Recursive Construction of Relative Phase Multiple Controlled Toffoli

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Abstract

We propose an efficient construction for multiple controlled-NOT gates that allows for relative phase difference in the output of the gate and uses no additional qubits other than n control bits and one target bit. We employ a recursive construction using three base cases: the phaseless CNOT, the phased Toffoli, and the phased triple controlled-NOT; the latter two are known constructions from previous literature on the subject. To prove its correctness, we use the method of exhaustion, checking all different gate and parameter combinations. Finally, we derive an upper bound on the complexity of our technique and compare it to the recently known construction of complexity $9n + \mathcal{O}(1)$ CNOT gates.

Contents

1 Introduction

The theory of quantum information and quantum computation allows us to exploit the phenomena present in quantum mechanics to solve computational problems that classical computers cannot; at least in theory. To take this theory into practice, among other things, depth of quantum circuits needs to be reduced such that it takes less time to run than the coherence time of the device it is running on. Papers like [Barenco et al., 1995] have proposed ways to write complex unitary gates in terms of simpler unitary gates efficiently.

One of the most commonly used two-qubit gates in quantum computation is the $CNOT$ gate. The $CNOT$ gate has a control and a target qubit, and its action is to flip the target qubit when the control qubit is set to $|1\rangle$. In other words, it performs the operation $CNOT(|a\rangle|b\rangle) = |a\rangle|a \oplus b\rangle$, where $|a\rangle$ is the control and $|b\rangle$ the target. This gate can be extended to the Toffoli gate that acts on three qubits. It has two control qubits and one target qubit, and its actino is to flip the target if the controls are $|11\rangle$.

The Toffoli gate can be further generalized to a gate with n control qubits and still one target qubit. We will denote this gate as C^nX for the rest of the paper. The matrix of CnX is definted as

$$\text{diag}\left\{1, 1, ..., 1, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right\} \tag{1}$$

Our focus is in optimizing the implementing C^nX gates in which a relative phase error can be introduced. Given a unitary U, its relative phase version is a unitary V such that $|u_{i,j}| = |v_{i,j}|$ for all i, j, i.e., the magnitude of all elements of U and V are equal. Thus, the relative phase C^nX is defined as

$$\mathrm{diag}\left\{ z_0, z_1, ..., z_{2^{n+1}-3}, \begin{pmatrix} 0 & z_{2^{n+1}-2} \\ z_{2^{n+1}-1} & 0 \end{pmatrix} \right\} \tag{2}$$

where every $z_i \in \mathbb{C}$ has $|z_i| = 1$.

2 Construction

We build the relative phase-error with no ancillae C^nX gates. Let's call these p-C^nX gates, where n is the number of control bits. Along with the normal CX gates, we use two known p-C^nX as base cases [Maslov, 2016]. These other base cases are $n = 2$ and $n = 3$. Let's take a look at these base constructions. When we have $n = 2$, the corresponding circuit is the following.

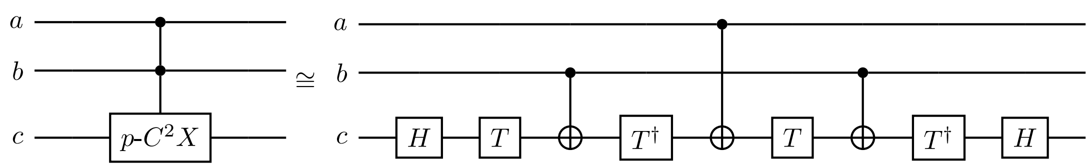

Figure 1: p-C^2X base construction

Where $\cong$ means that the circuit on the right is a relative phase version of the circuit on the left. In the final decomposition and gate count, the circuit in the right is considered. And for $n = 3$ we have the following circuit.

