Smaller Circuits for Arbitrary $n$-qubit Diagonal Computations*

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Abstract

Several known algorithms for synthesizing quantum circuits in terms of elementary gates reduce arbitrary computations to diagonal [1, 2]. Circuits for $n$-qubit diagonal computations can be constructed using one $(n-1)$-controlled one-qubit diagonal computation [3] and one inverter per pair of diagonal elements, not unlike the construction of classical AND-OR-NOT circuits based on the lines of a given truth table of a one-output Boolean function. More economical quantum circuits for diagonal computations are known [5, 6] in special cases.

We propose a construction for combinational quantum circuits without ancilla qubits that allows one to implement arbitrary $n$-qubit diagonal computations exactly. Compared to known constructions, our circuits are an order of magnitude smaller and asymptotically smaller if no ancilla can be used.

Rather than synthesize a pair of diagonal values at a time, our technique seeks tensor-product decompositions with $2 \times 2$ diagonal matrices and is applied recursively. In this process, we use $2^{n-1} - 1$ sub-circuits that perform diagonal computations. Each contains a diagonal rotation of the last qubit surrounded by two CNOT-chains, and can be viewed as an “XOR-controlled” rotation — a new type of composite gate.

1 Introduction

Logic circuits provide a notation for computations of multiple functions, often bearing computational semantics. For example, $F[g(x), h(y)]$ might be represented by three gates labelled $F$, $g$ and $h$. Input lines of gates $g$ and $h$ are then labelled $x$ and $y$, and their output lines enter the gate $F$, whose output lines carry the result of the computation. Observe that if $g$ and $h$ are viewed as one gate, any pair $(x, y)$ is a valid input, which is how classical bits are combined into bit-strings. The situation is similar in quantum computing, except that qubits are complex two-dimensional vectors. Combined gates are applied to tensor-product vector spaces and represented mathematically by matrix tensor products. With an appropriate gate library, a logic circuit outlines how to implement a given computation in hardware. This motivates circuit synthesis, i.e., finding circuits that implement functionally-specified computations.

We briefly recall the following Definitions [9]. First, an $n$-qubit state vector is an element of $\otimes^n_1\mathbb{C}[|0\rangle,|1\rangle]$, with abbreviations such as $|01\rangle = |0\rangle \otimes |1\rangle$ being typical. In this work, measurements are not allowed midcomputation. Thus, a quantum computation is a $2^n \times 2^n$ matrix with complex entries which is moreover unitary, i.e., $A^\dagger A = I$. Here, $A$ is written in terms of the computational basis $|00\ldots0\rangle, |00\ldots1\rangle, |01\ldots0\rangle, \ldots$

With more than three qubits, some quantum computations can be specified more compactly using quantum circuit diagrams such as those in Figure 3. The more significant qubits correspond to higher lines. Gates are applied left to right and are chosen from the following universal gate library [1]:

- A $y$-axis Bloch sphere rotation $R_y(\theta) = 
  \begin{pmatrix}
  \cos \theta/2 & \sin \theta/2 \\
  -\sin \theta/2 & \cos \theta/2
  \end{pmatrix}
$, where $0 \leq \theta < 2\pi$.
- A $z$-axis Bloch sphere rotation $R_z(\alpha) = 
  \begin{pmatrix}
  e^{-i\alpha/2} & 0 \\
  0 & e^{i\alpha/2}
  \end{pmatrix}
$, where $0 \leq \alpha < 2\pi$.
- A CNOT gate $CNOT_{j}$, which is controlled on the $j$th line and changes the $\ell$th. Given a bit string $b_1 \ldots b_n$ and letting $\oplus$ denote the XOR operation also known as addition in the field of two elements $F_2$, the gate $CNOT_{j}$ exchanges basis states $|b_1b_2\ldots b_{j-1}b_jb_{j+1}\ldots b_n\rangle \leftrightarrow |b_1b_2\ldots b_{j-1}(b_j \oplus b_{j+1})b_{j+1}\ldots b_n\rangle$.

The three types of gates above can be applied to any qubits and are considered elementary. We will also use several types of composite gates as shortcuts for frequently used circuits. For example, the one-qubit NOT gate (also known as Pauli-X or $\sigma_x$) is expressed using two elementary gates, up to a global phase:

$$X = NOT = 
\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
\approx R_x(\pi) \cdot R_z(-\pi)
$$

We recall that the term CNOT means “Controlled-NOT”, i.e., applied on the controlled line iff the control line carries 1. Along the same lines, we define the $k$-controlled NOT gate denoted $k$-CNOT which preserves the values $b_1, b_2, \ldots, b_k$ on its $k$ control lines and produces $b_1 \oplus (b_2, b_3, \ldots, b_k)$ on the controlled line $\ell$, i.e., the inverter is applied iff all control lines carry 1. The 2-CNOT is also called the Toffoli gate. In Section 4 we outline how $k$-CNOT gates are implemented in terms of elementary gates and consider a more general construction of $k$-controlled one-qubit gates in which a given one-qubit gate is applied iff all control lines carry 1. When using such gates in a broader context, one may want to specify the $k$-control lines as a subset $S$ of all lines. Then we say that the gate is $S$-controlled. We denote such $S$-controlled $R_z(\theta)$ rotations by $CR_z(S, \theta)$ and point out that their decompositions into elementary gates are given in [11, 17]. These composite quantum gates are used in circuit synthesis algorithms in Section 4. Furthermore, we consider a less common type of control which applies a given one-qubit gate iff the values on control lines XOR to one rather than AND to one. In Section 4 such XOR-controlled gates are denoted by $XR_z(S, \theta)$ and used in circuit synthesis algorithms. We also decompose them into elementary gates as shown in Figure 3.

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As in prior work [2], our main goal is to produce quantum circuits with elementary gates for a specified sort of quantum computation. Our main result is a generalization of a prior result [2][2.2] to n-qubit computations. The prior result asserts that any 2-qubit unitary matrix whose off-diagonal entries in the computational basis vanish could be synthesized in 5 elementary gates or less.

**Definition 1.1** An n-qubit unitary matrix $A = (a_{ij})$ is diagonal iff $a_{ij} = 0$ whenever $i \neq j$. We describe a quantum computation as diagonal when its associated matrix in terms of the computational basis is diagonal. Finally, the notation $A = \text{diag}(b_1, \ldots, b_n)$ means $A$ is an $n \times n$ diagonal matrix $A = (a_{ij})$ with $a_{ii} = b_i$.

**Proposition 1.2** Let $A = \text{diag}(z_1, \ldots, z_{2^n})$ be an n-qubit diagonal quantum computation. Then there exists an $(n-1)$-qubit diagonal quantum computation $B = \text{diag}(w_1, \ldots, w_{2^n-1})$ and a one-qubit diagonal $C = \text{diag}(y_1, y_2)$ so that $A = B \otimes C$ if and only if

$$z_1z_2^{-1} = z_3z_4^{-1} = z_5z_6^{-1} = \cdots = z_{2^n-1}z_2^{-1} \tag{2}$$

The check that such a tensor satisfies the chain of equalities is routine. For the opposite implication, begin with $\text{diag}(z_1, z_2, \ldots, z_{2^n})$. Then define the $C$ of the statement by $C = \text{diag}(z_1, z_2)$. Now $A$ being unitary demands $z_1 \neq 0$. Thus, choose $B = \text{diag}(1, z_3/z_1, z_5/z_1, \ldots, z_{2^n-1}/z_1)$. The chain equality then implies $A = B \otimes C$.

Before giving a key definition, we recall that in Lie theory the term character denotes a continuous complex-valued function $\chi$ with the property $\chi(ab) = \chi(a)\chi(b)$ whose arguments are typically matrices. Our manuscript does not assume the familiarity with Lie theory, and we state all necessary properties of characters explicitly, e.g., for a character $\chi$ we typically consider the function $\log \chi$ which has the property $\log \chi(ab) = \log \chi(a) + \log \chi(b)$.

