, \ldots, n\), and an Oracle function \(f(x)\) that acts on a marked element \(s\) as follows,

\[
f(x) = \begin{cases} 1, & x = s, \\ 0, & x \neq s, \end{cases}
\]

Grover’s algorithm finds the marked element in as few calls to \(f(x)\) as possible \([2]\). More in detail, the database is encoded into a superposition of quantum states with each element being assigned to a corresponding basis state. Grover’s algorithm searches over each possible outcome, which is represented as a basis vector \(|x\rangle\) in an \(n\)-dimensional Hilbert space in \(d\)-ary quantum system. Correspondingly, the marked element is encoded as \(|s\rangle\). Thus, after applying unitary operations as oracle function to the superposition of the different possible outcomes, the search can be done in parallel. Then the generalized diffusion operator, which is also known as inversion about the average operator amplifies the amplitude of the marked state to increase its measurement probability using constructive interference, while attenuating all other amplitudes, and searches the marked element in \(O(\sqrt{N})\) steps, where \(N = d^n\).

The circuit diagram for generalized Grover’s algorithm in a \(d\)-ary quantum system is presented in Figure 2. As shown in Figure 2, To perform Grover’s search algorithm in a \(d\)-ary quantum system, at least \(n + 1\) qudits are required. More elaborately, the steps of the Grover’s algorithm are as follows:

**Initialization:** The algorithm starts with the uniform superposition of all the basis states on the \(n\) input qudits in \(|0\rangle\) by incorporating generalized Hadamard or quantum DFT gate. The last ancilla qudit is used as an output qudit which is initialized to \(F_d|d-1\rangle\). Thus, we obtain the \(d\)-ary quantum state \(|a\rangle\):

\[
|a\rangle = F_d^{\otimes n}|0_d\rangle = \frac{1}{\sqrt{d^n}} \sum_{x=1}^{d^n} |x\rangle
\]

**Oracle query:** By phase shift, the oracle \((O_s)\) of Grover search marks the marked state \(|s\rangle\) and keeps other states unaltered through phase shift \(\phi_s\), which can be expressed as:

\[
O_s(\phi_s) = 1 + (e^{i\phi_s} - 1) |s\rangle \langle s|\]

The oracle block \(U_f\) as shown in Figure 2 of Grover’s algorithm depends on the problem instance. One needs to design the oracle using Unitary transformation as per requirement.

**Diffusion operation:** This diffusion operation \((D_a)\) is a reflection about the initial vector \(|a\rangle\) with a phase \(\phi_a\):

\[
D_a(\phi_a) = 1 + (e^{i\phi_a} - 1) |a\rangle \langle a|
\]
The diffusion operator of Grover’s search is generic and not problem specific. As shown in Figure 2, the diffusion operator is initialized with generalized Hadamard ($F^d \otimes |0^n\rangle \langle 0^n| - I_d$) and generalized Hadamard ($F^d \otimes |0^n\rangle \langle 0^n|$) again. The matrix representation of generalized diffusion operator [35] for $d$-ary quantum system is shown below:

$$diff_d = \begin{pmatrix}
\frac{2^d - 1}{2^d} & \frac{2^d}{2^d} & \cdots & \frac{2^d}{2^d} \\
\frac{2^d}{2^d} & \frac{2^d - 1}{2^d} & \cdots & \frac{2^d}{2^d} \\
\cdots & \cdots & \cdots & \cdots \\
\frac{2^d}{2^d} & \frac{2^d}{2^d} & \cdots & \frac{2^d - 1}{2^d}
\end{pmatrix}$$

The generalized circuit for Grover’s diffusion operator in $d$-ary quantum system as shown in Figure 3 can be constructed using generalized Hadamard gate, generalized NOT gate and generalized $n$-qudit Toffoli gate. As discussed in the previous section, to implement Grover’s algorithm in technology specific physical devices, this $n$-qudit Toffoli gate needs to be decomposed using one-qudit or two-qudit gates. While decomposing the $n$-qudit Toffoli gate, if the depth and the ancilla qubits arbitrarily increase then automatically the time complexity of Grover’s algorithm also increases, which is undesirable. In the next subsection, we have shown a novel approach for decomposition of $n$-qudit Toffoli gate with optimized depth as compared to the state-of-the-art. Thus, the time complexity of Grover’s algorithm will also be optimized.

