Both Toffoli and Controlled-NOT need little help to do universal quantum computation

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Abstract

What additional gates are needed for a set of classical universal gates to do universal quantum computation? We answer this question by proving that any single-qubit real gate suffices, except those that preserve the computational basis.

The result of Gottesman and Knill implies that any quantum circuit involving only the Controlled-NOT and Hadamard gates can be efficiently simulated by a classical circuit. In contrast, we prove that Controlled-NOT plus any single-qubit real gate that does not preserve the computational basis and is not Hadamard (or its alike) are universal for quantum computing.

Previously only a “generic” gate, namely a rotation by an angle incommensurate with π, is known to be sufficient in both problems, if only one single-qubit gate is added.

Key words: quantum circuit, universal quantum computation, universal basis, Toffoli, Controlled-NOT.

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1 Introduction

A set of quantum gates $G$ (also called a basis) is said to be universal for quantum computation if any unitary operator can be approximated with arbitrary precision by a circuit involving only those gates (called a $G$-circuit). Since complex numbers do not help in quantum computation, we also call a set of real gates universal if it approximates arbitrary real orthogonal operators.

Which set of gates are universal for quantum computation? This basic question is important both in understanding the power of quantum computing and in the physical implementations of quantum computers, and has been studied extensively. Examples of universal bases are: (1) Toffoli, Hadamard, and $\frac{\pi}{4}$-gate, due to Kitaev [5] (2) CNOT, Hadamard, and $\frac{\pi}{8}$-gate, due to Boykin, Mor, Pulver, Roychowdhury, and Vatan [2], and (3) CNOT plus the set of all single-qubit gate, due to Barenco, Bennett, Cleve, DiVincenzo, Margolus, Shor, Sleator, Smolin, and Weinfurter [1].

Another basic question in understanding quantum computation is, Where does the power of quantum computing come from? Motivated by this question, we rephrase the universality question as follows: Suppose a set of gates $G$ already contains universal classical gates, and thus can do universal classical computation, what additional quantum gate(s) does it need to do universal quantum computation? Are there some gates that are more “quantum” than some others in bringing more computational power?

Without loss of generality, we assume that $G$ contains the Toffoli gate, since it is universal for classical computation. The above three examples of universal bases provide some answers to this question. It is clear that we need at least one additional gate that does not preserve the computational basis. Let us call such a gate basis-changing. Our main result is that essentially the basis-changing condition is the only condition we need:

**Theorem 1.1.** The Toffoli gate and any basis-changing single-qubit real gate are universal for quantum computing.

The beautiful Gottesman-Knill Theorem [3] implies that any circuit involving CNOT and Hadamard only can be simulated efficiently by a classical circuit. It is natural to ask what if Hadamard is replaced by some other gate. We know that if this replacement $R$ is a rotation by an irrational (in degrees) angle, then $R$ itself generates a dense subset of all rotations, and thus is universal together with CNOT, by Barenco et al. [1]. What if the replacement is a rotation of rational angles? We show that Hadamard and its alike are the only exceptions for a basis-changing single-qubit real gate, in conjunction with CNOT, to be universal.

**Theorem 1.2.** Let $T$ be a single-qubit real gate and $T^2$ does not preserve the computational basis. Then $\{\text{CNOT}, T\}$ is universal for quantum computing.

A basis is said to be complete if it generates a dense subgroup of $U(k)$ modular a phase, or $O(k)$ for some $k \geq 2$. We actually prove that each of the two bases in the above theorems...
gives rise to a complete basis. By the fundamental theorem of Kitaev [5] and Solovay [9], any complete basis can efficiently approximate any gate (modular a phase), or real gate if the basis is real. Therefore, any real gate can be approximated with precision \( \epsilon \) using \( \text{polylog}(\frac{1}{\epsilon}) \) gates from either basis, and any circuit over any basis can be simulated with little blow-up in the size.