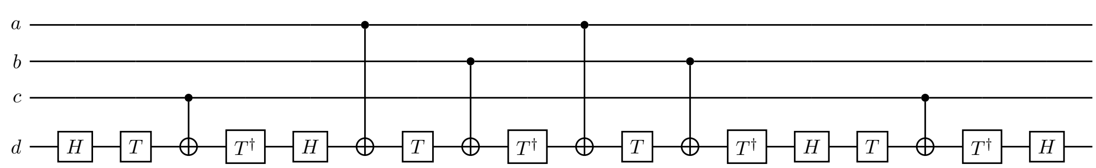

Figure 2: p-C^3X base construction

Notice how C^3X has 3 CX pairs, one on qubit a, one on qubit b, and one on qubit c. Looking at the structure of p-C^3X, we can build p-C^4X by first extending the CX to a C^2X as follows.

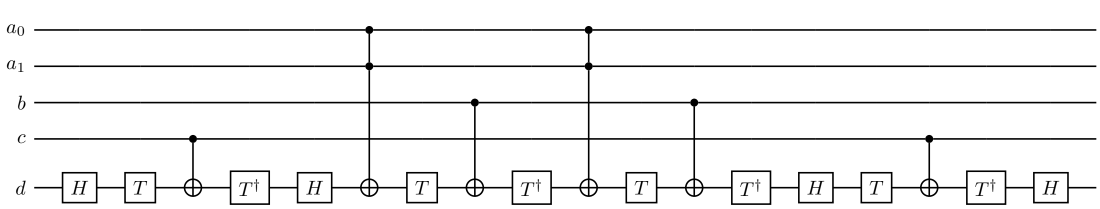

Figure 3: p-C^4X from p-C^3X

Then, we can replace the normal C^2X with the p-C^2X base case shown in Figure 1.

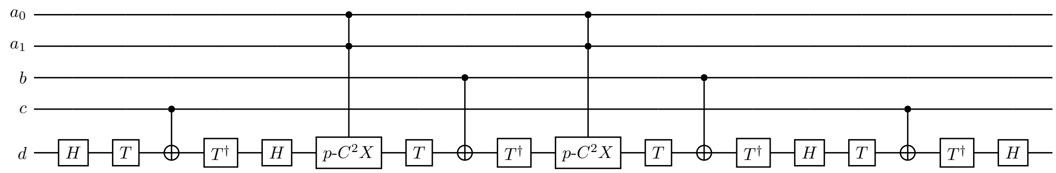

Figure 4: Replacing normal C^2X with p-C^2X

Similarly for p-C^5X, and p-C^6X, we can again extend the CX pairs into C^2X from the $n = 3$ structure, and replace these with p-C^2X. For p-C^7X, p-C^8X, and p-C^9X, we repeat the same process as above, however this time extend the CX pairs into C^3X, and replace these with p-C^3X. For p-$C^{10}X$, p-$C^{11}X$, and p-$C^{12}X$, we extend the CX pairs into C^4X, and replace these with the p-C^4X gates that we previously built.

Overall, to build an arbitrary p-C^nX where $n > 3$, extend the a qubit CX pairs to $C^{\lceil \frac{n}{3} \rceil}X$, the b qubit CX pairs to $C^{\lfloor \frac{n}{3} \rfloor}X$, and the c qubit CX pairs to $C^{(n-\lceil \frac{n}{3} \rceil - \lfloor \frac{n}{3} \rfloor)}X$. We repeat the process until all the gates decompose to the gates in the base cases. At the end, we repeat these gates with their corresponding phase gates.

3 CX count

For an arbitrary C^nX, we will denote the cost of building such gate as the number of CX gates used. This cost depends on the cost of p-$C^{\lceil \frac{n}{3} \rceil}X$, p-$C^{\lfloor \frac{n}{3} \rfloor}X$ and p-$C^{(n-\lceil \frac{n}{3} \rceil - \lfloor \frac{n}{3} \rfloor)}X$. We aim to provide a strict bound for the growth of this cost with respect to number of control qubits, n.

