

QUANTUM CIRCUIT IDENTITIES

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ABSTRACT. There are quantum circuit identities that simplify quantum circuits, reducing the effort needed physically to implement them. This paper constructs all identities made from 3 or fewer operations taken from a common set of one qubit operations, and explains how they may be used to simplify the cost of constructing quantum circuit identities.

1. INTRODUCTION

Since the breakthrough algorithms of Grover [9] and Shor [17], their generalizations to the hidden subgroup problem (HSP) by Kitaev [13], and beyond [10, 16], there has been intense interest in building quantum computers. But building quantum circuits is a challenging task, and one important part is being able to reduce a circuit to simple building blocks that are easily implemented. Some blocks are more costly to implement in terms of time, effort, and cost, for different physical realizations of quantum gates, so exchanging some operations for equivalent operations can be useful. Some different physical approaches are Raman-coupled low-energy states of trapped ions [3, 8], electron spins in quantum dots [6], linear optics [4], nuclear spins in silicon [12], and atomic cavity quantum electrodynamics [7]. Furthermore, when building quantum simulators [11, 15], it is useful to simplify constructions to equivalent circuits using fewer or faster operations. A slightly old list of quantum simulators is at [18].

Often placing two larger circuit blocks in series allows the adjacent blocks to have some gates merged. This can be done by realizing when certain combinations of elementary operations can be replaced by equivalent operations which lower the cost metric. For a good introduction to quantum circuits see [5].

Identities can be generated automatically with reasonable effort, but when automatically reducing circuits, doing so at runtime is too slow for longer identities. It is therefore important to have on hand a large list of identities, so simplifications can be automated. The purpose of this paper is to start with a relatively flexible set of matrices, and construct all identities up to a given length from them. The value of this paper is a simple set of rules to simplify many quantum circuits automatically and deterministically. This is done explicitly for one qubit identities made from products of 3 or less “elementary” gates. Since most simplifications in practice should come from merging a few gates in adjacent larger circuit blocks, choosing length 3 should encompass most needs.

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This paper is laid out as follows: section 2 defines the matrices used in the identities and their relevance, section 3 explains the procedure to obtain the identities (filtering out trivial or redundant identities, and proving their validity), section 4 contains a list of identities, and finally section 5 contains concluding remarks.

2. DEFINITIONS

Single qubit operations are in one-to-one correspondence with 2×2 unitary matrices, but certain of these matrices have special importance in the quantum computing literature [2, Chapter 4]. Most circuits in the literature are constructed from the following eleven unitary matrices:

$$\begin{aligned}
 I &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & X &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & Y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} & Z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
 S &= \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} & T &= \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} & H &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} & P(\theta) &= e^{i\theta/2} I \\
 R_x(\theta) &= \cos \frac{\theta}{2} I - i \sin \frac{\theta}{2} X & R_y(\theta) &= \cos \frac{\theta}{2} I - i \sin \frac{\theta}{2} Y \\
 R_z(\theta) &= \cos \frac{\theta}{2} I - i \sin \frac{\theta}{2} Z
 \end{aligned}$$

X , Y , and Z are the Pauli spin matrices, and R_x , R_y , and R_z are the corresponding exponential matrices, giving rotations on the Bloch sphere [2, Exercise 4.6]. H is the Hadamard matrix, used extensively in quantum algorithms. S is the phase gate, and T is called the $\pi/8$ gate (even though $\pi/4$ appears in it). Trivially $S = T^2$ and $Z = S^2$; they are each included since they appear in many quantum circuit constructions. P is a phase rotation by $\theta/2$ to help match identities automatically.

3. PROCEDURE

Infinite families of qubit operations are likely to be hard to construct physically, except in special cases, so we arbitrarily chose a *finite* subset of the matrices in section 2 - small enough so that automatically generating identities is not too time consuming, yet large enough to yield a useful set of identities. We start with 35 matrices $\Lambda = \{I, X, Y, Z, H, S, T, R_x(\theta_j), R_y(\theta_j), R_z(\theta_j), P(\theta_j)\}$ where $\theta_j = \frac{4\pi}{8}j$, for $j = 1, 2, \dots, 7$. Note that R_x , R_y , R_z , and P all have period 4π and equal the identity when their argument is 0, thus the choices for θ_j . Taking fewer choices for θ_j results in much fewer identities, but enlarging the number by a factor of 2 made the process unbearably slow. In order to shorten notation later, let $X_j = R_x(\frac{4\pi}{8}j)$, $j = 1, 2, \dots, 7$. Similarly define Y_j , Z_j , and P_j .