We also provide an alternative prove for theorem 1.1 by directly constructing the approximation circuit for an arbitrary real single-qubit gate, instead of using Kitaev-Solovay theorem. The drawback of this construction is that the approximation is polynomial in \( \frac{1}{\epsilon} \); however, it is conceptually simpler, and uses some new idea that does not seem to have appeared before (for example, in the approximation for Control-sign-flip).

There is a broader concept of universality based on computations on encoded qubits, that is, fault-tolerant quantum computing. We do not discuss this type of computation, an interested reader is referred to the survey of Preskill [8]. For a more detailed reference to related works, refer to the book of Nielsen and Chuang [7].

2 Preliminary

Denote the set \( \{1, 2, \cdots, n\} \) by \([n]\). We will mostly follow the notations and definitions from the book by Kitaev, Shen, and Vyalyi [4].

The (pure) state of a quantum system is a unit vector in its state space. The state space of one quantum bit, or qubit, is the two dimensional complex Hilbert space, denoted by \( \mathcal{H} \). A prechosen orthonormal basis of \( \mathcal{H} \) is called the computational basis and is denoted by \( \{|0\rangle, |1\rangle\} \). The state space of a set of \( n \) qubits is the tensor product of the state space of each qubit, and the computational basis is denoted by

\[
\{|b\rangle = |b_1\rangle \otimes |b_2\rangle \otimes \cdots \otimes |b_n\rangle : b = b_1 b_2 \cdots b_n \in \{0, 1\}^n\}.
\]

A gate is a unitary operator \( U \in \mathcal{U}(\mathcal{H}^\otimes r) \), for some integer \( r > 0 \). For an ordered subset \( A \) of a set of \( n \) qubits, we write \( U[A] \) to denote applying \( U \) to the state space of those qubits.

A set of gates is also called a **basis**. A **quantum circuit** over a basis \( G \), or a \( G \)-circuit, on \( n \) qubits and of size \( m \) is a sequence \( U_1[A_1], U_2[A_2], \cdots, U_m[A_m] \), where each \( U_i \in G \) and \( A_i \subseteq [n] \). Sometimes we use the same notation for a circuit and for the unitary operator that it defines. The following definition generalizes the definition in [3].

**Definition 2.1.** The operator \( U : \mathcal{H}^\otimes r \rightarrow \mathcal{H}^\otimes r \) is approximated by the operator \( \hat{U} : \mathcal{H}^\otimes N \rightarrow \mathcal{H}^\otimes N \) using the ancilla state \( |\Psi\rangle \in \mathcal{H}^\otimes N - r \) if, for arbitrary vector \( |\xi\rangle \in \mathcal{H}^\otimes r \),

\[
\left\| \hat{U}(|\xi\rangle \otimes |\Psi\rangle) - U|\xi\rangle \otimes |\Psi\rangle \right\| \leq \epsilon \|\xi\|.
\]

Let \( G \) be a basis. A **\( G \)-ancilla state**, or an ancilla state when \( G \) is understood, of \( \ell \) qubits is a state \( A|b\rangle \), for some \( G \)-circuit \( A \) and some \( b \in \{0, 1\}^\ell \). A basis \( G \) is said to be **universal for quantum computing** if any gate (modular a phase), or any real gate when each gate in \( G \) is real, can be approximated with arbitrary precisions by \( G \)-circuits using \( G \)-ancillae. By a
phase, we mean the set \( \{ \exp(i\alpha) : \alpha \in \mathbb{R} \} \). The basis is said to be complete if it generates a dense subgroup of \( U(k) \) modular a phase, or \( O(k) \) when its real for some \( k \geq 2 \). A complete basis is clearly universal.