The growth of the gate depends on the transition difference when we extend one of these gates by one control bit, like shown in Figure 3. Let the first difference be defined as the cost of transition between p-$C^{n-1}X$ to p-C^nX.

$$\text{first diff. at } n = \text{cost}(p\text{-}C^nX) - \text{cost}(p\text{-}C^{n-1}X) \tag{3}$$

Let the second difference be defined as the difference in of transition cost from p-C^nX to p-$C^{n+1}X$ and transition cost from p-$C^{n-1}X$ to p-C^nX.

$$\text{second diff. at } n = \big(\text{cost}(p\text{-}C^{n+1}X) - \text{cost}(p\text{-}C^nX)\big) - \big(\text{cost}(p\text{-}C^nX) - \text{cost}(p\text{-}C^{n-1}X)\big) \tag{4}$$

If we look at the data (attached in appendix A), we see that the second difference is zero when the transition cost of p-C^nX to p-$C^{n+1}X$ is equal to that of p-$C^{n-1}X$ to p-C^nX. As n increases, the second difference presents itself in sequences of 0s. For each value of $n \geq 4$, the ith sequence that governs the second difference at n is defined by $i = \lfloor \log_3(n-1) \rfloor$. These sequence comes in pairs, where each ends in a second difference of 2^i and each has length 3^i where i refers to the ith sequence of 0.

We can estimate the average second difference of each sequence by diving the 2^i value at the end of the sequence by length of the sequence. We can use this fact to find the average second difference centered at n.

$$\text{average second diff. of the } i\text{th sequence} = \left(\frac{2}{3}\right)^i \tag{5}$$

$$= \left(\frac{2}{3}\right)^{\lfloor \log_3(n-1) \rfloor} = \text{average second diff. at } n \tag{6}$$

Let's define a continuous function $u(x)$ that serves as an upper bound of $f(n) = \left(\frac{2}{3}\right)^{\lfloor \log_3(n-1) \rfloor}$. Since $f(n)$ contains the floor function, we need to multiply by a constant factor when removing the floor to get an upper bound. Thus, $u(x) = \frac{3}{2}\left(\frac{2}{3}\right)^{\log_3(x+2)}$.

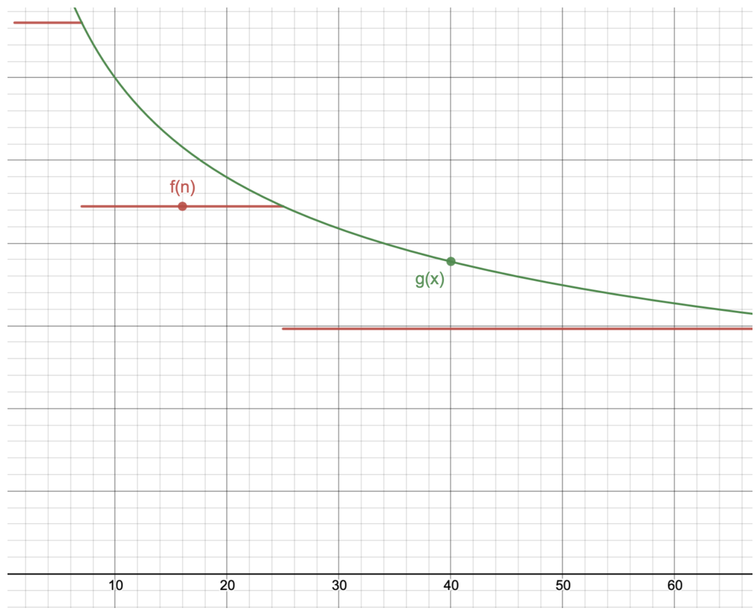

Figure 5: Graph showing that $u(x)$ (denoted as $g(x)$) is an upper bound of $f(n)$

Recall that $u(x)$ is the continuous upper bound of the average second difference of the cost when centered at n. Since $u(x)$ is strictly decreasing, $u(x)$ is also the upper bound of the second derivative of the continuous cost function at n. Let us define this cost function as $y(x)$.

