Synthesis of unitaries with Clifford+T circuits

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We describe a new method for approximating an arbitrary $n$ qubit unitary with precision $\varepsilon$ using a Clifford and T circuit with $O(4^n(n(\log(1/\varepsilon) + n))$ gates. The method is based on rounding off a unitary to a unitary over the ring $\mathbb{Z}[i, 1/\sqrt{2}]$ and employing exact synthesis. We also show that any $n$ qubit unitary over the ring $\mathbb{Z}[i, 1/\sqrt{2}]$ with entries of the form $(a + b\sqrt{2} + ic + id\sqrt{2})/2^k$ can be exactly synthesized using $O(4^n nk)$ Clifford and T gates using two ancillary qubits. This new exact synthesis algorithm is an improvement over the best known exact synthesis method by B. Giles and P. Selinger requiring $O(3^{2^n} nk)$ elementary gates.

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Implementing a unitary operation using a universal gate set is a fundamental problem in quantum computing. The problem naturally arises when we want to implement some quantum algorithm on a fault tolerant quantum computer. Most fault tolerant protocols allow one to implement only Clifford circuits (those generated by CNOT, Hadamard and Phase gates). To achieve universal quantum computation one needs to add at least one non-Clifford gate. One of the common examples is a $T := \left( \begin{array}{cc} 1 & 0 \\ 0 & e^{i\pi/4} \end{array} \right)$ gate. Many unitaries that occur in quantum algorithms cannot be implemented exactly using the Clifford and T gate set and must be approximated. However, the study of unitaries that can be implemented exactly using Clifffords and T has been useful for finding more efficient approximations. An example is an asymptotically optimal algorithm for approximating single qubit rotations using Clifford and T gates[11]. This algorithm achieves polynomial speed-up over the Solovay-Kitaev algorithm[2, 5] (which is applicable to generic universal gate sets). The key ingredients of this algorithm are: an algorithm for synthesizing optimal single qubit circuits given a unitary that can be implemented exactly[7] and an efficient round-off procedure that approximates an arbitrary single qubit unitary by the one that is exactly implementable. We extend these ideas to the approximate synthesis of unitaries acting on multiple qubits and show that any $n$ qubit unitary can be approximated with precision $\varepsilon$ using at most $O(4^n(n(\log(1/\varepsilon) + n))$ Clifford and T gates and two ancillae. Our decomposition does not require taking square roots. We use only addition, subtraction and multiplication by $1/\sqrt{2}$; these operations preserve elements of $\mathbb{Z}[i, 1/\sqrt{2}]$.

We also improve multiple qubit exact synthesis of unitaries over the ring $\mathbb{Z}[i, 1/\sqrt{2}]$. B. Giles and P. Selinger[3] showed that any $n$ qubit unitary over the ring $\mathbb{Z}[i, 1/\sqrt{2}]$ with entries of the form $(a + b\sqrt{2} + ic + d\sqrt{2})/\sqrt{2}$ can be synthesized exactly using at most one ancilla. However, their synthesis method requires $O(3^{2^n} nk)$ gates, which is far from information theoretic bounds. In this paper we propose a synthesis method that uses two ancillae and requires $O(4^n nk)$ gates. The main results of the paper are summarized in the following theorems:

**Theorem 1.** Any $n$ qubit unitary can be approximated within Frobenius distance $\varepsilon$ using $O(4^n(n(C\log(1/\varepsilon) + n))$ Clifford and T gates and at most two ancillae.

**Theorem 2.** Any $n$ qubit unitary with entries of the form $(a + b\sqrt{2} + ic + d\sqrt{2})/\sqrt{2}$ can be exactly implemented using $O(4^n nk)$ Clifford and T gates using at most two ancillae.

To prove both results we use a variant of the Householder decomposition which expresses a matrix as a product of reflection operators and a diagonal unitary matrix. In our case the diagonal unitary matrix is always the identity. We define a reflection operator constructed from a unit vector $|\psi\rangle$ as $R_{\psi} = I - 2 |\psi\rangle\langle\psi|$. Our structure-preserving decomposition is given by the following lemma:

**Lemma 1.** Let $U$ be a unitary acting on $n$ qubits and let $\{u_1, \ldots, u_{2^n}\}$ be the columns of $U$. The unitary $U$ can be simulated using the unitary

$$U' = |0\rangle\langle 1| \otimes U + |1\rangle\langle 0| \otimes U^\dagger.$$
Unitary $U'$ is a product of reflection operators constructed from the family of unit vectors

$$|w_j^\pm\rangle = (|j\rangle \otimes |j\rangle \pm |0\rangle \otimes |u_j\rangle) / \sqrt{2}, \text{ for } j = 1, \ldots, 2^n.$$