Now we introduce the standard notations for some gates we shall use later. Denote the identity operator on \( \mathcal{H} \) by \( I \). We often identify a unitary operator by its action on the computational basis. The Pauli operators \( \sigma^x \) and \( \sigma^z \), and the Hadamard gate \( H \) are

\[
\sigma^x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad H := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.
\]

If \( U \) is a gate on \( r \) qubits, for some \( r \geq 0 \) (when \( r = 0 \), \( U \) is a phase factor), \( \Lambda^k(U) \) is the gate on \( k + r \) qubits that applies \( U \) to the last \( r \) qubits if and only if the first \( k \) qubits are in \( |1\rangle^{\otimes k} \). The superscript \( k \) is omitted if \( k = 1 \). Changing the control condition to be \( |0\rangle^{\otimes k} \), we obtain \( \Lambda^k(U) \). The Toffoli gate is \( \Lambda^2(\sigma^x) \), and CNOT is \( \Lambda(\sigma^z) \). Evidently the latter can be realized by the former. From now on we only consider real gates. As in the previous section, a gate \( g \) is said to be basis-changing if it does not preserve the computational basis.

### 3 Completeness proofs

In this section we prove the following theorems, from which Theorem 1.2 and Theorem 1.1 follow immediately.

**Theorem 3.1.** Let \( S \) be any single-qubit real gate that is basis-changing after squaring. Then \( \{ \text{CNOT}, S \} \) is complete.

**Theorem 3.2.** The set \( \{ \Lambda^2(\sigma^z), H \} \) is complete.

We need the following two lemmas, which fortunately have been proved.

**Lemma 3.3 (Włodarski [10]).** If \( \alpha \) is not an integer multiple of \( \pi/4 \), and \( \cos \beta = \cos^2 \alpha \), then either \( \alpha \) or \( \beta \) is an irrational multiple of \( \pi \).

**Lemma 3.4 (Kitaev [5]).** Let \( \mathcal{M} \) be a Hilbert space of dimension \( \geq 3 \), \( |\xi\rangle \in \mathcal{M} \) a unit vector, and \( H \subset SO(\mathcal{M}) \) be the stabilizer of the subspace \( \mathbb{R}(|\xi\rangle) \). If \( V \in O(\mathcal{M}) \) does not preserve \( \mathbb{R}(|\xi\rangle) \), \( H \cup V^{-1}HV \) generates a dense subgroup of \( SO(\mathcal{M}) \).

**Proof of Theorem 3.1.** Define

\[
U := (S \otimes S \cdot \Lambda(\sigma^z)[1, 2])^2.
\]

It suffices to prove that \( U \) and \( \Lambda(\sigma^x) \) generate a dense subgroup of \( SO(4) \). Without loss of generality, we assume that \( U \) is a rotation by an angle \( \theta \), the other case can be proved similarly. Then by the assumption, \( \theta \) is not an integer multiple of \( \pi/4 \).
Direct calculation shows that $U$ has eigenvalues $\{1, 1, \exp(\pm i\alpha)\}$, where
\[
\alpha = 2 \arccos \cos^2 \theta.
\]
The two eigenvectors with eigenvalue 1 are
\[
|\xi_1\rangle := \frac{1}{2}(|00\rangle - |01\rangle + |10\rangle + |11\rangle),
\]
and
\[
|\xi_2\rangle := \frac{\sin \theta}{\sqrt{2}}(-|0\rangle + |1\rangle) + \frac{\cos \theta}{\sqrt{2}}(|0\rangle - |1\rangle).
\]
Let $\{|\xi_i\rangle : i \in \mathbb{Z}\}$ be a set of orthonormal vectors.