As $\lim_{x\to\infty} u(x) = 0$, we can bound $u(x)$ from above by a non-zero constant α such that $\Theta(\alpha) > \Theta(u(x))$. This implies that

$$\Theta(\alpha) > \Theta(y''(x)) \tag{7}$$

Integrating the inequality twice, we get

$$\Theta(x^2) > \Theta(y(x)) \tag{8}$$

And thus, we have a tight upper bound on the growth of our cost function. It is sub-quadratic.

The exact complexity, however, is a bit harder to find. By trial and error we found that the function $x^{\log_3(6)}$ approximates the actual data very well, with an uncertainty of about $\pm 320\, CX$ or $\pm 2\%$ for the first 400 values of n.

4 Naive comparison to the $9n + \mathcal{O}(1)$ construction

We compare the performance of our technique to the $3n + \mathcal{O}(1)$, where n is the number of Toffoli gates, technique outlined by Craig Gidney in [Gidney, 2021]. Since the $3n + \mathcal{O}(1)$ is in terms of the Toffoli (C^2X) gates, we multiply by a factor of 3 when converted to CX using the p-C^2X gates. After doing this, we are dealing with a complexity of $9n + \mathcal{O}(1)$.

Here, let's assume that gates of both techniques are interchangeable in applications, so we can compare them directly without considering any other constant factors. Provided in the post is an example of a 10-control bits gate. This gate is made up of 16 p-C^2X (each cost $3\, CX$) and $3\, C^2Z($ each cost $6\, CX)$ for a total of $66\, CX$ gates. Using point-slope form, we have the regression line $y = 9(n - 10) + 66$, where y is the number of CX gates used.

We can see from Figure 6 that the cost of our technique is superior to that of the $9n + \mathcal{O}(1)$ technique up until $n = 27$. It is to be seen how much more or how many fewer cases our technique is useful in specific applications.

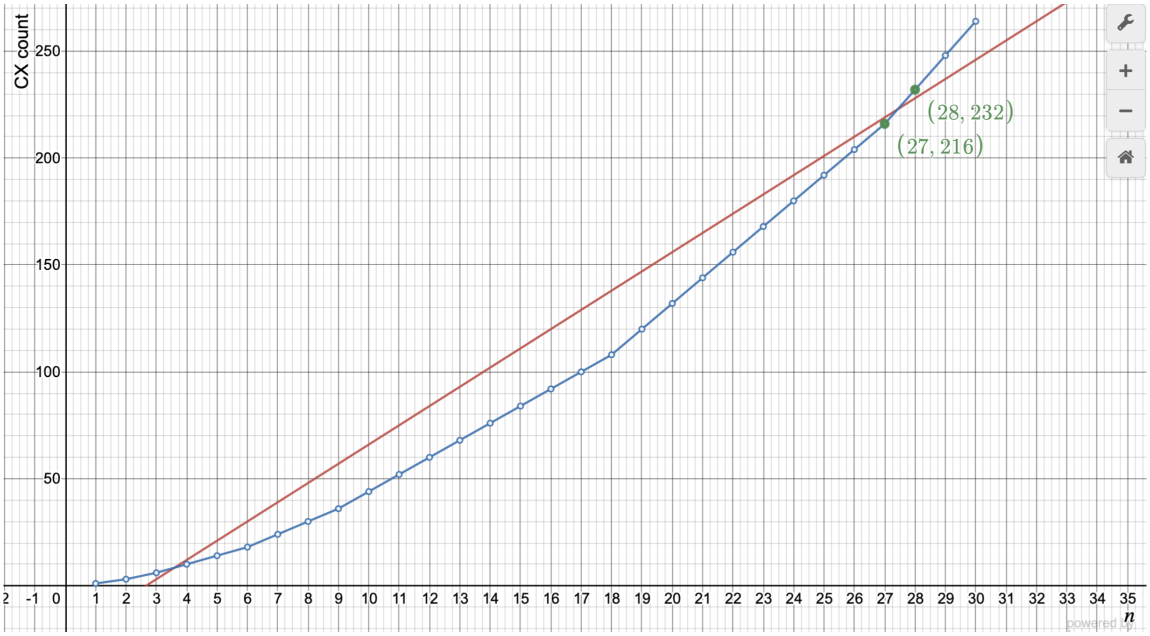

Figure 6: Red: growth of the $3n + \mathcal{O}(1)$ technique. Blue: growth of our technique.