The combination of the oracle and the diffusion gives generalized Grover operator $G$,

$$G = O_s(\phi_s)D_a(\phi_a)$$

We need to iterate this Grover operator $O(\sqrt{N})$ times to get the coefficient of the marked state $s$ large enough that it can be obtained from measurement with probability close to 1 and thus conclude the Grover algorithm.

4 Improved Circuit Design of Grover’s Algorithm in $d$-ary Quantum System

In order to execute Grover’s algorithm on physical quantum devices, it has to be ideally decomposed using single-qudit and/or two-qudit gates. It is important to carry out the effective low depth and low gate count decomposition in near term quantum device and beyond [36].

4.1 Proposed $n$-qudit Toffoli Gate Decomposition

The most important aspect of our proposed work is the decomposition of $n$-qudit $d$-dimensional Toffoli Gate. For this, as an initial step, the understanding of the decomposition of generalized Toffoli Gate is necessary. All the figures below have inputs and outputs as $d$-dimensional qudits, but the states $|d\rangle$ and $|d + 1\rangle$ may be temporarily used during the computation. The idea of keeping $d$-ary input/output enables these circuit constructions to be applied for any already existing $d$-ary qudit-only circuits.

A generalized Toffoli decomposition in $d$-ary system using $|d\rangle$ state is shown in Figure 3. A similar construction for the Toffoli gate in binary using qutrit is evident from previous state-of-the-art work [34], we have extended it for $d$-ary quantum system. The aim is to carry out an $X_d$ operation on the target qudit.
(third qudit) as long as the two control qudits, are both $|d - 1\rangle$. First a $|d - 1\rangle$-controlled $X_{d+1}^{\pm 1}$, where $+1$ and $d + 1$ are used to denote that the target qudit is incremented by 1 (mod $d + 1$), is performed on the first qudit and second qudit. This upgrades second qudit to $|d - 1\rangle$. First a $|d - 1\rangle$-controlled $X_{d+1}^{\pm 1}$, where $+1$ and $d + 1$ are used to denote that the target qudit is incremented by 1 (mod $d + 1$), is performed on the first qudit and second qudit. This upgrades second qudit to $|d - 1\rangle$ if and only if first qudit and second qudits were $|d - 1\rangle$. Then a $|d - 1\rangle$-controlled $X_{d+1}^{\pm 1}$, where $+1$ and $d + 1$ are used to denote that the target qudit is incremented by 1 (mod $d + 1$), is performed on the first qudit and second qudit. This upgrades second qudit to $|d\rangle$ if and only if first qudit and second qudits were $|d - 1\rangle$ as expected. The controls are reinstated to their original states by a $|d - 1\rangle$-controlled $X_{d+1}^{\pm 1}$ gate, which revokes the effect of the first gate. The $|d\rangle$ state from $d + 1$-ary quantum system can be used instead of ancilla to store temporary information, is the important aspect in this decomposition.

![Diagram](image)

**Figure 4: Generalized Toffoli in $d$-ary quantum system**

As in [34], the circuit decomposition of generalized Toffoli gate is realized in terms of ternary Toffoli gate instead of 1-qutrit and 2-qutrit gates in order to obtain lower circuit depth. Even though, during simulation, they decomposed the ternary Toffoli gate into six 2-qutrit and seven 1-qutrit physically implementable quantum gates. We have also followed the similar approach for extending the decomposition of generalized $n$-qudit Toffoli gate in terms of $d + 1$-ary Toffoli gate. But, the approach of further Toffoli decomposition for simulation has not been inherited. Instead, the $d + 1$-ary Toffoli gate has been decomposed into $d + 2$-ary CNOT gates. Let us consider a generalized CNOT gate for $d + 2$-ary quantum system as $C_{X,d+2}^{+1}$, where $+1$ and $d + 2$ are used to denote that the target qudit is incremented by 1 (mod $d + 2$) only when the control qudit value is $d + 1$. The $((d + 2)^2 \times (d + 2)^2)$ matrix representation of the $C_{X,d+2}^{+1}$ gate is as follows:

$$
C_{X,d+2}^{+1} = 
\begin{pmatrix}
I_{d+2} & 0_{d+2} & 0_{d+2} & \cdots & 0_{d+2} \\
0_{d+2} & I_{d+2} & 0_{d+2} & \cdots & 0_{d+2} \\
0_{d+2} & 0_{d+2} & I_{d+2} & \cdots & 0_{d+2} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0_{d+2} & 0_{d+2} & 0_{d+2} & \cdots & X_{d+2}^{+1}
\end{pmatrix}
$$