By Lemma 3.3, $\alpha$ is incommensurate with $\pi$, therefore, $U$ generates a dense subgroup of $H_1 := SO(\text{span}\{|\xi_3\rangle, |\xi_4\rangle\})$. Note that $\Lambda(\sigma^x)[1, 2]$ preserve $|\xi_1\rangle$, but not $\text{span}\{|\xi_2\rangle\}$. Therefore, by Lemma 3.4, the set
\[
H_1 \bigcup \Lambda(\sigma^x)[1, 2] H_1 \Lambda(\sigma^x)[1, 2]
\]
generates a dense subgroup of
\[
SO(\text{span}\{|\xi_i\rangle : i = 2, 3, 4\}) =: H_2,
\]
thus so does $\{U, \Lambda(\sigma^x)[1, 2]\}$. Finally, observe that $\Lambda(\sigma^x)[2, 1]$ does not preserve $\text{span}\{|\xi_1\rangle\}$, therefore, apply Lemma 3.4 again we conclude that $\{U, \Lambda(\sigma^x)[1, 2], \Lambda(\sigma^x)[2, 1]\}$ generates a dense subgroup of $SO(4)$.

**Proof of Theorem 3.2.** Define
\[
U := (H \otimes H \otimes H \cdot \Lambda^2(\sigma^x)[1, 2, 3])^2.
\]
Direct calculation shows that $U$ has eigenvalue 1 with multiplicity 6, and the other two eigenvalues $\lambda_{\pm} := \exp(\pm i\alpha)$, where $\alpha = \pi - \arccos \frac{3}{4}$. Since $\lambda_{\pm}$ are roots of the irreducible polynomial
\[
\lambda^2 - \frac{3}{2} \lambda + 1,
\]
which is not integral, therefore $\lambda_{\pm}$ are not algebraic integers. Thus $\alpha$ is incommensurate with $\pi$, which implies that $U$ generates a dense subgroup of the rotations over the corresponding eigenspace (denote the eigenvectors by $|\xi_7\rangle$ and $|\xi_8\rangle$).

By direct calculation, the eigenvectors correspond to eigenvalue 1 are:
\[
\{|000\rangle, |010\rangle, |100\rangle, |001\rangle + |011\rangle, |101\rangle + |110\rangle + |111\rangle, |011\rangle - |101\rangle\}.
\]
Label the above eigenvectors by $|\xi_i\rangle$, $i \in [6]$. It is easy to verify that each $U_i$, $i \in [6]$, constructed below preserves $\{ |\xi_j\rangle : 1 \leq j < i \}$, but not span$\{|\xi_i\rangle\}$.

\[
U_1 := I \otimes I \otimes H, \quad U_2 := U_1 \cdot \Lambda^2(\sigma^x)[2, 3, 1] \cdot U_1, \\
U_3 := U_1 \cdot \Lambda^2(\sigma^x)[1, 3, 2] \cdot U_1, \quad U_4 := \Lambda^2(\sigma^x)[2, 3, 1], \\
U_5 := U_1 \cdot \Lambda^2(\sigma^x)[2, 3, 1] \cdot U_1, \quad U_6 := \Lambda^2(\sigma^x)[1, 3, 2].
\]

Applying Lemma \[3.4\] several times, we see that \{$U_i, U_i U_{i+1}, \ldots, U_6$\} generates a dense subgroup of span$\{|\xi_j\rangle : i \leq j \leq 8 \}$. Thus \{$\Lambda^2(\sigma^x), H$\} generates a dense subgroup of $SO(8)$. We leave the details for the interested readers.

### 4 Alternative proof for Theorem \[1.1\]

Fix an arbitrary basis-changing real single-qubit gate $S$, and the basis

\[ \mathcal{B} := \{ S, \Lambda^2(\sigma^x) \} \]

In this section we give an explicit construction to approximate an arbitrary real gate using the basis $\mathcal{B}$. Due to the following result by Barenco et al. \[1\], we need only consider approximating single-qubit real gates:

**Proposition 4.1 (Barenco et al. \[1\]).** Any gate on $r$ qubits can be realized by $O(r^2 4^r)$ CNOT and single-qubit gates.

Fix an arbitrary single-qubit gate $W$ that we would like to approximate. Without loss of generality, we can assume that $S$ and $W$ are rotations, for otherwise $\sigma^x S$ and $\sigma^x W$ are.