5 Applications in Phaseless Circuits

Recall that our relative phase C^nX is defined as the following matrix.

$$p\text{-}C^nX = \text{diag}\left\{ z_0, z_1, ..., z_{2^{n+1}-3}, \begin{pmatrix} 0 & z_{2^{n+1}-1} \\ z_{2^{n+1}-2} & 0 \end{pmatrix} \right\} \tag{9}$$

By [Maslov, 2016], this can also be written as a product of a phased-diagonal matrix D^n and the phaseless Toffoli.

$$p\text{-}C^nX = D^n(C^nX), \tag{10}$$

where $D^n := \text{diag}\{z_0, z_1, ..., z_2^{n+1} - 2, z_2^{n+1-1}\}$. Since $p\text{-}C^nX$ is a unitary matrix, it follows that its inverse is its conjugate transposed.

$$\left(p\text{-}C^nX\right)^{-1} = \left(p\text{-}C^nX\right)^{\dagger} \tag{11}$$

Thus, we can see that $\left(p\text{-}C^nX\right)^{\dagger}$ is also a relative phase C^nX.

$$\left(p\text{-}C^nX\right)^{\dagger} = \text{diag}\left\{ z_0^*, z_1^*, ..., z_{2^{n+1}-3}^*, \begin{pmatrix} 0 & z_{2^{n+1}-1}^* \\ z_{2^{n+1}-2}^* & 0 \end{pmatrix} \right\} \tag{12}$$

Again, this can be written as

$$\begin{aligned} \left(p\text{-}C^nX\right)^{\dagger} &= C^nX^{\dagger}(D^n)^{\dagger} \\ &= C^nX(D^n)^{\dagger} \end{aligned} \tag{13}$$

Since we know that C^nX is its own inverse.

To construct the $\left(p\text{-}C^nX\right)^{\dagger}$ circuit, we take the original $p\text{-}C^nX$ circuit, and reverse its gate order. Then we substitute all the gates by their inverse. Since H and CX are their own inverse, we only need to perform the replacement $T \longleftrightarrow T^{\dagger}$. Also since this substitution doesn't change the number of gates or gate types, the cost of $p\text{-}C^nX$ and its inverse is identical.

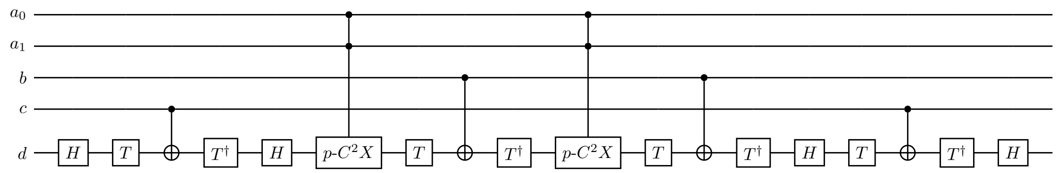

Figure 7: $p\text{-}C^4X$

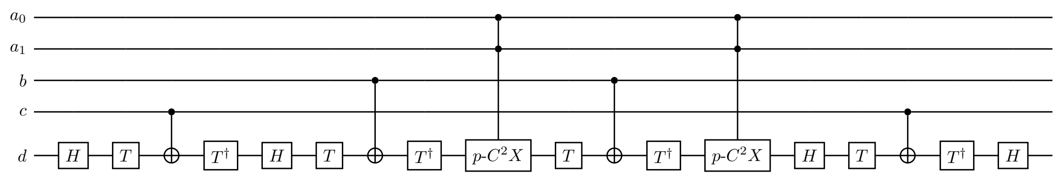

Figure 8: $\left(p\text{-}C^4X\right)^\dagger$. Note that $p\text{-}C^2X$ is its own inverse so we don't need to replace it

When we apply a relative phase C^nX and its inverse consecutively, we get the phaseless identity I. Therefore, we propose the following application. Consider U to be defined as $U : t \to f(t)$.