**Definition 1.3** Let $\mathcal{D}(n)$ be the set of n-qubit diagonal quantum computations. Then for $j = 1, \ldots, 2^n - 1$, we define character functions $\chi_j : \mathcal{D} \rightarrow \mathbb{C}$ by $\chi_j[\text{diag}(z_1, \ldots, z_{2^n})] = z_1^{-1}z_j^{-1}z_jz_2^{-1}z_2^{-1}z_3z_4^{-1}$. Also, $\ker \chi_j = \chi_j^{-1}(\{1\})$.

By Proposition 1.2 the elements of $\mathcal{D}(n)$ which are tensors are precisely the elements of $\cap_{j=1}^{2^n-1} \ker \chi_j$. The circuit synthesis algorithm then proceeds as follows for the diagonal input matrix $A$.

- For each nonempty subset $S$ of the lines $\{1, \ldots, n - 1\}$, we build a circuit $XR_S(S, \theta)$ whose effect depends on a variable $R_s(\theta)$ gate within the block. However, each translates the vector $[\log \chi_1(A) \ldots \log \chi_{2^n-1}(A)]^T$ by a $\theta$ dependent multiple of some nonzero vector.
- An appropriate check shows that the various vectors of the last item are all linearly independent. Thus, we may choose $\theta$’s so that all characters vanish on $XR$-circuits $\circ A$, given that there are $2^n - 1$ nonempty subsets of $\{1, \ldots, n - 1\}$ and similarly $2^n - 1$ characters.
- This produces a circuit decomposition $A = XR_{\text{Circuits }}(S \otimes C)$ with $B$ an $(n - 1)$-qubit diagonal and $C$ a 1-qubit diagonal.
- Recurse on $B$.

The gate count implied by this construction is given below.

**Theorem 1.4** Any n-qubit diagonal computation is performed by a circuit with $(\frac{2n}{2})2^n - 2n - 1$ elementary gates. No ancilla qubits are necessary.
from AND–OR decompositions, e.g., along the lines of \((b_1 \text{ OR } b_2) = b_1 \oplus b_2 \oplus (b_1 \text{ AND } b_2)\). Publicly available tools for such ESOP-decomposition include, EXORCISM-4 \(^6\). \(^8\).

While our main focus is on quantum circuits, we observe that classical two-level AND–OR circuits can be constructed with every nonzero value in the truth table separately, by means of a sub-circuit responsible only for that line of the truth table. A number of parallels exist between the synthesis of classical two-level logic on \(n\) inputs and diagonal \(n\)-qubit computations. However, note that the present work focuses on arbitrary diagonal \(n\)-qubit computations and worst-case complexities, which are often similar to average-case for both classical and quantum circuits. Yet industrial benchmarks are often easier than a randomly chosen functions or circuits. This work does not consider parallels to specific two-level logic optimization tools which target industrial circuits.

In reversible logic circuits, AND gates are not available, but \(k\)-CNOT gates allow for a similar construction. These gates act on a bit-string by computing the conjunction of the \(k\) control bits and then XOR'ing the result to the prior value of the controlled bit. Inverters, necessary at some inputs of some AND gates in classical two-level circuits, can be modelled by pairs of inverters on control lines of \(k\)-CNOT gates — one before and one after. To this end, we denote the collection of parallel inverters on lines from a subset \(S\) by \(\otimes X\), where \(X\) stands for an inverter. \(^1\) The giant \(\otimes X\) gates are then modelled by chaining multiple \(k\)-CNOT gates that share the same controlled bit through the circuit. In fact, such circuits correspond one-to-one to XOR-SUM decompositions of the Boolean function computed on the controlled bit and have been studied in the context of ROM-based classical and quantum computation \(^{10}\) where signals on only some lines can be modified.

More generally, we consider other \(k\)-controlled one-qubit units besides the \(k\)-CNOT gates which are directly analogous to \(k\)-input AND gates. Specifically, the multi-argument AND gates will be replaced by the quantum computations \(CA(S, \theta, \phi)\) realized by the circuit diagram of Figure \(11\). In analogy to the giant \(\otimes\) gate we compose \(CA(S, \theta, \phi)\) acting on the same \(n\)th qubit. In this case, the effect of all \(CA\) is cumulative, and each one-qubit computation is applied only when its control qubits have the right values. Classical two-level circuit decompositions can be viewed similarly.

**Definition 2.1** Let \(S \subseteq \{1, \ldots, n-1\}\) and \(S \neq \emptyset\), and let \(\theta, \phi \in \mathbb{R}\). Put \(A = e^{\theta B}R_z(\phi)\) a one-qubit diagonal computation for \(R_z(\phi)\) the Bloch sphere rotation of the interaction. Then \(CA(S, \theta, \phi)\) is that quantum computation whose action on the computational basis states is given as follows:

\[
CA(S, \theta, \phi)|b_1 b_2 \cdots b_n\rangle = \begin{cases} 
|b_1 b_2 \cdots b_{n-1}\rangle \otimes A|b_n\rangle, & b_j = 1 \text{ for all } j \in S \\
|b_1 b_2 \cdots b_{n-1}\rangle \otimes |0\rangle, & b_j = 0 \text{ for some } j \in S 
\end{cases}
\]

For \(S\) and \(\theta\) as above, we also introduce the notation \(CR_z(S, \theta) = CA(S, \theta, 0)\).

Direct computation verifies that the \(CA(S, \theta, \phi)\) are diagonal and moreover each is associated with a circuit diagram in Figure \(11\). Although some gates in Figure \(11\) are not elementary, their decompositions are known \(^{11}\). Using appropriate placement of inverters around the \(CA\{1, n-1\}, \theta, \phi\) gate, i.e., \(\otimes X \circ CA\{1, n-1\}, \theta, \phi\) \(\otimes X\), even-numbered pairs of consecutive diagonal matrix elements may be modified to any two values in \(U(1)\). Composing such computations one can synthesize an arbitrary diagonal quantum computation.

According to the decomposition in Figure \(11\), \(^{11}\) Lemma 7.11, such a \(k\)-controlled one-qubit diagonal computation may be viewed as an elementary one-qubit computation flanked by two \(k\)-CNOTs if one reusable ancilla qubit initialized to \(0\) is available. Also \(^{11}\) Lemma 7.4, a \(k\)-CNOT can be implemented using \(8(k - 3)\) Toffoli gates for any \(k \geq 5\) given an ancilla qubit. Accounting for further normalizations and cancellations, a \(k\)-CNOT is implemented with \(48k - 116\) elementary gates and one ancilla qubit initialized to \(0\).

To produce an overall gate count (or, rather an upper bound), we observe that any two diagonal quantum computations \(U, V\) can be reordered \((UV = VU)\). In particular, this is true for circuits \(\otimes X \circ CA\{1, n-1\}, \theta, \phi\) \(\otimes X\). To set each pair of entries of a given diagonal computation, we choose one such circuit for every subset of \(S \subseteq \{1, \ldots, n-1\}\). To summarize, we have \(2^{n-1} CA\{1, n-1\}, \theta, \phi\) gates, each taking up to \(48n - 164\) elementary gates. To count elementary gates in the inverters, we note that every possible \(S\) occurs exactly once. Therefore, we have \(\sum_{j=0}^{n-1} j \binom{n-1}{j} = (n - 1)2^{n-2} - 1\) gates, which count for \((n - 1)2^{n-1}\) elementary gates.