where $X_{d+2}^{+1}$ and $0_{d+2}$ are both $(d + 2) \times (d + 2)$ matrices as shown below:

$$
X_{d+2}^{+1} = 
\begin{pmatrix}
0 & 0 & \cdots & 0 & 1 \\
1 & 0 & \cdots & 0 & 0 \\
0 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & 0
\end{pmatrix}
$$

$$
0_{d+2} = 
\begin{pmatrix}
0 & 0 & \cdots & 0 & 0 \\
0 & 0 & \cdots & 0 & 0 \\
0 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & 0
\end{pmatrix}
$$

As for example, let there be 8-qudit Toffoli gate as shown in Figure 5(a). Firstly, we decompose it as in [34] as shown in Figure 5(b). Further, we decompose all the $d + 1$-ary Toffoli gate into $(d + 2)$-ary CNOT gates as shown in Figure 5(c) with the help of the proposed decomposition of generalized Toffoli in any dimensional quantum system. As shown in Figure 5(c), all the $d + 1$-controlled Toffoli gates are decomposed into $d - 1$-controlled and $d$-controlled CNOT gates. Similarly, all the $d$-controlled Toffoli gates are decomposed into
$d$-controlled and $d + 1$-controlled CNOT gates. Thus, with the help of $|d\rangle$ and $|d + 1\rangle$ quantum state of $(d + 2)$-ary system, $X_d$ is executed if all the controlled qudits are in $|d - 1\rangle$ state. In this manner, an $n$-qudit Toffoli gate can be decomposed. Now, if we want to realise our approach in binary quantum system, then it could be easily carried out if ququads of quaternary [37] or 4-ary quantum system comes into play. Moreover, we also achieved logarithmic depth and on top of that we reduce the constant factor to 3 from 13, which is thoroughly discussed in the next subsection with the help of an example. By simulation, we have verified our circuits. The simulation result for 8-qubit Toffoli gate, Figure 6(c), is shown in the Appendix. In Table 3 as in Appendix, we have shown the input and output states as well as intermediate states for each time cycle of the circuit for all possible combination of input states $|00000000\rangle$, $|00000010\rangle$, $|00000100\rangle$, ..., $|11111110\rangle$. We have shown that only for the input state $|11111110\rangle$, the output state changes to $|11111111\rangle$, otherwise there is no change of output states for corresponding input states.

4.2 Comparative Analysis

A comparative study of our Toffoli decomposition with some previous works [34, 38, 23, 39, 40, 29, 41] is shown in Table 1. Our work outperforms all of them in terms of depth of the circuit, even the best in the business [34]. We simulate our work taking the conventional Gokhale construction [22] into account, since it is so far the benchmark in the ancilla-free frontier zone. This technique makes the decomposition typically exorbitant in gate count and depth as a large number for constant factor of gate-count is required as compared to our approach. This would be better explained with the following example.

As shown in Figure 6(a), a Multi-controlled Toffoli gate with 7 controls and 1 target is considered. Figure 6(b) depicts the decomposition of the generalized 8-qubit Toffoli gate as shown in Figure 6(a) with the help of Gokhale design [34]. Their circuit temporarily stores information directly in the qutrit $|2\rangle$ state of the controls, so does our approach. However, instead of storing temporary results further with ququads $|3\rangle$ state, they simply decompose their ternary Toffoli into 13 1-qutrit and 2-qutrit gates [32] as mentioned in their paper [34], but in our case, we further decompose ternary Toffoli into three 4-ary CNOT gates using ququads $|3\rangle$ state as control, which is shown in Figure 6(c). This leads to the minimization of the constant factor of gate-count from 13 to 3 for single Toffoli decomposition and our approach becomes qudit generalizable.