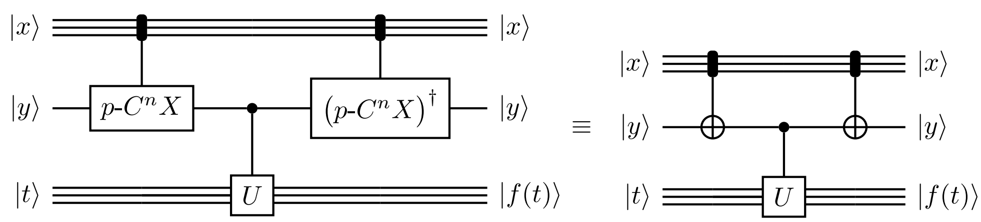

Figure 9: Specific application of relative phase C^nX

Let I be the identity matrix of appropriate size depending on the context and $\oplus$ denote addition modulo 2. We can write the effect of the circuit on the right of Figure 9 as

$$((p\text{-}C^nX)^\dagger \otimes I)(I \otimes CU)(p\text{-}C^nX \otimes I)|x\rangle|y\rangle|t\rangle \tag{14}$$

$$= ((p\text{-}C^nX)^\dagger \otimes I)(I \otimes CU)\left[(D^n)|x\rangle \left|y \oplus \prod x_i\right\rangle |t\rangle\right] \tag{15}$$

Recall that D^n is the phase component added by our relative phase C^nX, as shown in (10). Carrying on, we get the following.

$$((p\text{-}C^nX)^\dagger \otimes I)(I \otimes CU)\left[(D^n)|x\rangle \left|y \oplus \prod x_i\right\rangle |t\rangle\right] \tag{16}$$

$$= ((p\text{-}C^nX)^\dagger \otimes I)\left[(D^n)|x\rangle \left|y \oplus \prod x_i\right\rangle \left|\left(y \oplus \prod x_i\right) f(t) + \left(1 \oplus y \oplus \prod x_i\right) t\right\rangle\right] \tag{17}$$

Taking the case in which $|y\rangle = |0\rangle$, we can simplify the equation above to the one below.

$$((p\text{-}C^nX)^\dagger \otimes I)\left[(D^n)|x\rangle \left|\prod x_i\right\rangle \left|\left(\prod x_i\right) f(t) + \left(1 \oplus \prod x_i\right) t\right\rangle\right] \tag{18}$$

$$= (D^n)^\dagger(D^n)|x\rangle \left|\prod x_i \oplus \prod x_i\right\rangle \left|\left(\prod x_i\right) f(t) + \left(1 \oplus \prod x_i\right) t\right\rangle \tag{19}$$

$$= |x\rangle|0\rangle \left|\left(\prod x_i\right) f(t) + \left(1 \oplus \prod x_i\right) t\right\rangle \tag{20}$$

Where $(D^n)^\dagger(D^n) = I$ and $(p\text{-}C^nX)^\dagger(p\text{-}C^nX) = I$. The state in the third register will take on $|f(t)\rangle$ if and only if all qubits in register $|x\rangle$ are in state $|1\rangle$ and will stay on $|t\rangle$ otherwise, which is the effect we intended to get. Also note that the controlled U gate showed in 9 cannot have any effect on $|y\rangle$.

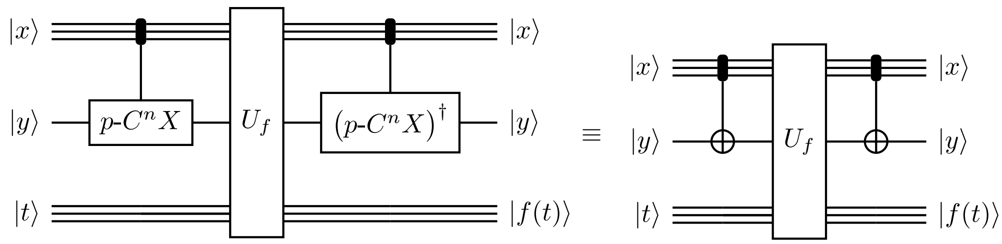

Figure 10: Generalized application of relative phase C^nX

The circuit shown in Figure 9 can be generalized to the one shown in Figure 10. The overall action of the left circuit on the input state $|x, y, t\rangle$ is defined by

$$\big[(p\text{-}C^nX)^\dagger \otimes I^m\big]U_f\big[(p\text{-}C^nX) \otimes I^m\big]\,|x, y, t\rangle \tag{21}$$