The overall count of \(2^{n-1}(49n - 165)\) elementary gates to implement an arbitrary \(n\)-qubit diagonal in the presence of an ancilla qubit may be improved by ordering the Figure \(11\)-circuits so as to cancel most of the inverters. This can be achieved via Gray-code ordering of subsets \(S\) where every two consecutive subsets differ by exactly one \(X\) gate. Thus a single inverter will separate every consecutive pair of \(CA\{1, n-1\}, \theta, \phi\) circuits. This decreases the overall gate count to \(2^{n-1}(48n - 164) + 2^{n-2}(2 - 2 = 2^{n-1}(48n - 163) - 2)\), barring further cancellations of CNOT gates in the implementations of \(CA\{1, n-1\}, \theta, \phi\). However, since lingering inverters are equally distributed on all possible lines, one does not expect that more than half of the \(1\)-CNOTs per \(CA\{1, n-1\}, \theta, \phi\) gate will cancel on average. Therefore, our estimated gate count is \(12n^2\). Interestingly, without the single ancilla qubit used above, a \(k\)-CNOT gate requires a quadratic rather than linear number of elementary gates. Moreover without the ancilla, the overall gate count becomes \(\theta(n^2\theta)\) rather than \(\theta(n^2\theta)\). The following sections accomplish two improvements, using characters defined on \(\theta\) as above:

- We achieve \(\theta(n^2\theta)\) without any ancilla qubit.
- We lower the leading term of the gatecount from \(12n^2\theta\) to \(\frac{3}{2}n^2\theta\).

Finally, we point out that special-case circuits for diagonal computations are proposed in \(\delta\). They use measurements on ancilla qubits (and thus are not purely combinational quantum circuits) and do not solve our generic synthesis problem for diagonal computations. Moreover, later steps of their algorithms depend on outcomes of earlier measurements, which is roughly equivalent to using multiplexor gates, also known as MUX or if-then-else gates, immediately after measurement. Furthermore, the emphasis of this work is on \(A = \text{diag}(a_1, \ldots, a_2) \in \mathbb{D}(n)\) for which at most \(p(n)\) of the \(a_j \neq 1\) for some polynomial in \(n\), where more is a function \(f(\bar{b})\ detecting nonunit entries may be evaluated using polynomial resources. Despite the radically different setting, we emphasize the following point. The generic measurement algorithm \(\delta\) [3] would need to synthesize \(2^n - 1 \approx 2^n\) nonunit diagonal phases within the tensor \(\otimes \delta_1 R_z(\theta_j)\) individually. Since, generically, phases are unlikely to repeat, the functions \(U_j\) in the worst case become \(U_{\delta_0}\) [p.1351] for \(\bar{b}\) an \(n - 1\) bit string and \(\delta_0\) the corresponding delta function. Thus in the present notation, \(U_{\delta_0}\) is \((n - 1)-conditioned\) CNOT. These cost roughly \(50n\) elementary gates \(\delta\) in the presence of an ancilla. The work in \(\delta\) approximates arbitrary rotation with binary digits, and approximating \(\otimes \delta_1 R_z(\theta_j)\) to one-bit precision requires at least \(100n2^n\) elementary gates in addition to \(2^n\) measurements. To improve the
3 Synthesis via Controlled Rotations

This section describes a different synthesis algorithm in terms of $CR_S(S, \theta)$ gates, compared to that analyzed in Section 2. This new algorithm motivates further synthesis algorithms in terms of $X_R(S, \theta)$ gates.

3.1 Subset Controlled Rotations

Following Definition 2.1, an $n – 1$ qubit computational basis state $\ket{b_1 b_2 \cdots b_{n-1}}$ with $b_i = 1$ for each $i \in S$ will be referred to as $S$-conditioned.

**Definition 3.1** Let $e_j$, $1 \leq j \leq 2^n – 1$, denote the standard basis vectors of $\mathbb{R}^{2^n-1}$, e.g. $\ket{0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0}$. The symbol $\bar{b}$ denotes the bit-string $b_1 \cdots b_{n-1}$ or the corresponding integer with this binary representation. These states are associated to vectors in $\mathbb{R}^{2^n-1}$ as follows. For the extremal computational basis states, set $v_{000 \cdots 0} = -e_1$ and $v_{111 \cdots 1} = e_{2^n-1}$, else let $v_{\bar{b}} = e_{\bar{b}} - e_{111 \cdots 1}$. Moreover, the vectors $\{v_{\bar{b}}\}_{\bar{b} \neq 0}$ form a basis for $\mathbb{R}^{2^n - 1}$.

Their application is Propositions 3.3 and 4.7.

**Example 3.2** In the case of $n = 4$ qubits where states above computational basis states of values on the top three lines, we form a basis of $\mathbb{R}^7$. In particular, $v_{0000} = -e_1$ does not count, while the basis consists of $v_{0001} = e_1 - e_2$, $v_{0010} = e_2 - e_3$, $v_{0101} = e_3 - e_4$, $v_{1001} = e_4 - e_5$, $v_{1010} = e_5 - e_6$, $v_{1100} = e_6 - e_7$, and $v_{1111} = e_7$. We will typically omit $v_{0000}$.

Now consider the map $\log : \mathcal{D}(n) \to \mathbb{R}^{2^n - 1}$ given by

$$\log \chi(A) = [\log \chi_1(A) \ A \ A \ A \ A]$$

This map is a group homomorphism between the commutative group $\mathcal{D}(n)$ and the commutative group $\mathbb{R}^{2^n-1}$ under vector addition. This means that for any $n$-qubit diagonal quantum computations $A, B \in \mathcal{D}(n)$, one has $\log \chi(A \circ B) = [\log \chi(A) + \log \chi(B)]$.

Moreover, $A \approx C \otimes R_S(\pi)$ is equivalent to $\log \chi(A) = 0$ by Proposition 1.2.

**Proposition 3.3** Let $C(S)$ denote the $S$-conditioned basis states for some nonempty $S \subseteq \{1, \ldots, n-1\}$. Then

$$\log \chi(CR_S(S, \theta)) = 0 \sum_{\bar{b} \in \mathcal{S}} v_{\bar{b}}$$

**Proof:** Put $A = CR_S(S, \theta) = \text{diag}(z_1, z_2, \cdots, z_{2^n})$. Then recall $\chi_j(A) = z_{j-1} z_{j} z_{j+1} z_{j+2}$. Now if the binary expression for $j$ represents an $S$ conditioned state, $z_{j-1} e^{-i \theta}$ and $z_{j+1} e^{i \theta}$. If the binary expression for $j$ is not $S$-conditioned, then each entry is one. Likewise, if the binary expression for $j + 1$ is an $S$-conditioned bit-string, $z_{j+1} e^{-i \theta} z_{j+2} e^{i \theta}$. If the binary expression for $j + 1$ is not $S$-conditioned on the other hand, each is $1$. Via a case study, this verifies the formula above holds for the $j$th component of $\log \chi(A)$.

**Example 3.4** Consider $n = 4$ qubits for the subset $S = \{1, 3\}$ and $\theta$ arbitrary. Let $\theta = -\pi / 2$, so that $R_S(\theta) = e^{i \theta} E_{13} + e^{-i \theta} E_{22}$. Since $A = CR_S(\{1, 3\}, \theta)$ is diagonal, we describe the quantum computation by specifying multiples on each computational basis state.

Thus, $\chi_1(A) = 1, \chi_2(A) = 1, \chi_3(A) = 1, \chi_S(A) = e^{-2i \theta}, \chi_6(A) = e^{2i \theta}$, and $\chi_7(A) = e^{i \theta}$. Thus we have directly computed that $\log \chi(CR_S(\{1, 3\}, \theta)) = -2 q(0 0 0 0 1 1 1)^f$.

The $\{1, 3\}$-conditioned states are $|101\rangle$, $|111\rangle$. Moreover, $v_{\bar{b}} = e_{\bar{b}} - e_{111}$ for $\bar{b} \neq 111$. Thus

$$v_{|101\rangle} + v_{|111\rangle} = (e_5 - e_6) + e_7 = [0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 1]^f$$

Thus we computed the right-hand side of Proposition 3.3.

3.2 Description of the Controlled Synthesis Algorithm

Note that there are $2^n - 1$ nonempty subsets of $\{1, \ldots, n - 1\}$ and $2^{n-1} - 1$ functions $\chi_j : \mathcal{D}(n) \to U(1)$, i.e. $\log \chi_j : \mathcal{D}(n) \to i \mathbb{R}^{2^{n-1} - 1}$. Thus, the following matrix is square.