**Proof.** By direct calculation we check that $U'$ maps $|1\rangle \otimes |\phi\rangle$ to $|0\rangle \otimes U|\phi\rangle$ for any $n$ qubit state $|\phi\rangle$. Next we observe that $|w_j^\pm\rangle$ are eigenvectors of $U'$ with eigenvalues $\pm 1$. Defining $P_j^\pm$ to be projectors on subspaces spanned by $|w_j^\pm\rangle$ and using the spectral theorem we express $U'$ as $\sum_{j=1}^{2^n} (P_j^+ - P_j^-)$. Since $\sum_{j=1}^{2^n} (P_j^+ + P_j^-)$ is the identity operator and all projectors $P_j^\pm$ are orthogonal we can write:

$$U' = I - 2 \sum_{j=1}^{2^n} P_j^- = \prod_{j=1}^{2^n} (I - 2P_j^-).$$

The right hand side is a product of $2^n$ reflection operators, as required. \qed

It is not difficult to see that if $|u_j\rangle$ has coordinates in the computational basis over the ring $\mathbb{Z} [i, 1/\sqrt{2}]$ then the unit vector $|w_j^\pm\rangle$ also does. This is the reason why we call our decomposition structure-preserving. Exactly synthesizing a reflection operator is not more difficult than exactly preparing corresponding unit vector:

**Lemma 2.** Any reflection operator $R_{|\phi\rangle}$ which $|\phi\rangle$ has coordinates in the computational basis of the form $((a + b\sqrt{2} + ic + d\sqrt{2})/\sqrt{2})$ can be implemented using $O(2^n n^k)$ Cliffords and $T$ gates and at most one ancilla.

**Proof of lemma 2.** Note that $UR_{|\phi\rangle}U^\dagger = R_{U|\phi\rangle}$. Therefore, to implement the reflection operator with corresponding unit vector $|\phi\rangle$ it is enough to find a $U$ that prepares $|\phi\rangle$ starting from $|0\rangle$. The column lemma [3] provides a construction for $U$ requiring $O(2^n n^k)$ Cliffords and $T$ gates and one ancilla. Unitary $R_{|\phi\rangle}$ is a multiple controlled $Z$ operator and can be implemented with $O(n)$ gates and one ancilla, for example using the construction from [9]. We conclude that we need $O(2^n n^k)$ Cliffords and $T$ gates in total to implement $R_{|\phi\rangle}$. \qed

Now we have all results required to proof Theorem 2:

**Proof of theorem 2.** The construction from lemma 1 allows one to simulate an $n$ qubit unitary using one ancilla and $2^n$ reflection operators. The unit vectors correspond to each reflection operator have coordinates of the form $((a + b\sqrt{2} + ic + d\sqrt{2})/\sqrt{2})$ in the computational basis. According to lemma 2 these reflection operators can be implemented using one ancilla and $O(2^n n^k)$ Cliffords and $T$ gates. Therefore we need $O(4^n n^k)$ Cliffords and $T$ gates and at most two ancillae to implement the unitary exactly. \qed

To show the approximation result we use the decomposition above and then approximate each reflection operator separately. First we note the following relation between approximating reflection operators and their corresponding unit vectors:

**Proposition 1.** The distance induced by the Frobenius norm between two reflection operators is bounded by the Euclidean distance between corresponding unit vectors as:

$$\|R_{|\psi\rangle} - R_{|\phi\rangle}\|_{F_r} \leq 2\sqrt{2}\|\psi - |\phi\rangle\|.$$

To prove the proposition it is enough to use the definition of the Frobenius norm $\|A\|_{F_r} = \text{Tr} (AA^\dagger)$, express $\|R_{|\psi\rangle} - R_{|\phi\rangle}\|_{F_r}$ in terms of $|||\phi\psi|||^2$, use that $\text{Re} (\phi \psi) \leq ||\phi \psi||$ and express $\text{Re} (\phi \psi)$ in terms of $|||\psi - |\phi\rangle\|^2$. Next we show how to approximate arbitrary reflection operator by at most two reflection operators with corresponding unit vectors over the ring $\mathbb{Z} [i, 1/\sqrt{2}]$.

**Lemma 3.** Any $n$ qubit reflection operator $R_{|\psi\rangle}$ can be approximated within Frobenius distance $\epsilon$ by the product of two reflection operators, such that coordinates in the computational basis of corresponding unit vectors have the form $(a + b\sqrt{2} + ci + di\sqrt{2})/2^m$ where $c(\epsilon) = [n/2] + O(\log(1/\epsilon))$ and using at most one ancilla. If unit vector $|\psi\rangle$ has at least two coordinates in the computational basis equal to zero it is sufficient to use one reflection operator and no ancilla is required.