Our circuit construction as shown in 6(c), as in the Gokhale design, can also be interpreted as a binary tree of gates. More elaborately, the inputs/outputs are qubits, but we grant inhibition of the $|2\rangle$ and $|3\rangle$ ququads states in between. The circuit maintains a tree structure and has the property that the intermediate qubit, of each sub-tree as well as root can only be upraised to $|2\rangle$ if all of its seven control leaves were $|1\rangle$. To verify this property, we perceive that the qubit $q_1$ can only become $|2\rangle$ if and only if it was originally $|1\rangle$ and qubit $q_6$ was previously $|3\rangle$. At the following level of the tree, we see qubit $q_6$ could have only been $|3\rangle$ if it was previously $|1\rangle$ and both $q_3$ and $q_7$ qubits were $|2\rangle$ before. If any of the controls were not $|1\rangle$, the $|2\rangle$ or $|3\rangle$ states would fail to move to the root of the tree. Hence, the $X$ gate is only carried out if all controls
are $|1\rangle$. The right half of the circuit undergoes computation to get back the controls to their original state. This construction applies more generally to any multi-controlled $U$ gate.

After each succeeding level of the tree structure, the number of qubits under inspection is reduced by a factor of $\sim 2$. This leads to the circuit depth being logarithmic in $n$, where $n$ is the number of controls. On top of that, each ququads is operated on by a small constant number of three gates, so the total number of gates is optimized. Since this is a first of its kind approach for $n$-qudit Toffoli decomposition, so we could not compare it with any other techniques for qudits, hence we have taken $d = 2$ as shown in Figure 6 for establishing our betterment as compare to the state-of-the-art techniques. We have shown 8-qudit Toffoli decomposition but, this can be extended to $n$-qudit also. For $n$-qudit Toffoli decomposition, the maximum number of CNOT gates requires is $3 \cdot n - 5$, which implies that the functional relation between gate count and number of qudit is linear. Thus, we have also shown an example with 16-qudit Toffoli and 32-qudit Toffoli decomposition elaborately in Figure 7 and Figure 8 respectively, mapping the structure to binary tree concept helps in establishing the logarithmic depth claim.

### Table 1: Asymptotic comparison of $n$-controlled gate decomposition.

|                      | This Work | Gokhale [34] | Gidney [40] | He [38] | Barenco [29] | Wang [39] | Lanyon [23], Ralph [41] |
|----------------------|-----------|--------------|-------------|---------|--------------|-----------|-------------------------|
| **Depth**            | $\log_2 n$ | $\log_2 N$   | $n$         | $\log_2 n$ | $n^*$        | $n$       | $n$                     |
| **Ancilla**          | 0         | 0            | Controls are qubits | Controls are qubits | Qubits | Controls are qubits | Target is $d = n$-level qudit |
| **Qudit Types**      | d-ary     | 3            | Binary      | Binary    | Binary       | Ternary   | Binary                  |
| **Generalization**   |           |              |             |           |              |           |                         |

As discussed in the previous section, in $d$-ary quantum system, generalized Grover’s algorithm for search over $N$ unstructured database items require just $O(\sqrt{N})$ iterations of Grover operator, where $N = d^n$ and $d \geq 2$. As discussed earlier, this Grover operator is the combination of the oracle and the diffusion. However in each iteration, Grover search has multi-controlled Toffoli gate in diffusion operator with $M = \lceil \log_d N \rceil$ controls [35]. In simpler words, each of the iterations has $(\log_d N)$-qudit or $n$-qudit Toffoli gate in Grover’s diffusion operator as already discussed in Figure 3. The best known Toffoli decomposition in qudit system [39] specifically in ternary quantum system shows that the depth of the realized circuit is linear, i.e. the depth is $\log_d N$ or $n$. But, our logarithmic depth with very small constant decomposition of $n$-qudit Toffoli gate leads to the reduction of a $\log_2 N$ factor of $n$-qudit Toffoli gate in Grover’s algorithm to $\log_2 \log_d N$ in each iteration. Hence, we reduce a logarithmic factor, i.e. $O(\log_2 \log_d N)$ in Grover search’s time complexity via our $n$-qudit Toffoli decomposition as compared to previous work [35, 42] as shown in Table 2.