**Definition 3.5** The matrix $\log \chi(CR_S(n))$ is the $(2^{n-1} - 1) \times (2^{n-1} - 1)$ matrix defined as follows. Order nonempty subsets $S_1, S_2, \ldots S_{2^n - 1}$ in dictionary order. Then for $1 \leq j \leq 2^{n-1} - 1$, the $j$th column of $\log \chi(CR_S(n))$ is $\log \chi(CR_S(S_j, 1))$. Thus, the following matrix is square.

**Lemma 3.6** Let $\bar{\theta} = \{\theta_1, \ldots, \theta_{2^{n-1} - 1}\}$.

For $S_1, S_2, \ldots S_{2^n - 1}$ the dictionary ordering of the nonempty subsets of $\{1, \ldots, n-1\}$,

$\log \chi(CR_S(S_1, \bar{\theta})) = \log \chi(CR_S(n)) \bar{\theta}$

**Proof:** Recall $\log \chi(A \circ B) = \log \chi(A) + \log \chi(B)$. It is brief computation to check that $\log \chi(CR_S(S, \theta)) = \log \chi(CR_S(S, 1 \text{ rad}))$. Thus we may expand the left-hand side as $\sum_{j=1}^{2^n - 1} \theta_j \log \chi(CR_S(S_j, 1))$, which can be seen equal to the right-hand side.

We now state the controlled rotation synthesis algorithm for a diagonal unitary computation. The proof of correctness in the next
subection verifies the assertions that $\log \tilde{Z}(\text{CR}_c(n))$ is invertible for all $n$ and that $D$ is as stated a tensor.

**Controlled Rotation Synthesis Algorithm** Begin with $A \in D(n)$, for which we wish to synthesize a circuit diagram in terms of the elementary gates of the introduction. Label $S_1, S_2, S_3, \ldots S_{2n-1}$ to be the nonempty subsets of the top $n - 1$ lines $\{1, \ldots, n - 1\}$ in dictionary order.

1. Compute $\bar{\psi} = \log \tilde{Z}(A)$.

2. Compute the inverse matrix $\{\log \tilde{Z}(\text{CR}_c(n))\}^{-1}$.

3. Compute $\bar{\theta} = \{\log \tilde{Z}(\text{CR}_c(n))\}^{-1} \bar{\psi}$, treating $\bar{\psi}$ as a column vector. Label $\bar{\theta} = \theta_1 \cdots \theta_{2n-1}$.

4. Compute the diagonal quantum computation
   $D = \text{CR}_c(S_1, -\theta_1) \circ \cdots \circ \text{CR}_c(S_{2n-1}, -\theta_{2n-1}) \circ A$. As is verified below, $D$ is a tensor.

5. Use the argument of prop. 1 to compute $D = B \otimes C$ for $B \in D(n - 1)$ and $C = R_c(\eta)$ for some angle $\eta$.

6. Thus $A = \text{CR}_c(S_{2n-1}, \theta_{2n-1}) \circ \cdots \circ \text{CR}_c(S_1, \theta_1) \circ [B \otimes R_c(\eta)]$. Techniques from the literature are then used to decompose each $\text{CR}_c(S, \theta)$ into elementary gates per Figure 2.

7. The algorithm terminates by recursively producing a circuit diagram for $B \in D(n - 1)$.

**Example 3.7**

Let $A = \text{diag}(e^{i\pi/6}, e^{i\pi/6}, e^{i\pi/6}, e^{i\pi/6}, e^{i\pi/6}, e^{i\pi/6}, e^{i\pi/6}, e^{i\pi/6}, e^{i\pi/6})$. Then one has $\chi_1(A) = e^{-i\pi/6}, \chi_2(A) = e^{-2i\pi/6}, \chi_3(A) = e^{-3i\pi/6}$ so that $\bar{\psi} = \log \tilde{Z}(A) = (i[2\pi/6 - 3\pi/6 - 2\pi/6], 0, 0, 0, 0, 0, 0, 0, 0, 0)$. We now must compute $\bar{\theta}$ by computing the inverse matrix $\{\log \tilde{Z}(\text{CR}_c(3))\}^{-1}$. For this matrix, first compute the following.

$$\log \tilde{Z}(\text{CR}_c(3)) = i \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & -1 \\ 0 & 1 & 1 \end{pmatrix}$$

(8)

The following inverse matrix results, and it may be reused for multiple specific diagonals $A$.

$$\{\log \tilde{Z}(\text{CR}_c(3))\}^{-1} = -i \begin{pmatrix} 1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

(9)

So $\bar{\theta} = \{\log \tilde{Z}(\text{CR}_c(3))\}^{-1} \bar{\psi} = [-\pi/6 - 4\pi/6, 2\pi/6]$. Hence $D$ as defined below is a tensor.

$$D = \text{CR}_c(\{1\}, \pi/6) \circ \text{CR}_c(\{1, 2\}, 4\pi/6) \circ \text{CR}_c(\{2\}, -\pi/6) \circ \text{diag}(1, \text{e}^{i\pi/12}, \text{e}^{i2\pi/12}, \text{e}^{i3\pi/12}, \text{e}^{i4\pi/12}, \text{e}^{i5\pi/12}, \text{e}^{i6\pi/12})$$

(10)

In order to verify this directly, we compute the eight diagonal matrix coefficients of each $\text{CR}_c(S, \theta)$.

$$\text{CR}_c(\{1\}, \pi/6) = \text{diag}(1, 1, 1, 1, e^{-\pi/12}, e^{\pi/12}, e^{-3\pi/12}, e^{3\pi/12})$$

$$\text{CR}_c(\{1, 2\}, 4\pi/6) = \text{diag}(1, 1, 1, 1, 1, 1, 1, e^{-4\pi/12}, e^{4\pi/12})$$

$$\text{CR}_c(\{2\}, -2\pi/6) = \text{diag}(1, 1, e^{2\pi/12}, e^{-2\pi/12}, 1, 1, e^{3\pi/12}, e^{-3\pi/12})$$

(11)

Then multiplying,

$$D = \text{diag}(e^{12\pi/12}, e^{6\pi/12}, e^{20\pi/12}, e^{14\pi/12}, e^{9\pi/12}, e^{3\pi/12}, e^{3\pi/12}, \text{e}^{18\pi/12})$$

(12)

Since $D$ is a tensor, we obtain the following decomposition of $A$.

$$A = \text{CR}_c(\{1\}, -\pi/6) \circ \text{CR}_c(\{1, 2\}, -4\pi/6) \circ \text{CR}_c(\{2\}, \pi/6) \circ \text{diag}(1, \text{e}^{8\pi/12}, \text{e}^{-3\pi/12}, \text{e}^{-2\pi/12}, \text{e}^{3\pi/12}, \text{e}^{6\pi/12})$$

(13)

The algorithm then recursively synthesizes the 2-qubit diagonal

$$(\text{diag}(1, \text{e}^{8\pi/12}, \text{e}^{-3\pi/12}, \text{e}^{-2\pi/12}, \text{e}^{3\pi/12}, \text{e}^{6\pi/12}))$$

\(\diamondsuit\)

**3.3 Proof of Correctness of Controlled Rotation Synthesis**

We briefly check that $D$ is as claimed a tensor $B \otimes C$. First note that

$$\log \tilde{Z}(\text{CR}_c(S_1, -\theta_1) \circ \cdots \circ \text{CR}_c(S_{2n-1}, -\theta_{2n-1}) \circ A) = -\bar{\psi} + \bar{\psi} = \bar{\theta}$$

(14)

Here, we have used the group homomorphism property of $\log \tilde{Z}(\cdot)$. This property further implies

$$\log \tilde{Z}(\text{CR}_c(S_1, -\theta_1) \circ \cdots \circ \text{CR}_c(S_{2n-1}, -\theta_{2n-1}) \circ A) = -\bar{\psi} + \bar{\psi} = \bar{\theta}$$

(15)

So by the restatement of Proposition 1, we must have $D = B \otimes C$.