For any $\beta \in [0, 2\pi)$, define

\[ |\phi_\beta\rangle := \cos \beta |0\rangle + \sin \beta |1\rangle, \quad \text{and}, \quad U_\beta := \begin{pmatrix} \cos \beta & -\sin \beta \\ \sin \beta & \cos \beta \end{pmatrix}. \]

Let $\theta, \alpha \in [0, 2\pi)$, and $\theta$ not an integral multiple of $\pi/2$, be such that $S \equiv U_\theta$ and $W \equiv U_\alpha$. The following proposition can be easily checked.

**Proposition 4.2.** Let $W_{\alpha/2}$ be a gate on $k + 1$ qubits such that $W_{\alpha/2} |0\rangle^{\otimes k+1} = |\phi_{\alpha/2}\rangle \otimes |0\rangle^{\otimes k}$. With

\[ W_\alpha := W_{\alpha/2} (-\bar{\Lambda}^{k+1}(-1)) W_{\alpha/2}^\dagger \sigma^z[1], \quad (1) \]

for any vector $|\xi\rangle \in \mathcal{H}$,

\[ U_\alpha |\xi\rangle \otimes |0\rangle^{\otimes k} = W_\alpha (|\xi\rangle \otimes |0\rangle^{\otimes k}). \quad (2) \]

Clearly $\bar{\Lambda}^{k+1}(-1)$ can be realized by $\Lambda^2(\sigma^x)$ and $\sigma^z$. Therefore, to approximate $U_\alpha$, it suffices to approximate $\sigma^z$ and $W_{\alpha/2}$, which we will show in the following subsections.

Define the constants

\[ \delta_\theta := 1/\log \frac{1}{\cos^4 \theta + \sin^4 \theta}, \quad \text{and}, \quad \delta'_\theta := 1/\log \frac{1}{\cos^2 \theta}. \]
4.1 Approximating $\sigma^z$

If $\theta$ is a multiple of $\pi/4$, say $\theta = \pi/4$, then we can easily do a sign-flip by applying a bit-flip on $U_\theta|1\rangle = \frac{1}{\sqrt{2}}(0) + \frac{1}{\sqrt{2}}|1\rangle$. But for a general $\theta$, $U_\theta|1\rangle = -\sin\theta|0\rangle + \cos\theta|1\rangle$ is “biased”. Immediately comes into mind is the well-known idea of von Neumann on how to approximate a fair coin by tossing a sequence of coins of identical bias\footnote{That is, toss two coins, declare “0” if the outcomes are “01”, declare “1” if the outcomes are “10”, and continue the process otherwise.}. To illustrate the idea, consider

$$U_\theta|0\rangle \otimes U_\theta|1\rangle = \sin \theta \cos(|11\rangle - |00\rangle) + \cos^2\theta|01\rangle - \sin^2\theta|10\rangle.$$ 

If we switch $|00\rangle$ and $|11\rangle$ and leave the other two base vectors unchanged, the first term on the right-hand side changes the sign, while the remaining two terms are unchanged. While we continue tossing pairs of “quantum coins” and do the $|00\rangle$-and-$|11\rangle$ switch, we approximate the sign-flip very quickly. The state defined below will serve the role of arbitrary unit vector $|b\rangle$.

**Definition 4.3.** For any integer $k \geq 0$, the phase ancilla of size $k$ is the state

$$|\Phi_k\rangle := (U_\theta|0\rangle \otimes U_\theta|1\rangle)^\otimes k.$$ 

Clearly $|\Phi_k\rangle$ can be prepared from $|0\rangle^\otimes 2k$ by a $\mathcal{B}$-circuit of size $O(k)$.

**Lemma 4.4.** The operator $\sigma^z$ can be approximated with precision $\epsilon$, for any $\epsilon > 0$, by a $\mathcal{B}$-circuit of size $O(k)$, using the phase ancilla $|\Phi_k\rangle$, for some integer $k = O\left(\delta_0 \log \frac{1}{\epsilon}\right)$.