### Table 2: Asymptotic comparison of Grover’s algorithm in any $d$-ary QuantumSystem, where $d > 2$.

|                      | This Work | Hunt [42] | Fei [35] |
|----------------------|-----------|-----------|----------|
| **Depth**            | $\log_2 (\log_2 N)$ | $\log_2 N$ | $\log_2 N$ |
5  Action of leakage error on the Toffoli decomposition

A $d$-dimensional quantum system, or qudit, is the span of $\{|0\rangle, |1\rangle, \ldots, |d-1\rangle\}$, called the computational subspace. However, it is an engineering challenge to prepare such a computational subspace. In general, the prepared system is a much larger space of dimension $D$ such that $D = d \oplus d_l$ where $\oplus$ denotes the direct sum. The qudit is embedded in this much larger space, and the excess $d_l$-dimensional subspace, which is the span of $\{|d\rangle, |d+1\rangle, \ldots, |D-1\rangle\}$, is termed as the leakage subspace [9, 10]. The system tends to leak from
the computational subspace to the leakage subspace, i.e. access the higher dimensions, leading to erroneous results. Such leakage is a serious obstacle for reliable computation since normal protection schemes against decoherence [43, 44, 45, 46] is unable to correct such a leakage error [9].

In this work, the generalized qudit Toffoli requires access to the $d + 2$-th dimension. Therefore, the system must be intentionally embedded in a subspace larger than its computational subspace, and the higher dimension is accessed occasionally. Therefore, the risk of leakage is high for such a decomposition. In
the authors have studied the effect of channel noise on ternary Toffoli gate. We show, however, that in the presence of different leakage error models, the proposed decomposition can lead to completely or partially erroneous result.

Let $\mathcal{H}_d$ and $\mathcal{H}_l$ be the Hilbert Space associated with the computational and leakage subspace respectively. The probability of a quantum state $\rho$ to leak out of the computational subspace, also called the leakage rate, under some evolution $\mathcal{E}$ is given by \[ L(\mathcal{E}(\rho)) = Tr\{P_{\mathcal{H}_l}\mathcal{E}(\rho)\} \]

where $P_{\mathcal{H}_l}$ is a projector on the leakage subspace. In other words, the above expression gives the probability of finding the qudit $\rho$ in the leakage subspace after the evolution via a CPTP map $\mathcal{E}$. If the system has not leaked to the leakage subspace, then the expression $Tr\{P_{\mathcal{H}_l}\mathcal{E}(\rho)\}$ would evaluate to 0 due to the projective measurement.

Two typical models of leakage error considers the two scenarios where the system either completely or partially leaks to the leakage subspace. They are mathematically expressed in terms of erasure model and a unitary model respectively. For the sake of simplicity, we shall henceforth consider that the leakage subspace is the span of $\{|d\rangle, |d + 1\rangle\}$, where $d$ is the dimension of the qudit. However, as described henceforth, the dimension of the computation or leakage subspace does not contribute to the effect of these two leakage models. The system, at occasion, is raised to the energy level $\geq d$ for the working principle of the Toffoli gate. Nevertheless, there is a non-zero probability of the system to leak into those higher dimensions spontaneously.

### 5.1 Erasure model of the leakage error

In this model, the system leaks completely into the leakage subspace with probability $p_l$. If $\rho = \sum_{i=0}^{d-1} \alpha_i |\psi_i\rangle \langle \psi_i|$ and $\rho_l = |\psi_D\rangle \langle \psi_D|$ be the states of the original system and the system in the leakage subspace respectively, then under the action of an evolution $\mathcal{E}$ on the quantum state

$$\mathcal{E}(\rho) = (1 - p_l)p + p_l |\psi_D\rangle \langle \psi_D|$$ \tag{3}$$

In Eq. (3), $|\psi_D\rangle \in$ span of $\{|d\rangle, |d + 1\rangle\}$. The depth of the circuit of an n-qudit Toffoli decomposition is $2[log(n)]$, where the first half is for the action of the Toffoli gate, and the second half is to restore the system to its original configuration. Therefore, the probability that the system stays in its computation subspace after the action of the Toffoli gate is $(1 - p_l)^{2[log(n)]}$. Interestingly the decay in probability is not exponential with the number of qudits (due to the $[log(n)]$ power). However, the decay can still be substantial for large $n$.

In our Toffoli decomposition (Fig. 4), a particular qudit $q_c$ is raised to the energy level $d$ (or $d + 1$) if the two corresponding control qudits $q_1^c$ and $q_2^c$ are both in an energy level $d - 1$ (or $d$). Then the corresponding target qudit $q_t$ undergoes addition by 1 (modulo d) if $q_c = |d\rangle$. However, under the erasure model of leakage, it is possible that the qudit $q_c$ creeps to the energy level $d$ or $d + 1$ due to the leakage error. In such a scenario

(i) If the control qudits $q_1^c$ and $q_2^c$ are not in an energy level $d - 1$, even then $q_c$ is in state $d$ (or $d + 1$), and the addition of $+1$ (modulo d) occurs on the qudit $q_t$.