**Proposition 3.8** $\log \tilde{Z}(\text{CR}_c(3))$ is an invertible $(2^n - 1) \times (2^n - 1)$ matrix.

**Proof:** It suffices instead to consider the similar matrix corresponding to a change of basis to $v_{j0}$ as $\bar{b}$ runs over the bitstrings representing binary expressions for $1, 2, \ldots, 2^n - 1$. Thus, if $B = [v_{j0-1}, v_{j0-2} \cdots v_{j1-1}]$ is the change of basis matrix, $M = B^{-1} \log \tilde{Z}(\text{CR}_c(n))B = (m_{jk})$ has $m_{jk} = 0$ if $\bar{b}_j$ is not $S_k$-conditioned and $m_{jk} = 1$ if $\bar{b}_j$ is $S_k$-conditioned. So for example, if $S_k = \{1, 2, \ldots, n - 1\}$, then the $k$th column of $M$ is $e_{2^n-1-k}$; $M$ is invertible since column operations reduce $M$ to a permutation matrix. Indeed, the $e_{2^n-1-k}$ column may be used to clear all other nonzero entries in the last row. Then each of the columns corresponding to $n - 2$ element subsets retain a single nonzero entry, and the corresponding rows may be cleared. Continuing by induction produces a permutation matrix. \(\square\)

**4 Synthesis via $\text{XOR}$-Controlled Rotations**

This section defines new composite $\text{XR}_c(S, \theta)$ gates. We then propose a new synthesis algorithm based on decomposing a circuit into such $\text{XR}$-gates, which are then broken down into elementary gates.

**4.1 $\text{XOR}$-Controlled Rotations**

**Definition 4.1** Let $S \subset \{1, \ldots, n - 1\}$ and $S \neq \emptyset$. Suppose $S = \{s_1, \ldots, s_k\}$ with $s_1 < s_2 < \cdots < s_k$. Then the circuit $\text{XR}_c(S, \theta)$ is defined by

$$\text{XR}_c(S, \theta) = \text{CR}_c(\{1\}, \pi/6) \circ \text{CR}_c(\{1, 2\}, 4\pi/6) \circ \text{CR}_c(\{2\}, -\pi/6) \circ \text{diag}(1, \text{e}^{i\pi/12}, \text{e}^{i2\pi/12}, \text{e}^{i3\pi/12}, \text{e}^{i4\pi/12}, \text{e}^{i5\pi/12}, \text{e}^{i6\pi/12})$$

(16)

Note that $\text{XR}_c(S, 4\pi\ell)$ is an identity computation for $\ell \in \mathbb{Z}$.

**Remark 4.2** The computation performed by $\text{XR}_c(S, \theta)$ is diagonal because it maps every computational basis state into a multiple of itself. Indeed, the $\text{CNOT}$ block at left is a permutation of basis states, and the $\text{CNOT}$ block at right is its inverse. \(\diamondsuit\)
Remark 4.3  It turns out that the circuits constructed above perform identical computations even if the elements of $S$ are read in any different order. To formalize this claim, let $\sigma$ be a permutation of $\{1, \ldots, k\}$. Then define

$$\begin{align*}
\text{CNOT}_{R_1}(\theta, \sigma) &= \begin{pmatrix} 1 & & & & & & & \\ & & & & e^{i\phi} & & & \\ & & & e^{-i\phi} & & & & \\ & & \vdots & & & & & \\ & & & & & & e^{i\phi} & \\ & & & & e^{-i\phi} & & & \\ & & & & & & & \end{pmatrix} \\
\text{CNOT}_{R_2}(\theta, \sigma) &= \begin{pmatrix} 1 & & & & & & & \\ & & & & e^{i\phi} & & & \\ & & & e^{-i\phi} & & & & \\ & & \vdots & & & & & \\ & & & & & & e^{i\phi} & \\ & & & & e^{-i\phi} & & & \\ & & & & & & & \end{pmatrix}
\end{align*}$$

We claim that $\text{XOR}(S, \theta, \sigma) = \text{XOR}(S, \theta)$ and show an example in Figure 3. The claim can be verified for basis states and then extended by linearity. Indeed, those circuits contain two symmetric chains of CNOT gates, and the second chain restores all lines except for the bottom to their input values. On the last line, $R_1(\theta)$ or $R_1(\theta) \otimes R_2(\theta)$ is applied, depending on the $\otimes$-sum of all input lines of the gate. 2. 

The ordering of the elements in $S$ affects the order in which the $\otimes$-sum is computed, but this does not affect the sum. This $\otimes$-sum, motivated by the notation for circuits $\text{XOR}(S, \theta)$ introduced in Figure 3.

Definition 4.4  A computational basis state $|b_1 b_2 \cdots b_{2^{n-1}}\rangle$ is an $S$-flip state for a nonempty $S \subset \{1, \ldots, n-1\}$ iff

$$|\beta_1 \beta_2 \cdots \beta_{2^{n-1}}\rangle = \text{CNOT}_{S_1} \otimes \text{CNOT}_{S_2} \otimes \cdots \otimes \text{CNOT}_{S_n}|b_1 b_2 \cdots b_{2^{n-1}}\rangle$$

has $\beta_k = 1$. Equivalently, S-flip states are those whose bits in lines listed in $S$ have an odd number of 1s (i.e., XOR to 1).

Example 4.5  Suppose $n = 4$ qubits, so the top line set is $\{1, 2, 3\}$. Then $\text{XOR}(\{1, 2, 3\}, \theta)$ is provided in Figure 4. Also shown is the circuit $\text{XOR}(\{1, 3\}, \theta, \sigma)$ for $\sigma$ the flip permutation of two elements. These two circuits realize the same diagonal quantum computation.

Example 4.6  Consider the special case of $n = 4$ qubits. The flip states of each nonempty subset of $\{1, 2, 3\}$ of the top three lines are given in the table below.

| subset | flip states |
|--------|-------------|
| \{1\}  | \{000\}, \{010\}, \{100\}, \{110\} |
| \{1, 2\} | \{010\}, \{101\}, \{100\}, \{010\} |
| \{1, 3\} | \{001\}, \{101\}, \{100\}, \{101\} |
| \{1, 2, 3\} | \{001\}, \{101\}, \{100\}, \{101\} |
| \{2\}  | \{010\}, \{101\}, \{110\}, \{111\} |
| \{2, 3\} | \{001\}, \{011\}, \{101\}, \{111\} |
| \{3\}  | \{100\}, \{101\}, \{110\}, \{111\} |

Shown are all bit-strings where bits in relevant positions XOR to 1.

Proposition 4.7  Let $\mathcal{S}$ be the set of flip states of a set $S$. Then

$$\log \text{XOR}(S, \theta) = -2\theta \sum_{|\psi\rangle \in \mathcal{S}} v_{|\psi\rangle}$$

Note that $|00 \cdots 0\rangle$ is never a flip state, so that $\sum_{|\psi\rangle \in \mathcal{S}} v_{|\psi\rangle}$ never appears within the above sum.

The proof is similar to that of Proposition 3.3. However, $\text{XOR}(S, \theta)$ never leaves any computational basis state fixed, which is why the factor of $\theta$ is doubled.

Example 4.8  Consider $n = 4$ qubits for the subset $S = \{1, 3\}$ and $\theta$ arbitrary. For convenience, label $\phi = -\theta/2$, so that $R_1(\theta) = e^{2i\phi}E_{11} + e^{-2i\phi}E_{22}$. We leave it to the reader to check that $A = \text{XOR}(\{1, 3\}, \theta)$ is diagonal and merely describes the multiples on each computational basis state.

$|00\rangle \to e^{i\theta} |00\rangle$,
$|01\rangle \to e^{i\theta} |01\rangle$,
$|10\rangle \to e^{-i\theta} |10\rangle$,
$|11\rangle \to e^{-i\theta} |11\rangle$.