The process to find the identities was programmed in both C++ and Mathematica 4.2 to help weed out errors and avoid missing any identities. An identity is an equivalence $lhs = rhs$, for example $Z = HXH$, where lhs and rhs are strings of matrix names. The length of an identity is the number of matrices on the right hand side. lhs always has length 1. To find all identities of length n , all $n^{|\Lambda|}$ products of combinations of matrices from Λ are computed, and then the results are compared numerically with a small tolerance to each matrix in Λ . Numerical computations were a lot faster than doing accurate symbolic comparisons in Mathematica, and they were much easier to implement on the C++ side. This generated a list of identities of the form $lhs = rhs$ where lhs is a single matrix, and rhs is a product of n matrices. Identities were passed through a filter (described in section 3.1) to

remove redundant identities, trivial identities, and to clean them up by applying obvious simplifications. Finally, the identities of length up to 3 are listed in section 4, modulo the filtering process. The final list of identities were verified symbolically in Mathematica 4.2 [1] and numerically by the C++ program to ensure that filtering did not introduce errors. C++ source code and a Mathematica 4.2 notebook implementing the programs are at [14], along with a file containing all (unfiltered) identities of length 4 and less, of which there are 400089 (see table 1).

3.1. Filtering identities. Each identity is run through the filtering process described below to remove redundant identities and those that can be shortened using previous identities. The filter performs the following steps on an identity:

The Filter

- (1) *Shrink*: If the length d of rhs is 3 or larger, remove the identity if any identity with a length of $2, 3, \dots, d-1$ can be applied to shorten rhs . This way, knowing $I = HH$, we avoid identities like $H = HHH$ which are deduced from shorter identities.
- (2) *Negate*: Apply the rules $\{Q_4 \rightarrow -I, Q_j \rightarrow -Q_{j-4}\}$ for $Q \in \{P, X, Y, Z\}$ and $j = 5, 6, 7$. This replaces expressions like $X_5Y_6 \rightarrow (-X_1)(-Y_2) = X_1Y_2$, making all subscripts less than 4, and shortening the list.
- (3) *Clean*: Merge the negative signs from the previous step, and move to the front of the string. This step is trivial mathematically, but must be performed symbolically in the computer.
- (4) *Phase*: Since the P_j commute with all matrices, merge them all to the front of rhs , except for a possible “-” in front. That is, replace expressions like $P_2 = -P_3SP_1Z_1$ with $I = -P_2SZ_1$.
- (5) *Normalize*: Apply the 90 commuting rules $\{QQ_j \rightarrow Q_jQ, TZ \rightarrow ZT, SZ \rightarrow ZS, ST \rightarrow TS, SZ_j \rightarrow Z_jS, TZ_j \rightarrow Z_jT, VQ_4 \rightarrow Q_4V\}$ for $Q \in \{X, Y, Z\}$, $V \in \Lambda$, and the rules on identities $\{II \rightarrow I, I \rightarrow\}$ to normalize the expression, and to allow further simplifications. For example, this allows the simplifications $ZZ_3SZSZ_2 \rightarrow ZZSZ_3Z_2 \rightarrow SZ_5 \rightarrow -SZ_1$.
- (6) *Collapse*: Combine any obvious expressions using the 196 identities $\{Q_iQ_j \rightarrow Q_k\}$ for $Q \in \{P, X, Y, Z\}$, $i, j \in \{1, 2, \dots, 7\}$, and $k = (i + j) \bmod 8$, where $Q_0 = I$. For example, X_2X_3 becomes X_5 and $Y_2Y_3Y_3$ becomes I .
- (7) *Merge*: Remove trivial identities such as when the lhs and rhs are symbolically identical, or $lhs = I$. Remove duplicate identities at this step.
- (8) *Rotate*: To avoid a lot of identities, if the identity is now made up only of rotations X_j, Y_j , and Z_j , (and treating $\pm I$ as rotations) it is discarded. Since these matrices act as rotations of the Bloch sphere they satisfy usual rotation identities, so this does not remove too many useful relations. For the online list [14] they are retained for completeness.
- (9) *Repeat*: Repeat the above steps until the list of length n identities becomes stable. Repetition is necessary; for example step 6 may allow step 2 to simplify the identity further.
- (10) *Grouping*: After the list is stable, group similar identities to shorten the list, using symbols $\{A, B, C\}$, chosen cyclically from $\{X, Y, Z\}$. For example, the three identities $I = XX$, $I = YY$, and $I = ZZ$ are replaced with the identity $I = AA$, and the three identities $Z_2 = -XY$, $Y_2 = -ZX$, and $X_2 = -YZ$ are replaced with $A_2 = -BC$.