(ii) If the control qudits $q_1^c$ and $q_2^c$ are in an energy level $d - 1$, then $q_c$, which was already in energy level $d$ due to leakage error, is changed to the energy level 0 by the actions of $q_1^c$ and $q_2^c$. Therefore, the action on the target qudit $q_t$ does not take place at all.

Therefore, a leakage error, which is of the form of an erasure model, leads to a completely erroneous outcome of the Toffoli gate. When this decomposition technique of Toffoli gate is applied on an $n$-qudit Grover’s Search algorithm, there are $O(\sqrt{n})$ iterations of the algorithm and the Toffoli gate is applied in each iteration. Therefore the probability of no leakage error in the entire algorithm procedure is $(1 - p_l)^{2[log(n)]} \sqrt{n}$. Fig. 5 shows the probability of no leakage error for various values of $p_l$ and $n$. The probability that the system remains noise-free reduces exponentially with the number of qudits, and the slope of the curve is determined by the probability of leakage error $p_l$. 

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5.2 Unitary model of the leakage error

This model considers a scenario where only the state $|d-1\rangle$ can leak into the immediately higher dimension $|d\rangle$, and the state from leakage subspace can return to the state $|d-1\rangle$. Assuming equal probability of both the processes, the corresponding Hamiltonian is

$$H = \frac{1}{2} (|d\rangle\langle d-1| + |d-1\rangle\langle d|)$$

Therefore, the unitary corresponding to this Hamiltonian is [10]

$$U = \exp(-iHt) = \mathbb{I} - \cos(t/2) (|d-1\rangle\langle d-1| + |d\rangle\langle d|) + \sin(t/2) (|d\rangle\langle d-1| + |d-1\rangle\langle d|)$$

where $t$ is the time duration for which the Hamiltonian is applied. The corresponding Leakage Rate of a quantum state $\rho$, as shown in [10], is

$$L(\rho(t)) = \sin^2(t/2)p_l.$$ (4)

Let us assume a quantum state $\psi = \sum_{i=0}^{d-2} \alpha_i |i\rangle + \alpha_{d-1} |d-1\rangle$, where $\alpha_i \in \mathbb{C}$ and $\sum_{i=0}^{d-1} |\alpha_i|^2 = 1$. If $p_l$ is the leakage probability, then the state changes to

$$\sum_{i=0}^{d-2} \alpha_i |i\rangle + \sqrt{p_l} \alpha_{d-1} |d-1\rangle + \sqrt{1-p_l} \alpha_{d-1} |d\rangle$$.

The leakage rate, according to Eq. 4, is $L(\rho(t)) = \sin^2(t/2)p_l|\alpha_{d-1}|^2$. For Grover’s search algorithm, initially the state is prepared in the equal superposition of the basis states. Therefore, considering $\alpha_{d-1} = \frac{1}{\sqrt{2}}$, we have the leakage rate as

$$L(\rho(t)) = \sin^2(t/2)\frac{p_l}{2}.$$.

However, according to our proposed decomposition technique, each 3-qubit Toffoli is designed using 3 CNOT gates. In current IBM superconductor devices, the average time duration of a single CNOT gate is

Figure 9: Performance of n-qudit Grover’s Search under erasure model of leakage error
930 ns (according to the calibration details of the Melbourne Device). Due to this small time duration of each gate, the leakage error probability of the entire circuit of an \( n \)-qudit Grover’s Search algorithm (for \( n = 50 \)) is negligible.

However, in the scenario that such a unitary model of leakage error occurs, we show next the action of such an error on the execution of the Toffoli gate. We consider the action on a 3-qudit Toffoli, which forms the basis of the \( n \)-qudit Toffoli realization. Consider a general 3-qudit Toffoli gate whose input is of the form

\[
\sum_{i,j=0}^{d-1} \alpha_{i,j} |i,j\rangle |t\rangle
\]

where the first two are the control qudits and \( t \) is the target qudit. The Toffoli gate will change the target only when both the inputs are \( d - 1 \). Here, we show the action of a Toffoli gate on such a superposition.