Thus, $\chi_1(A) = e^{i\theta}$, $\chi_2(A) = e^{-i\theta}$, $\chi_3(A) = e^{i\theta}$, $\chi_4(A) = 1$, $\chi_5(A) = e^{-i\theta}$, $\chi_6(A) = e^{i\theta}$ and $\chi_7(A) = e^{-i\theta}$. Thus we have established that $\log \text{XOR}(\{1, 3\}, \theta)$ is diagonal in $|1 1 0 1 0 1 0 -1\rangle$.

On the other hand, flip states for $\{1, 3\}$ are given by $|011\rangle, |101\rangle, |100\rangle$ and $|110\rangle$. Moreover, treating integers via their binary representation, $v_{|\psi\rangle} = e_j - e_{j+1}$ for $j \neq 111$. Thus

$$(e_1 - e_2) + (e_3 - e_4) + (e_5 - e_6) + (e_7 - e_8) = |1 1 1 1 0 1 1 1 0\rangle.$$ 

This concludes the example.

4.2 Description of XOR-Controlled Synthesis Algorithm

The $-0.5$ radians in the definition of the following matrix cancels the $-2$ coefficient in equation 15. It is similar to the Definition 4.5.

Definition 4.9  The matrix $\log \text{XOR}(S, n)$ is the $(2^{n-1} - 1) \times (2^{n-1} - 1)$ matrix defined as follows. Order nonempty subsets $S_1, S_2, \ldots, S_{2^{n-1}-1}$ in dictionary order. Then for $1 \leq j \leq 2^{n-1} - 1$, the $j$th column of $\log \text{XOR}(S, n)$ is $\log \text{XOR}(S_j, -0.5)$.

Example 4.10  Computing $\log \text{XOR}(S, 4)$ is most quickly accomplished using the table of example 4.6 and Proposition 4.7 as was done for a column in 4.8. The result is

$$\log \text{XOR}(S, 4) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}.$$ (19)

The third column recalls example 4.8.

Lemma 4.11  Let $\bar{\theta} = \{01 \cdots 2^{n-1}-1\}$, then for $S_1, S_2, \ldots, S_{2^{n-1}-1}$ the dictionary ordering of the nonempty subsets of $\{1, \ldots, n-1\}$, we have

$$\log \text{XOR}(S_1, \theta_1) \circ \cdots \circ \text{XOR}(S_{2^{n-1}-1}, \theta_{2^{n-1}-1}) = -2\log \text{XOR}(S, \bar{\theta})$$ (20)

The proof is quite similar to Lemma 3.6. The multiple of $-2$ is due to the definition of $\log \text{XOR}(S, n)$, where we chose entries of $\pm i$ over entries of $\pm i/2$.

We now state the synthesis algorithm. It is critical in the following to note that $\log \text{XOR}(S, n)$ is invertible for all $n \geq 1$, so that
one may refer to the inverse matrix. This result will be proven in Proposition 4.13 below.

**Synthesis Algorithm** Begin with \( A \in \mathcal{D}(n) \). Label \( S_1, S_2, S_3, \ldots S_{2^n-1} \) to be the nonempty subsets of the top \( n-1 \) lines \( \{1, \cdots, n-1\} \) in dictionary order.

1. Compute \( \tilde{\psi} = \log \tilde{Z}(A) \).
2. Compute the inverse matrix \( \{\log \tilde{Z}[XR_c(n)]\}^{-1} \).
3. Compute \( \tilde{\theta} = (-1/2)\{\log \tilde{Z}[XR_c(n)]\}^{-1} \tilde{\psi} \), treating \( \tilde{\psi} \) as a column vector. Label \( \tilde{\theta} = [\theta_1 \cdots \theta_{2^n-1}]^T \).
4. Compute the diagonal quantum computation \( D = XR_c(S_1, \theta_1) \circ \cdots \circ XR_c(S_{2^n-1}, \theta_{2^n-1}) \circ A \). As is verified below, \( D \) is a tensor.
5. Use the argument of prop. 4.2 to compute \( D = B \otimes C \) for \( B \in \mathcal{D}(n-1) \) and \( C = R_c(\eta) \) for some angle \( \eta \).
6. Thus \( A = XR_c(S_{2^n-1}, \theta_{2^n-1}) \circ \cdots \circ XR_c(S_1, \theta_1) \circ [B \otimes R_c(\eta)] \). The algorithm terminates by recursively producing a circuit for \( D \in \mathcal{D}(n-1) \).

**Example 4.12** Consider the following 3-qubit computation:

\[
A = \text{diag}(e^{4\pi i/12}, e^{2\pi i/12}, e^{\pi i/12}, e^{3\pi i/12}, e^{8\pi i/12}, e^{11\pi i/12}, e^{10\pi i/12})
\]

(21)

We begin by computing \( \log \tilde{Z}[XR_c(3)] \). Since \( \{1\} \in \{1,2\} \) has flip states \( |01\rangle, |11\rangle \), we see the first column is \( e_2 - e_3 + e_3 = [010]^T \). Continuing this produces the matrix \( \log \tilde{Z}[XR_c(3)] \).

\[
\log \tilde{Z}[XR_c(3)] = i \begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & -1 \\
0 & -1 & 1
\end{pmatrix}
\]

(22)

The inverse matrix appears in the algorithm and may be reused for multiple diagonal computations.

\[
\{\log \tilde{Z}[XR_c(3)]\}^{-1} = (-i)\{1/2 \begin{pmatrix}
1 & 2 & 1 \\
1 & 0 & -1 \\
1 & 0 & 1
\end{pmatrix}\}
\]

(23)

Now \( \tilde{\psi} = \log \tilde{Z}(A) = i\log \chi_A(A) \log \chi_A(A) \log \chi_A(A)^T = i\{0 \ 7\pi/12 \ -6\pi/12 \}^T \).

Thus computing the parameters for the \( XR_c(S, \theta) \), \( \theta = (-1/2)\{\log \tilde{Z}[3]\}^{-1} \tilde{\psi} = [-4\pi/24 \ -3\pi/24 \ 3\pi/24 \}^T \).

It should be the case that

\[
D = XR_c(\{1\}, -3\pi/24) \circ XR_c(\{1,2\}, 3\pi/24) \circ XR_c(\{1\}, 4\pi/24) \circ A
\]

(24)

has \( D = B \otimes C \) for \( B \) a two-qubit diagonal and \( C \) a one-qubit diagonal. Note that the subset circuits above commute, so the order is immaterial.

The first step in computing \( D \) is to write \( XR_c(\{1\}, 4\pi/24) \) as a diagonal matrix. Begin by noting that

\[
1 \otimes 1 \otimes R_c(4\pi/24) = \text{diag}(e^{4\pi i/48}, e^{4\pi i/48}, e^{-4\pi i/48}, e^{4\pi i/48}, e^{-4\pi i/48}, e^{4\pi i/48}, e^{4\pi i/48}, e^{4\pi i/48})
\]

(25)

Associating the entries with \( |000\rangle, |001\rangle \), etc., we reverse those pairs whose two most significant bits are a flip state of \( \{1\} \).

\[
XR_c(\{1\}, 4\pi/24) = \text{diag}(e^{4\pi i/48}, e^{4\pi i/48}, e^{-4\pi i/48}, e^{4\pi i/48}, e^{4\pi i/48}, e^{-4\pi i/48}, e^{4\pi i/48}, e^{-4\pi i/48})
\]

(26)

We may similarly construct \( XR_c(\{1,2\}, 3\pi/24) \). The result is the following diagonal matrix.

\[
XR_c(\{1,2\}, 3\pi/24) = \text{diag}(e^{-3\pi i/48}, e^{-3\pi i/48}, e^{-3\pi i/48}, e^{-3\pi i/48}, e^{3\pi i/48}, e^{-3\pi i/48}, e^{-3\pi i/48}, e^{3\pi i/48})
\]

(27)

Finally, the flip states of \( \{2\} \) are \( |01\rangle \) and \( |11\rangle \). Thus we thus have the following.

\[
XR_c(\{2\}, -3\pi/24) = \text{diag}(e^{3\pi i/48}, e^{-3\pi i/48}, e^{-3\pi i/48}, e^{3\pi i/48}, e^{3\pi i/48}, e^{-3\pi i/48}, e^{3\pi i/48}, e^{-3\pi i/48})
\]

(28)

Collecting all terms, we arrive at

\[
D = \text{diag}(e^{-4\pi i/48}, e^{4\pi i/48}, e^{-4\pi i/48}, e^{4\pi i/48}, e^{4\pi i/48}, e^{-4\pi i/48}, e^{4\pi i/48}, e^{-4\pi i/48})
\]

(29)

Thus \( D = \text{diag}(e^{12\pi i/48}, e^{32\pi i/48}, e^{22\pi i/48}, e^{2\pi i/48}, e^{2\pi i/48}, e^{2\pi i/48}) \). The odd happenstance that the latter tensor fact is an identity saves one gate. To decompose \( D \) in five gates, call the routine recursively \( \Box \).