So roughly the filter applies known identities to try to shorten a given one, and returns standardized, simplified (using certain rules) identities.

3.1.1. *Filtering effects.* Table 1 shows the effects of filtering on the number of identities returned. The first row lists the counts with no filtering from section 3.1 applied. In this case, both Mathematica 4.2 and C++ find 47 identities of length 1 (almost all are trivial except $X_4 = Y_4 = Z_4 = P_4 = -I$). Going to length 2 added 625 identities, giving the total 672 in the table, and length 3 added 15068 identities, totaling 15740. The C++ program was fast enough to find the length 4 identities, but the Mathematica program is too slow for this length and longer. This case needed to compute all $|\Lambda|^4 = 35^4 = 1,500,625$ combinations, and compare them. Length 5 and 6 are probably computable, but will take a lot of resources.

The second row of the table is the number of identities returned when filtering is enabled, but not applying step 8 (rotation removal) and step 10 (grouping similar patterns) from section 3.1. The third line contains the counts when only step 10 is skipped, and the last line has counts obtained by applying all filtering steps.

Filter	Length 1	Length ≤ 2	Length ≤ 3	Length ≤ 4
No filtering	47	672	15740	400089
Keep rots, No groups	12	66	293	1330
Drop rots, No groups	6	54	185	982
All filtering	2	36	155	931

TABLE 1. Identity counts

Looking at the table, and noting that even the 931 filtered length 4 identities are too tedious to put in a paper, I decided to put the more manageable 155 length 3 and less identities. However the unfiltered lists can be found online [14].

4. IDENTITIES

The identities in table 2 are all the identities resulting from 3 or fewer products of matrices from Λ in section 2, after filtering. They are sorted alphabetically on the right hand side for quick reference. When the symbols A, B , or C appear in the identities, that identity stands for the three identities where A, B, C are a cyclic permutation of X, Y, Z , as explained in step 10 in section 3.1.

4.1. **Hand simplification.** Simplifying diagrams by hand is quite tedious, but can be assisted using these tables. Apply the procedure listed in section 3 to simplify the product until it simplifies no further, then look for identities in the list that apply.

4.1.1. *Example 1.* We verify the identity $Y = -XYX$. Starting with XYX , we see no identities in the table starting with $XY\dots$ or $YX\dots$, so we look for a grouping pattern, and find $A_2 = -BC$, which we apply as $Z_2 = -XY$, giving $XYX \rightarrow -Z_2X$. Expand using $A_2 = CB$ and collapse $I = AA$ giving the complete transformation $XYX \rightarrow -Z_2X \rightarrow -YXX \rightarrow -Y$, proving $Y = -XYX$.