**Proof of lemma 3.** First we construct the approximating unitary in a special case where no ancilla are required. Consider the reflection operator $R_{|\psi\rangle}$. Let $\{\alpha_k\}$ be the coordinates of $|\psi\rangle$ in computational basis. First we consider the case when $|\psi\rangle$ has at least two zero entries, say $\alpha_j$ and $\alpha_l$. We use an idea similar to [6] and define the approximating unitary as a reflection operator $R_{|\psi\rangle}$ corresponding to the vector

$$|\phi\rangle = \frac{a + bi}{2^m} |j\rangle + \frac{c + di}{2^m} |l\rangle + \sum_{k=1, k \neq j,l}^{2^n} \beta_k |k\rangle,$$

$$\beta_k = \frac{[2^m \text{Re} \alpha_k] + i [2^m \text{Im} \alpha_k]}{2^m}, a,b,c,d \in \mathbb{Z}.$$

The norm of $|\phi\rangle$ must be equal to 1, therefore:

$$a^2 + b^2 + c^2 + d^2 = 4^m \left(1 - \sum_{k=1, k \neq j,l}^{2^n} |\beta_k|^2\right).$$

The Diophantine equation above always has a solution according to Lagrange’s four-square theorem and it can be efficiently found using a probabilistic algorithm [10] that has runtime polynomial in number of bits required to write the right hand side of equation (1).

By Proposition 1, to estimate the distance between the reflection operator and its approximation it is enough to estimate the square of the distance between $|\psi\rangle$ and $|\phi\rangle$. We approximated each non-zero entry with precision $2^{-m} \sqrt{2}$, therefore

$$|||\psi - |\phi\rangle||^2 \leq 2^n \left(2^{-m} \sqrt{2}\right)^2 + 4^{-m} (a^2 + b^2 + c^2 + d^2).$$
The second summand of the right hand side of the inequality above can be estimated as:
\[
1 - \sum_{k=1, k \neq j, l} 2^n |\beta_k^2| = \sum_{k=1, k \neq j, l} (|\alpha_k^2| - |\beta_k^2|) \\
\leq \sum_{k=1, k \neq j, l} ||\alpha_k - |\beta_k|| (|\alpha_k| + |\beta_k|) \\
\leq 2^{-m} \sqrt{2} \sum_{k=1, k \neq j, l} (|\alpha_k| + |\beta_k|) \\
\leq 2^{-m} \sqrt{2} \left(2 \cdot 2^{n/2}\right).
\]

We used the Cauchy–Schwarz inequality to estimate sums involving $|\alpha_k|$ and $|\beta_k|$. For example:
\[
\sum_{k=1, k \neq j, l} |\alpha_k|^2 \leq \sqrt{2^n} \sum_{k=1, k \neq j, l} |\alpha_k|^2 = 2^{n/2}.
\]

In summary we get:
\[
||\psi| - |\phi||^2 \leq 2 \cdot 2^{n-2m} + 2^{3/2} \cdot 2^{(n/2-m)}.
\]

By choosing $m = \left\lceil n/2 + \log_2 \left(1/\epsilon^2\right) \right\rceil + 5$ and using Proposition 1 we get $\|R(\psi) - R(\phi)\|_{Fr} \leq \epsilon$ when $\epsilon \leq 1$.

In the case when all entries of $|\psi\rangle$ in the computational basis are non-zero, we add an ancilla and express the reflection around $|\psi\rangle$ using two reflection operators with unit vectors that can be approximated without using ancilla:
\[
I_1 \otimes R(\psi) = I_1 \otimes I_n - 2I_1 \otimes |\psi\rangle \langle \psi| \\
= I_1 \otimes I_n - 2 (|0\rangle \langle 0| + |1\rangle \langle 1|) \otimes |\psi\rangle \langle \psi| \\
= R_{I(\psi)} R_{I(\psi)}.
\]

Now we have all tools needed to prove Theorem 1:

\textbf{Proof of theorem 1.} We use construction from lemma 1 to simulate an $n$ qubit unitary using one ancilla and $2^n$ reflection operators. The unit vectors corresponding to each reflection operator have at least two zero coordinates in the computational basis, therefore we can use lemma 3 to approximate each reflection with a reflection operator without using ancillae with precision $2^{-m} \epsilon$. Unit vectors of each approximating reflection have entries of the form $(a + b\sqrt{2} + ci + di\sqrt{2})/2^{m(n,\epsilon)}$ for $m(n,\epsilon) = \left\lceil n/2 + O \left(\log \left(1/\epsilon\right)\right) \right\rceil$. Each reflection operator requires one ancillae and $O \left(2^{n-n} \cdot m(n,\epsilon)\right)$ Clifford and T gates according to lemma 2. Therefore, in total we need two ancillae and $O \left(4^n n \left(\log \left(1/\epsilon\right) + n\right)\right)$ Clifford and T gates to approximate the unitary within Frobenius distance $\epsilon$.

Our improved method for multi qubit exact synthesis outputs circuits with an exponential number of gates as a function of the number of qubits. This improves previously known method[3] which requires doubly exponential number of gates. The further improvements over our result may be possible: for example, removing the factor of $n$ from an expression $O \left(4^n n \left(\log \left(1/\epsilon\right) + n\right)\right)$.

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