4.3 Proof of Correctness

**Proposition 4.13** \( \log \tilde{Z}[XR_c(n)] \) is an invertible \( (2^{n-1} - 1) \times (2^{n-1} - 1) \) matrix for \( n \geq 1 \).

**Proof:** It is equivalent to consider the question for an alternate basis of \( \mathbb{R}^{2^n-1} \). Thus, choose instead the vectors \( v_b \in \mathbb{R}^{2^n-1} \). Then this number of elements corresponds to \( n \) in each column, i.e. a entry of \( 1 \) for the \( v_b \) component whenever the binary string for \( b \) describes a flip state of \( S \).

Fix \( S \). We first claim there precisely \( 2^{n-2} \) flip states for \( S \). To see this, observe that the equation \( \sum_b v_b \neq 1 \) is satisfied by \( S \)-flip states defines an affine linear \( \mathbb{F}_2 \) subspace of the finite dimensional vector space \( (\mathbb{F}_2)^{2^n-1} \). Then this number of elements corresponds to the dimension count, since any \( k \) dimensional vector space of \( \mathbb{F}_2 \) must contain \( 2^k \) elements.

Next, fix \( S_1 \neq S_2 \) distinct nonempty subsets. Then the associated columns of \( M \) span precisely \( 2^{n-2} \) positions in which each has a nonzero, unit entry. This is again a dimension count. Note that since \( S \)-flip states satisfy \( \sum_{b \in S} v_b = 1, S_1 \neq S_2 \). Thus the codimension one subspaces corresponding to \( S_1 \) and \( S_2 \) intersect transversally in a codimension two subspace.

Given these claims, label \( M = (m_{ij}) \) and recall \( \delta_i^j \) the Kronecker delta which is 1 for \( i = j \) and zero else. Now considerations of the last two paragraphs demand that \( MM' = (m_{ij})(m'_{ik}) = 2^{n-2}(\delta_i^j + 1) \). An omitted argument then shows \( 0 \neq \det(MM') \), yet this expression is also \( \det(M)^2 \). Thus the rows of \( M \) are linearly independent, concluding the proof. \( \square \)

**Example 4.14** This example explicitly computes the matrix \( M \) of the proof of Proposition 4.13 for \( n = 4 \) qubits. In the \( v_{\{001\}} \cdots v_{\{111\}} \)
basis, the $j$th column of $M$ encodes the flip states of $S_j$ the $j$th subset of $\{1,2,3\}$ in the dictionary order. Thus, the table of example 4.6 is rewritten as follows.

$$M = \begin{pmatrix}
0 & 0 & 1 & 1 & 0 & 1 & 1 \\
0 & 1 & 0 & 1 & 1 & 1 & 0 \\
0 & 1 & 1 & 0 & 1 & 0 & 1 \\
1 & 1 & 1 & 1 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 1 & 1 \\
1 & 0 & 1 & 0 & 1 & 1 & 0 \\
1 & 0 & 0 & 1 & 1 & 0 & 1 \\
\end{pmatrix}$$

Hence the matrix $M'M$ of the argument has the asserted form:

$$M'M = \begin{pmatrix}
4 & 2 & 2 & 2 & 2 & 2 & 2 \\
2 & 4 & 2 & 2 & 2 & 2 & 2 \\
2 & 2 & 4 & 2 & 2 & 2 & 2 \\
2 & 2 & 4 & 2 & 2 & 2 & 2 \\
2 & 2 & 2 & 4 & 2 & 2 & 2 \\
2 & 2 & 2 & 2 & 4 & 2 & 2 \\
2 & 2 & 2 & 2 & 2 & 4 & 2 \\
\end{pmatrix}$$

Hence, $\det(M) \neq 0$, implying that $M$ is invertible.

5 Gate Counts

An upper bound can be produced by adding gate counts in separate parts of synthesized circuits, but that does not account for possible gate cancellations between the parts.

CANCELLATIONS OF CNOTs IGNORED. Since each $XR_c(S, \theta)$ contains a total of $2^{|S|} + 1$ elementary gates (assuming $\theta \neq 0$),

$$#(XR_c(S, \theta)) = \frac{3^n}{2} - 1$$

For example, the zeroing block in three qubits requires $3 + 3 = 11$ gates, and in four qubits $-3 + 3 + 3 + 5 + 5 + 7 = 31$ gates.

Thus recursively synthesizing an $n$-qubit diagonal $A$ will require the following number of elementary gates

$$(n)2^{n-1} + (n-1)2^{n-2} + \cdots + (2)2^2 - 1 + 1 = (n-1)2^n + 1$$

Note that Theorem 5.3 is based upon not this number but the cancellations described in the next section.

A CNOT CANCELLATION HEURISTIC.

Given that some CNOT gates in neighboring XR subcircuits in $XR_c(S, \theta)$ may cancel, one wishes to reorder such subcircuits to facilitate more cancellations. This can be achieved with a tie-breaking scheme described here, which additionally optimizes another degree of freedom related to the structure of each XR block.

Definition 5.1 Let $S = \{j_1, j_2, \ldots, j_k\}$ for $j_1 < j_2 < \cdots < j_k$, and let $\theta \in R$. For $\sigma: \{1, \ldots, k\} \rightarrow \{1, \ldots, k\}$ a permutation, the circuit diagram $XR_c([j_{\sigma(1)} j_{\sigma(2)} \cdots j_{\sigma(k)}], \theta)$ corresponds to the sequence of CNOTs and $R_\sigma(\theta)$ gate of Equation (39) for $XR_c(S, \theta, \sigma)$.

Thus the circuit diagram $XR_c([j_{\sigma(1)} j_{\sigma(2)} \cdots j_{\sigma(k)}], \theta)$ realizes the quantum computation $XR_c(S, \theta, \sigma) = XR_c(S, \theta)$.

Remark 5.2 The choice of $\sigma$ does not affect the quantum computation performed, but it may change the number of CNOT cancellations in consecutive XR blocks. For example, the diagram implementing $XR_c([34521], \theta_1) \circ XR_c([3452], \theta_2)$ has two cancelling pairs of CNOTs, while the diagram for $XR_c([54321], \theta_1) \circ XR_c([3452], \theta_2)$ has none.

The sets $S_1, \ldots, S_{2^{n-1}}$ are the nonempty subsets of $\{1, \ldots, n-1\}$, in some order.

Figure 4: In this copy of $\mathcal{T}(4)$, for every label we only show the last integer. Full labels can be reconstructed as shortest paths from the root (the top vertex). All of the edges are directed downward. Thus, $v(1) = 3$, $v(2) = 3$, $v(3) = 2$, $v(2) = 2$, $b(1) = 2$ and $b(2) = 1$.

Lemma 5.3 Consider the circuit diagram $XR_c([j_1 j_2 \cdots j_k], \theta_1) \circ XR_c([k_1 k_2 \cdots k_m], \theta_2)$, and suppose $\theta_1, \theta_2 \notin 4\pi \mathbb{Z}$. Then the number of pairs of cancelling CNOTs in this diagram is 0 if $j_1 \neq k_1$ and $-1 + \max\{n \geq 1 \mid j_p = k_p \forall p \leq n\}$ else.