**Proof.** Let $k$ be an integer to be determined later. The following algorithm is a description of a circuit approximating $\sigma^z$ using $|\Phi_k\rangle$.

**Algorithm 1.** A $\mathcal{B}$-circuit $\hat{\sigma}^z$ approximating $\sigma^z$ using the phase ancilla $|\Phi_k\rangle$.

Let $|b_0\rangle \otimes |b\rangle$ be a computational base vector, where $b_0 \in \{0,1\}$ is the qubit to which $\sigma^z$ is to be applied, and $b = b_1b_2b_3 \cdots b_{k}$, $b' = b_1'b_2'b_3' \cdots b_k'$, $b, b' \in \{0,1\}^{2k}$ are the ancilla qubits. Condition on $b_0$ (that is, if $b_0 = 0$, do nothing, otherwise do the following),

Case 1: There is no $i$ such that $b_i \oplus b'_i = 0$, do nothing.

Case 2: Let $i$ be the smallest index such that $b_i \oplus b'_i = 0$, flip $b_i$ and $b'_i$.

Clearly the above algorithm can be carried out by $O(k)$ applications of Toffoli. Fix an arbitrary unit vector $|\xi\rangle \in \mathcal{H}$. Since neither $\sigma^z$ nor $\hat{\sigma}^z$ changes $|0\rangle \langle 0|(|\xi\rangle \otimes |\Phi_k\rangle)$,

$$||\sigma^z|\xi\rangle \otimes |\Phi_k\rangle - \hat{\sigma}^z(|\xi\rangle \otimes |\Phi_k\rangle)|| \leq ||-|1\rangle \otimes |\Phi_k\rangle - \hat{\sigma}^z(|1\rangle \otimes |\Phi_k\rangle)||.$$ \hspace{1cm} (3)

Let $|\Phi^+_k\rangle$ ($|\Phi^-_k\rangle$) be the projection of $|\Phi_k\rangle$ to the subspace spanned by the base vectors satisfying Case (1) (Case (2)), it is easy to prove by induction that

$$\hat{\sigma}^z(|1\rangle \otimes |\Phi^+_k\rangle) = |1\rangle \otimes |\Phi^+_k\rangle, \quad \text{and,} \quad \hat{\sigma}^z(|1\rangle \otimes |\Phi^-_k\rangle) = -|1\rangle \otimes |\Phi^-_k\rangle.$$
Furthermore,

$$\|\Phi_k^\perp\| = (\cos^4 \theta + \sin^4 \theta)^{k/2}.$$  

Therefore, the left-hand side of Equation 3 is upper bounded by

$$2 \|\Phi_k^\perp\| = 2 (\cos^4 \theta + \sin^4 \theta)^{k/2}.$$  

Since $\theta$ is not a multiple of $\pi/2$, the right-hand side is $< 1$. Thus choosing $k = O(\delta_\theta \log \frac{1}{\epsilon})$, the right-hand side in the above can be made $\leq \epsilon$.

### 4.2 Creating $|\phi_{\alpha/2}\rangle$

We would like to construct a circuit that maps $|0\rangle \otimes |0\rangle \otimes^k$ to a state close to $|\phi_{\alpha/2}\rangle \otimes |0\rangle \otimes^k$. The main idea is to create a “logical” $|\phi_{\alpha/2}\rangle$:

$$|\hat{\phi}_{\alpha/2}\rangle := \cos \frac{\alpha}{2} |0\rangle + \sin \frac{\alpha}{2} |\hat{1}\rangle,$$

where $|\hat{0}\rangle$ and $|\hat{1}\rangle$ are two orthonormal vectors in a larger space spanned by ancillae, and then undo the encoding to come back to the computational basis. To create $|\hat{\phi}_{\alpha/2}\rangle$, we first create a state almost orthogonal to $|\hat{0}\rangle$, and then apply Grover’s algorithm to rotate this state toward $|\hat{\phi}_{\alpha/2}\rangle$. Define the operator $T_{\theta}$ on 2 qubits as