$I = AA$	$Y = HY_3Z_2$	$Z_3 = -P_2Z_1Z$	$S = X_2SY_2$	$X = Y_3HY_2$
$I = -AC_2B$	$Y_1 = HZ$	$Z = P_2Z_2$	$Y = X_2Y_3H$	$H = Y_3HY_3$
$A_1 = -BA_1C$	$X_1 = HZ_1H$	$I = P_2Z_2Z$	$H = -X_2Y_3Y$	$S = -Y_3SX_1$
$A_1 = -BA_3B$	$X_2 = HZ_2H$	$Z_1 = P_2Z_3Z$	$H = -X_3HZ_1$	$H = -Y_3X$
$A_3 = BA_3C$	$Y_3 = HZ_2Y$	$Z_1 = -P_3S$	$S = X_3SY_3$	$X_2 = Y_3YH$
$A_2 = -BC$	$Y = -HZ_2Y_1$	$Z_2 = -P_3Z_1S$	$Y = X_3YX_3$	$H = Y_3ZY_2$
$A = BC_2$	$X_3 = HZ_3H$	$Z_3 = -P_3Z_2S$	$Y = -X_3ZX_1$	$Y = -Y_3Z_2H$
$A = B_2C$	$Z_3 = -P_1ZS$	$I = P_3Z_3S$	$Z = X_3ZX_3$	$H = Y_3Z_2Y$
$A = B_3AB_3$	$S = P_1Z_1$	$S = P_3Z_3Z$	$Y_1 = YHX_2$	$Y_3 = -ZH$
$A = B_3CB_1$	$A_2 = -P_2A$	$A_4 = P_4$	$Z_2 = -YHY_3$	$X_1 = ZX_1Y$
$A_3 = -CA_3B$	$A_3 = -P_2A_1A$	$I = P_4A_4$	$Y_3 = YHZ_2$	$X_3 = -ZX_1Z$
$A_1 = -CA_3C$	$A = P_2A_2$	$X_3 = -SHS$	$S = YSX$	$Y_1 = -ZY_2H$
$A_2 = CB$	$I = P_2A_2A$	$Z = SS$	$X_3 = -YX_1Y$	$I = -ZY_2X$
$A = -CB_2$	$A_1 = P_2A_3A$	$X_2 = -SXS$	$Y_3 = YX_2H$	$H = -ZY_3$
$A = C_1BC_3$	$Y_3 = -P_2HX_2$	$H = SX_1S$	$H = YX_2Y_3$	$I = -ZY_3H$
$A = -C_2B$	$I = P_2HX_2Y_1$	$X = SX_2S$	$I = -YX_2Z$	$H = -Z_1HX_3$
$A = C_3AC_3$	$X_2 = P_2HY_3$	$Y_2 = -SYS$	$Z_1 = YZ_1X$	$X = Z_1XZ_1$
$I = HH$	$I = -P_2HY_3X_2$	$Y = SY_2S$	$Z_3 = -YZ_1Y$	$Y = -Z_1XZ_3$
$Y_3 = -HX$	$Y_1 = P_2HZ_2$	$S = TT$	$Z_1 = -YZ_3Y$	$Y = Z_1YZ_1$
$Z_1 = HX_1H$	$I = -P_2HZ_2Y_3$	$Y_1 = XH$	$X = Y_1H$	$H = -Z_2HX_2$
$Z_2 = HX_2H$	$Y_2 = -P_2Y$	$H = XY_1$	$S = -Y_1SX_3$	$Y_1 = Z_2HY$
$Y = -HX_2Y_3$	$Y_3 = -P_2Y_1Y$	$Y_2 = -XY_3H$	$Y = -Y_1X_2H$	$Y = -Z_2HY_3$
$Z_3 = HX_3H$	$H = P_2Y_1Z_2$	$Z_3 = -XZ_1X$	$Z_2 = Y_1YH$	$Y_1 = -Z_2YH$
$Y_1 = -HYX_2$	$I = P_2Y_1Z_2H$	$Z_1 = -XZ_3X$	$H = -Y_1YX_2$	$H = -Z_2Y_1Y$
$Z = HY_1$	$Y = P_2Y_2$	$Z_3 = XZ_3Y$	$H = Y_1Z$	$H = -Z_3HX_1$
$Y_2 = -HY_2H$	$I = P_2Y_2Y$	$H = -X_1HZ_3$	$H = Y_2HY_2$	$X = -Z_3YZ_1$
$Y_1 = -HY_2X$	$Z_2 = P_2Y_3H$	$S = X_1SY_1$	$Z = Y_2HY_3$	$Y = Z_3YZ_3$
$X = -HY_3$	$I = -P_2Y_3HZ_2$	$Y = X_1YX_1$	$S = -Y_2SX_2$	
$Y_1 = -HY_3H$	$H = -P_2Y_3X_2$	$Z = -X_1YX_3$	$H = Y_2XY_3$	
$I = -HY_3X$	$I = -P_2Y_3X_2H$	$Z = X_1ZX_1$	$Z = -Y_3H$	
$Z_2 = HY_3Y$	$Y_1 = P_2Y_3Y$	$Y_3 = X_2HY$	$Y = -Y_3HX_2$	
$Y_2 = -HY_3Z$	$Z_2 = -P_2Z$	$H = -X_2HZ_2$	$X_2 = -Y_3HY$	

TABLE 2. The 155 filtered identities up to length 3

4.1.2. *Example 2.* Another way to approach this is to try to get all expressions into X, Y, Z, X_j, Y_j, Z_j , and then commute them to get X 's together, etc., until simplified. Thus to simplify HXH , we have

$$HXH \xrightarrow{H=XY_1} XY_1XXY_1 \xrightarrow{I=AA} XY_1Y_1 \xrightarrow{\text{step 6}} XY_2 \xrightarrow{A=BC_2} Z$$

where the rules applied are above each arrow, resulting in $Z = HXH$.

5. CONCLUSIONS AND FUTURE WORK

There are several ways to speed up the search process, like adding the phase matrices only to the front, and not using the identity except for comparisons. But the speed improvements are minimal.

Other directions are to extend this to understanding the 2 and 3 qubit operations. For example, the Toffoli gate can be implemented with 5 basic 2 qubit gates [5]. I believe it is unknown if this can be done with 4 gates, although it seems unlikely. A computer search should be able to shed light on this, and perhaps open up new understanding about minimal number of quantum gates needed for some other constructions.

Finally, length 2, 3, and 4 filtered and unfiltered identities are online [14], as well as the C++ code and the Mathematica 4.2 code.

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