Using the alternative representation from (9) and (12), we can rewrite the above expression as

$$\begin{aligned}&\big[C^nX(D^n)^\dagger \otimes I^m\big]U_f\big[(D^n)C^nX \otimes I^m\big]\,|x, y\rangle\,|t\rangle &(22)\\ &\quad= \big[C^nX(D^n)^\dagger \otimes I^m\big]U_f\big[(D^n) \otimes I^m\big]\,\Big|x, y \oplus \prod x, t\Big\rangle &(23)\end{aligned}$$

The overall action of the right circuit is equivalent to that of the left and is given by

$$\begin{aligned}\big[C^nX \otimes I^m\big]U_f\big[C^nX \otimes I^m\big]\,|x, y\rangle\,|t\rangle &= \big[C^nX \otimes I^m\big]U_f\big[C^nX\,|x, y\rangle \otimes I^m\,|t\rangle\,\big] &(24)\\ &= \big[C^nX \otimes I^m\big]U_f\,\Big|x, y \oplus \prod x, t\Big\rangle &(25)\end{aligned}$$

By definition, both give the output $|x, y \oplus \prod x, f(t)\rangle$. So by comparing the two circuits, we get the equality

$$\big[C^nX \otimes I^m\big]\big[(D^n)^\dagger \otimes I^m\big]U_f\big[(D^n) \otimes I^m\big]\,\Big|x, y \oplus \prod x, t\Big\rangle = \big[C^nX \otimes I^m\big]U_f\,\Big|x, y \oplus \prod x, t\Big\rangle \tag{26}$$

By canceling the common factor $\big[C^nX \otimes I^m\big]$ from both sides, we derive a meaningful constraint for U_f that allows it to operate between two relative phase C^nX without evoking any of their drawbacks, namely unwanted phase or bit flips in registers $|x\rangle$ and $|y\rangle$. In all cases, U_f satisfies

$$\big[(D^n)^\dagger \otimes I^m\big]U_f\big[(D^n) \otimes I^m\big] = U_f \tag{27}$$

The circuit acts in a way that leaves the input state $|x\rangle\,|y\rangle$ unaffected. In fact, many circuit constructions have this structure. Most notably, the quadratic multiple-controlled Toffoli in Lemmas 7.2, 7.3 and 7.5 of [Barenco et al., 1995] uses this structure. This will work as long as the states $|x\rangle\,|y\rangle$ going into $p\text{-}C^nX$ are the same as that going into $\big(p\text{-}C^nX\big)^\dagger$. If this is the case, we can enjoy a substantial cost reduction of relative phase C^nX.

References

[Barenco et al., 1995] Barenco, A., Bennett, C. H., Cleve, R., DiVincenzo, D. P., Margolus, N., Shor, P., Sleator, T., Smolin, J. A., and Weinfurter, H. (1995). Elementary gates for quantum computation. *Physical Review A*, 52(5):3457–3467.

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[Maslov, 2016] Maslov, D. (2016). Advantages of using relative-phase toffoli gates with an application to multiple control toffoli optimization. *Physical Review A*, 93(2).