$$T_{\theta} := U_{-\theta}[1] \Lambda(\sigma^x)[1, 2] U_{\theta}[1].$$

Since for any $\beta$, $U_{-\beta} = \sigma^x U_{\beta} \sigma^x$, $T_{\theta}$ and $\Lambda(T_{\theta})$ can be realized by the basis $\mathfrak{B}$. Let

$$\mathfrak{B}_1 := \{\Lambda^2(\sigma^x), \sigma^z, U_{\theta}, U_{-\theta}, T_{\theta}, \Lambda(T_{\theta})\}.$$  

**Lemma 4.5.** For any $\epsilon > 0$ there exists a $\mathfrak{B}_1$-circuit $\tilde{W}_{\alpha/2}$ of size $O(\delta_\theta \frac{1}{\epsilon} \log \frac{1}{\epsilon})$ that uses $O(\delta_\theta \frac{1}{\epsilon} \log \frac{1}{\epsilon})$ ancillae and satisfies

$$\left\|\tilde{W}_{\alpha/2}[0] \otimes^k 1 - |\phi_{\alpha/2}\rangle \otimes |0\rangle \otimes^k\right\| \leq \epsilon.$$

**Proof.** Figure 4 illustrates our proof. Let $k > 0$ be an integer to be specified later. Define

$$|\hat{0}\rangle := |0\rangle \otimes^k, \quad |\hat{1}\rangle := T_{\theta}^\perp |\hat{0}\rangle, \quad \text{and,} \quad \gamma := \arcsin \left(\cos 2k \theta\right).$$

Notice that $\pi/2 - \gamma$ is the angle between $|\hat{0}\rangle$ and $|\hat{1}\rangle$, and $0 < \gamma < \pi/2$, since $\sin \gamma = \langle \hat{0}| \hat{1}\rangle$. Let $S$ be the plane spanned by $|\hat{0}\rangle$ and $|\hat{1}\rangle$. Let $|\hat{1}\rangle$ be the unit vector perpendicular to $|\hat{0}\rangle$ in $S$ and the angle between $|\hat{1}\rangle$ and $|\hat{0}\rangle$ is $\gamma$.

Observe that on $S$ we can do the reflection along $|\hat{1}\rangle$ and the reflection along $|\hat{0}\rangle$. The former is simply $\Lambda^2(\sigma^z)$, which can be implemented using $\Lambda^2(\sigma^x)$ and $\sigma^z$. Since $T_{\theta}^{-1} = T_{\theta}$, the reflection along $|\hat{1}\rangle$ is

$$R := T_{\theta}^\perp \Lambda(\sigma^z) T_{\theta}^\perp.$$
Without loss of generality we can assume $\alpha/2 < \pi/2$; otherwise we will rotate $|\bar{1}\rangle$ close to $\Lambda^{2k}(\sigma^z)|\hat{\phi}_{\alpha/2}\rangle$ and then apply $\Lambda^{2k}(\sigma^z)$. Choose $k$ sufficiently large so that $\gamma < \pi/2 - \alpha/2$.

Now we can apply Grover’s algorithm to rotate $|\bar{1}\rangle$ to a state very close to $|\hat{\phi}_{\alpha/2}\rangle$. After that we do a “controlled-roll-back” to map $|\bar{1}\rangle$ (approximately) to $|1\rangle^k$ and does not change $|\tilde{\psi}_3\rangle$. This will give us an approximation of $|\hat{\phi}_{\alpha/2}\rangle$ in the state space of the controlling qubit.