Given this lemma, cancellations within $XR_c(S, \theta)$ will depend on both the choice of ordering of the $S_j$, $1 \leq j \leq 2^{n-1} - 1$ and also on a choice of ordering of the elements of each $S_j$. Below we show that a good ordering can be found by performing depth-first traversals of an appropriately defined rooted tree. In such a tree, every leaf corresponds to one XR block, and they can be ordered by DFS. Indeed, an XR block is uniquely identified by its subset $S_j$, which can be encoded by a decreasing sequence of non-repeating integers. Moreover, a decomposition of such an XR block into elementary gates is determined by an ordering of set elements, and we always use the decreasing order.

Definition 5.4 The tree $\mathcal{T}(n)$ is a rooted tree where vertices are (labelled by) all integer sequences $(n-1)a_2a_3 \cdots a_j$ with $n-1 > a_2 > a_3 > \cdots a_j \geq 0$. The root is labelled $(n-1)$. The directed edges begin at the vertex $(n-1)a_2a_3 \cdots a_j$ and end at the vertex $(n-1)a_2a_3 \cdots a_j a_{j+1}$ for $a_{j+1} < a_j$.

Figure 4 shows $\mathcal{T}(4)$.

In any $\mathcal{T}(n)$ the depth of the vertex labelled $(n-1)a_2 \cdots a_j$ is $j$, and the leaves of $\mathcal{T}(n)$ have labels of the form $(n-1)a_2a_3 \cdots a_j0$. Therefore each leaf is associated with a sequence $(n-1)a_2a_3 \cdots a_j$. All in all, there are $2^{n-2}$ leaves since subsets of $\{1,2,\ldots,n-1\}$ containing $n-1$ are correspond to subsets of $\{1,2,\ldots,n-2\}$.

Definition 5.5 Let $v(j)$ denote the number of vertices of $\mathcal{T}(n)$ of depth $j$ and $l(j)$ the number of internal vertices, i.e., not leaves. We then define the number of bends at depth $j$ in $\mathcal{T}(n)$ as $b(j) = v(j+1) - v(j)$.

Lemma 5.6 Within $\mathcal{T}(n)$, the following hold.

1. $v(j) = \binom{n-1}{j-1}$.

2. The number of leaves at depth $j$ is $l(j) = \binom{n-2}{j-2}$.

3. $\delta(j) = \binom{n-1}{j-1} - \binom{n-2}{j-2} = \binom{n-2}{j-1}$.

4. $b(j) = \binom{n-1}{j} - \binom{n-2}{j-1}$.

Proof: 1. and 2. are proven by induction, 3. and 4. follow by popular combinatorial identities.
Definition 5.7 Consider the set of all strictly-decreasing integer sequences
\[ S(n) = \{ (n-1)a_2a_3 \cdots a_j | (n-1) > a_2 > a_3 > a_j \geq 0 \} \] (32)
Assume a particular depth-first traversal of \( \tau(n) \), which in particular induces an ordering of the leaves and, hence, \( S(n) \) because the leaves correspond to subsets. Furthermore, subsets correspond to \( \mathbb{Z} \) blocks, and therefore any DFS induces an ordering of those blocks. Our circuits use this ordering and, furthermore, implement each \( \mathbb{Z} \) block as \( XR_t([S],0) \), according to the decomposition of Definition 5.1.

Below we count the number of cancelling \( \text{CNOT} \)s when decompositions of \( XR_t([S],0) \) blocks into elementary gates are concatenated. This count is independent on how ties are broken in DFS.

Example 5.8 A particular DFS on \( \tau(6) \) produces the following ordering of decreasing subsequences of \( \{1,2,3,4,5\} \).
\[
54321, 5432, 5431, 54321, 5421, 542, 541, 54, 5321, 532, 531, 53, 521, 52, 51, 5
\] (33)
This corresponds to the decomposition \( XR_t([54321],[0]) \cdots XR_t([1],[0]) \) with \( 3+3+2+2+1+2+1+1+0+0+2+1+1+0+1+0+0 = 17 \) pairs of cancelling \( \text{CNOT} \) gates, for a total of 34 elementary gates cancelled.

Proposition 5.9 If \( \mathbb{Z} \) blocks are ordered and implemented according to a DFS traversal of \( \tau(n) \), then the number of cancelling pairs of \( \text{CNOT} \)s is at least
\[
\sum_{j=2}^{n-2} (j-1)b(j) = (n-2)2^{n-3} - 2^{n-2} + 1
\] (34)
This count corresponds to the generic and simultaneously worst case when no \( \mathbb{Z} \) gate is trivial.

Proof: Every \( \mathbb{Z} \) block corresponds to a leaf of \( \tau(n) \). We therefore consider unique shortest paths from root to leaves. Every edge on such a path corresponds to a \( \text{CNOT} \) in our decomposition for \( \mathbb{Z} \). Indeed, consider the last (smallest) two integers \( j > \ell \), in the label of the vertex that is further from the root. Then the corresponding gate is \( \text{CNOT}^{\ell} \). Moreover, the \( \text{CNOT} \)s in the implementation of \( \mathbb{Z} \) are ordered just like the edges are ordered on the shortest path.4

Consider two leaves that are neighbors in a DFS-induced ordering. Then the shortest paths from the root to each leaf coincide to a certain depth \( j \), in which \( j-1 \) pairs of \( \text{CNOT} \)s cancel. The furthest vertex shared by the two paths is seen to be the least common ancestor (LCA) of the two leaves in the tree. Observe that the number leaf pairs whose LCAs are at depth \( j \) equals the number of bends \( b(j) \). The right-hand-side follows using the fourth identity in Lemma 5.6 and the differentiation of the binomial theorem. □

Corollary 5.10 The computation performed by the circuit block
\[
XR_t([S],[0]) \cdots XR_t([S_{(n-2)},0],[n-1])
\]
may be implemented so as to produce \( (n-5)2^n - 2^{n-1} - 2n - 1 \) elementary gates.

Proof: The tree \( \tau(n) \) produces \( (n-5)2^n - 2^{n-2} + n + 1 \) cancelling pairs of \( \text{CNOT} \)s by ordering those non-empty subsets of \( \{1,\ldots,n-1\} \) which contain \( n-1 \). We obtain the totals by summation
\[
\sum_{k=2}^{n} [(k-2)2^{k-3} - 2^{k-2} + 1] = (n-5)2^{n-2} + n + 1
\] (35)
\[
[(n-1)2^n + 1] - 2[(n-5)2^{n-2} + n + 1] = (n+3)2^{n-1} - 2n - 1. \]

Example 5.11 Ignoring \( \text{CNOT} \) cancellations, a 6-qubit diagonal computation requires \( 5(2)^6 + 1 = 321 \) elementary gates. Recall that Example 5.5 creates 17 cancelling \( \text{CNOT} \) pairs by arranging subsets \( \{1,2,3,4,5\} \) containing 5. Continue by choosing \( XR_t([1],[0]) \) for the ordering of sequences
\[
4321, 432, 431, 4321, 421, 421, 41, 4, 321, 321, 32, 3, 21, 2, 1
\] (36)
to discover 6 more cancelling pairs. Thus 46 \( \text{CNOT} \)s cancel out. Then any 6-qubit computation may be realized in \( 321 - 46 = 275 = 9(2)^3 - 12 - 1 \) elementary gates.

6 Conclusions and On-going Work

We describe new generic circuit synthesis procedures for diagonal quantum computations that use no ancilla qubits and reduce gate counts compared to previously known algorithms by a factor of twenty-four. If prior techniques may not use ancilla qubits, our techniques lead to asymptotic improvements. These results directly impact existing circuit synthesis algorithms for arbitrary \( n \)-qubit circuits [14] whose subroutines decompose diagonal computations.

These dramatic reductions are enabled by a new circuit decomposition based on “XOR-controlled rotations” — new composite gates with particularly simple elementary-gate decompositions.

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