\[
\sum_{i,j} \alpha_{i,j} |i,j\rangle |t\rangle + \alpha_{d-1,d-1} |d-1,d-1\rangle |t\rangle
\]

\[
\rightarrow \sum_{i,j} \alpha_{i,j} |i,j\rangle |t\rangle + \alpha_{d-1,d-1} |d-1,d\rangle |t\rangle
\]

\[
\rightarrow \sum_{i,j} \alpha_{i,j} |i,j\rangle |t\rangle + \alpha_{d-1,d-1} |d-1,d\rangle |t+1\rangle
\]

\[
\rightarrow \sum_{i,j} \alpha_{i,j} |i,j\rangle |t\rangle + \alpha_{d-1,d-1} |d-1,d-1\rangle |t+1\rangle
\]

In case there is a leakage error, the probability amplitude of the state \( |d-1,d-1\rangle |t\rangle \) changes from \( \alpha_{d-1,d-1} \) to \( p\alpha_{d-1,d-1} \) where \( p \) depends on whether leakage error occurred on single or multiple qudits. Therefore, the probability associated with the correct Toffoli action decreases \( p \) times. Furthermore, some of the states of the form \( |l,d-1\rangle |t\rangle \), where the first qudit can be in any state 0, 1, \ldots, \( d-2 \) (the scenario of \( |d-1,d-1\rangle \) is already discussed), changes to \( |l,d\rangle |t\rangle \). The action of the Toffoli gate will lead the target qubit to change from \( |t\rangle \) to \( |t+1\rangle \).

In other words, the unitary model of leakage error reduces the probability associated with the correct action of the Toffoli gate, and associates some probability of incorrect Toffoli gate action. However, due to its dependency on the time of action, the action of this leakage error model seems to be less severe than that of the erasure model.

### 6 Conclusion

In this work, we have proposed a novel approach to decompose generalized \( n \)-qudit Toffoli gate to 2-qudit gates with logarithmic depth without using any ancilla qudit. We have shown an instance of 8-qudit Toffoli gate decomposition to establish the logarithmic depth as an example. We have shown a comparative study in which it is depicted that our approach is better than the existing state-of-the-art approaches. We have also shown that Grover’s algorithm can be implemented in any \( d \)-ary quantum system with the proposed \( n \)-qudit Toffoli gate so as to get the advantage of optimized depth as compared to state-of-the-art approaches. Using this novel proposed decomposition of \( n \)-qudit Toffoli gate, any quantum algorithm can be optimized that employs generalized Toffoli gate. Finally, we have studied the effect of leakage error on this decomposition technique. Our study shows that the decomposition is more fallible to the erasure model of leakage noise than the unitary model. Nevertheless, for low error probability, the gate can operate with high fidelity. A future scope of this study is to look into resource-efficient noise mitigation techniques to protect the functionality of the Toffoli gate from leakage error.

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A Simulation Results

The simulation result for 8-qubit Toffoli gate, Figure 6(c), is shown in this section. In Table 3, we have shown that only for the input state $|11111110\rangle$, the output state changes to $|11111111\rangle$, which is highlighted in Table 3, otherwise there is no change of output states for corresponding input states. The simulation is carried out on Google Colab platform [47] and the code is available at https://github.com/N-Qudit-Toffoli-Decomposition.
Table 3: Simulation result for 8-qubit Toffoli shown in Figure [6]

| Circuit State | After 1st time cycle | After 2nd time cycle | After 3rd time cycle | After 4th time cycle | After 5th time cycle | After 6th time cycle | After 7th time cycle | Original State | After 8th time cycle |
|---------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|---------------|----------------------|
| 00000000      | 00000000             | 00000000             | 00000000             | 00000000             | 00000000             | 00000000             | 00000000             | 00000000       | 00000000             |
| 00000001      | 00000001             | 00000001             | 00000001             | 00000001             | 00000001             | 00000001             | 00000001             | 00000001       | 00000001             |
| ...            | ...                  | ...                  | ...                  | ...                  | ...                  | ...                  | ...                  | ...            | ...                  |
| 10000111      | 10000111             | 10000111             | 10000111             | 10000111             | 10000111             | 10000111             | 10000111             | 10000111       | 10000111             |
| 10000110      | 10000110             | 10000110             | 10000110             | 10000110             | 10000110             | 10000110             | 10000110             | 10000110       | 10000110             |
| ...            | ...                  | ...                  | ...                  | ...                  | ...                  | ...                  | ...                  | ...            | ...                  |

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