**Algorithm 2.** A $\mathfrak{B}_1$-circuit $\tilde{W}_{\alpha/2}$ that maps $|0\rangle \otimes |0\rangle^{\otimes k}$ to a state close to $|\hat{\phi}_{\alpha/2}\rangle \otimes |0\rangle^{\otimes k}$.

1. Apply $I \otimes T_{\tilde{\theta}}^{\otimes k}$.
2. (Grover’s algorithm) Apply $(R \Lambda^{2k}(\sigma^z))^T$.
3. (Sub-circuit $A_3$) For a computational base vector $|b\rangle$ of the ancillae, if $|b\rangle \neq |\tilde{0}\rangle$, flip the first bit.
4. (Sub-circuit $A_4$) Use the first bit as the condition bit, apply $\Lambda(T_{\tilde{\theta}}^{\otimes k})$.

It can be easily verified that

$$\left\| \tilde{W}_{\alpha/2}(|0\rangle \otimes |0\rangle^{\otimes k}) - |\phi_{\alpha/2}\rangle \otimes |0\rangle^{\otimes k} \right\| \leq 2\gamma.$$  

Setting $\gamma \approx \epsilon/2$, by direct computation the number of ancillae is $O(k) = O(\delta_{\tilde{\theta}}' \log \frac{1}{\epsilon})$, and the size of $\tilde{W}_{\alpha/2}$ is $O(k/\gamma) = O(\delta_{\tilde{\theta}}' \frac{1}{\epsilon} \log \frac{1}{\epsilon})$. 

\[\square\]
4.3 Approximating $U_\alpha$

Theorem 1.1 is a straightforward corollary of the following theorem and Proposition 4.1.

**Theorem 4.6.** For any $\epsilon > 0$, the operator $U_\alpha$ can be approximated with precision $\epsilon$ by a $B$-circuit of size \( O(\delta_\theta \cdot \frac{1}{\epsilon} \cdot \log \frac{1}{\epsilon}) \) and using \( O(\delta_\theta \cdot \log \frac{1}{\epsilon}) \) ancillae.

**Proof.** We first compose a $B_1$-circuit that approximates $U_\alpha$, according to Equation 1, 2, and Algorithm 2, and use $k_1$ (different) ancillae in each call to the latter, for an integer $k_1$ to be specified later. Let $\gamma := \cos^{2k_1} \theta$. Then the precision is $O(\gamma)$. After implementing $\Theta_\theta$ and $\Lambda(\Theta_\theta)$, there are in total $O(\frac{1}{\epsilon})$ uses of $\sigma^z$.

Finally we apply Algorithm 3 to approximate each $\sigma^z$ using the same phase ancilla $|\Phi_{k_2}\rangle$ for $k_2 = O(1/\gamma^3)$. Let $\delta_\theta := 2(\cos^4 \theta + \sin^4 \theta)^{k_2/2}$ be the error of one call to $\tilde{\sigma}^z$ using exactly $|\Phi_{k_2}\rangle$. Observe that using the same phase ancilla for $O(\frac{1}{\gamma})$ times causes error at most $1 + 2 + \cdots + O(\frac{1}{\gamma}) = O(\frac{1}{\gamma})$. Setting $\delta_\theta = \gamma^3$, the total error caused by $\tilde{\sigma}^z$ is $O(\gamma)$. Thus the total error of the whole circuit is still $O(\gamma)$. Setting $\gamma \approx \epsilon$, $k_1 = O(\delta_\theta \log \frac{1}{\epsilon}) = O(\delta_\theta \log \frac{1}{\epsilon})$ and $k_2 = O(\delta_\theta \log \frac{1}{\epsilon})$. Therefore the number of ancillae is $O(k_1 + k_2) = O(\delta_\theta \frac{1}{\epsilon} \log \frac{1}{\epsilon})$. The size of the circuit is $O((k_1 + k_2) \frac{1}{\epsilon}) = O(\delta_\theta \frac{1}{\epsilon} \log \frac{1}{\epsilon})$.

\[\Box\]

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