Appendices

A Difference data for first 400 cases

n	CX count	First diff.	Second diff.	Length	i
1	1	N/A	N/A	N/A	N/A
2	3	2	N/A	N/A	N/A
3	6	3	1	1	0
4	10	4	1	1	0
5	14	4	0	3	1
6	18	4	0	3	1
7	24	6	2	3	1
8	30	6	0	3	1
9	36	6	0	3	1
10	44	8	2	3	1
11	52	8	0	9	2
12	60	8	0	9	2
13	68	8	0	9	2
14	76	8	0	9	2
15	84	8	0	9	2
16	92	8	0	9	2
17	100	8	0	9	2
18	108	8	0	9	2
19	120	12	4	9	2
20	132	12	0	9	2
21	144	12	0	9	2
22	156	12	0	9	2
23	168	12	0	9	2
24	180	12	0	9	2
25	192	12	0	9	2
26	204	12	0	9	2
27	216	12	0	9	2
28	232	16	4	9	2
29	248	16	0	27	3
30	264	16	0	27	3
31	280	16	0	27	3
32	296	16	0	27	3
33	312	16	0	27	3
34	328	16	0	27	3
35	344	16	0	27	3
36	360	16	0	27	3
37	376	16	0	27	3
38	392	16	0	27	3
39	408	16	0	27	3
40	424	16	0	27	3
41	440	16	0	27	3
42	456	16	0	27	3
43	472	16	0	27	3
44	488	16	0	27	3
45	504	16	0	27	3
46	520	16	0	27	3
47	536	16	0	27	3
48	552	16	0	27	3

49	568	16	0	27	3
50	584	16	0	27	3
51	600	16	0	27	3
52	616	16	0	27	3
53	632	16	0	27	3
54	648	16	0	27	3
55	672	24	8	27	3
56	696	24	0	27	3
57	720	24	0	27	3
58	744	24	0	27	3
59	768	24	0	27	3
60	792	24	0	27	3
61	816	24	0	27	3
62	840	24	0	27	3
63	864	24	0	27	3
64	888	24	0	27	3
65	912	24	0	27	3
66	936	24	0	27	3
67	960	24	0	27	3
68	984	24	0	27	3
69	1008	24	0	27	3
70	1032	24	0	27	3
71	1056	24	0	27	3
72	1080	24	0	27	3
73	1104	24	0	27	3
74	1128	24	0	27	3
75	1152	24	0	27	3
76	1176	24	0	27	3
77	1200	24	0	27	3
78	1224	24	0	27	3
79	1248	24	0	27	3
80	1272	24	0	27	3
81	1296	24	0	27	3
82	1328	32	8	27	3
83	1360	32	0	81	4
84	1392	32	0	81	4
85	1424	32	0	81	4
86	1456	32	0	81	4
87	1488	32	0	81	4
88	1520	32	0	81	4
89	1552	32	0	81	4
90	1584	32	0	81	4
91	1616	32	0	81	4
92	1648	32	0	81	4
93	1680	32	0	81	4
94	1712	32	0	81	4
95	1744	32	0	81	4
96	1776	32	0	81	4
97	1808	32	0	81	4
98	1840	32	0	81	4
99	1872	32	0	81	4
100	1904	32	0	81	4
101	1936	32	0	81	4
102	1968	32	0	81	4

103	2000	32	0	81	4
104	2032	32	0	81	4
105	2064	32	0	81	4
106	2096	32	0	81	4
107	2128	32	0	81	4
108	2160	32	0	81	4
109	2192	32	0	81	4
110	2224	32	0	81	4
111	2256	32	0	81	4
112	2288	32	0	81	4
113	2320	32	0	81	4
114	2352	32	0	81	4
115	2384	32	0	81	4
116	2416	32	0	81	4
117	2448	32	0	81	4
118	2480	32	0	81	4
119	2512	32	0	81	4
120	2544	32	0	81	4
121	2576	32	0	81	4
122	2608	32	0	81	4
123	2640	32	0	81	4
124	2672	32	0	81	4
125	2704	32	0	81	4
126	2736	32	0	81	4
127	2768	32	0	81	4
128	2800	32	0	81	4
129	2832	32	0	81	4
130	2864	32	0	81	4
131	2896	32	0	81	4
132	2928	32	0	81	4
133	2960	32	0	81	4
134	2992	32	0	81	4
135	3024	32	0	81	4
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