UNIVERSAL QUANTUM GATES

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Abstract. In this paper we study universality for quantum gates acting on qudits. Qudits are states in a Hilbert space of dimension $d$ where $d$ can be any integer $\geq 2$. We determine which 2-qudit gates $V$ have the properties (i) the collection of all 1-qudit gates together with $V$ produces all $n$-qudit gates up to arbitrary precision, or (ii) the collection of all 1-qudit gates together with $V$ produces all $n$-qudit gates exactly. We show that (i) and (ii) are equivalent conditions on $V$, and they hold if and only if $V$ is not a primitive gate. Here we say $V$ is primitive if it transforms any decomposable tensor into a decomposable tensor. We discuss some applications and also relations with work of other authors.

1. Statements of main results

We determine which 2-qudit gates $V$ have the property that all 1-qudit gates together with $V$ form a universal collection, in either the approximate sense or the exact sense. Here $d$ is an arbitrary integer $\geq 2$. Our results are new for the case of qubits, i.e., $d = 2$ (which for many is the case of primary interest). We treat the case $d > 2$ as well because it is of independent interest and requires no additional work.

Since Deutsch [3] found a universal gate (on 3 qubits), universal gates for qubits have been extensively studied. We mention in particular the papers [1], [2], [4], [5] and [6] which will be further discussed in §2.

First we set up some notations. A qudit is a (normalized) state in the Hilbert space $\mathbb{C}^d$. An $n$-qudit is a state in the tensor product Hilbert space $H = (\mathbb{C}^d)^\otimes n = \mathbb{C}^d \otimes \cdots \otimes \mathbb{C}^d$. The computational basis of $H$ is the orthonormal basis given by the $d^n$ classical $n$-qudits

$$|i_1i_2\cdots i_n\rangle = |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \quad (1.1)$$

where $0 \leq i_j \leq d - 1$. The general state in $H$ is a superposition

$$|\psi\rangle = \sum \psi_{i_1i_2\cdots i_n} |i_1i_2\cdots i_n\rangle \quad (1.2)$$

where $||\psi||^2 = \sum |\psi_{i_1i_2\cdots i_n}|^2 = 1$. We say $\psi$ is decomposable when it can be written as a tensor product $|x_1 \cdots x_n\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_n\rangle$ of qudits.

A quantum gate on $n$-qudits is a unitary operator $L : (\mathbb{C}^d)^\otimes n \rightarrow (\mathbb{C}^d)^\otimes n$. These gates form the unitary group $U((\mathbb{C}^d)^\otimes n) = U(d^n)$. A sequence $L_1, \ldots, L_k$ of gates constitutes a quantum circuit on $n$-qudits. The output of that circuit is the product gate $L_1 \cdots L_k$. In
practice, one wants to build circuits out of gates $L_i$ which are local in that they operate on only a small number of qudits, typically 1, 2 or 3.

We can produce local gates in the following way. A 1-qudit gate $A$ gives rise to $n$ different $n$-qudit gates $A(1), \ldots, A(n)$ obtained by making $A$ act on the individual tensor slots. So

$$A(l)|x_1 \cdots x_l \cdots x_n\rangle = |x_1\rangle \otimes \cdots \otimes |x_{l-1}\rangle \otimes A|x_l\rangle \otimes |x_{l+1}\rangle \otimes \cdots \otimes |x_n\rangle$$  \hspace{1cm} (1.3)

Similarly, for a 2-qudit gate $B$, we have $n(n-1)$ different $n$-qudit gates $B(p,q)$ obtained by making $B$ act on pairs of slots. For $B = \sum S_i \otimes T_i$ we have $B(p,q) = \sum S_i(p)T_i(q)$.

A basic problem in quantum computation is to find collections of gates which are universal in the following sense.

**Definition 1.1.** A collection of 1-qudit gates $A_i$ and 2-qudit gates $B_j$ is called universal if, for each $n \geq 2$, every $n$-qudit gate can be approximated with arbitrary accuracy by a circuit made up of the $n$-qudit gates produced by the $A_i$ and $B_j$.

We also have the stronger notion, which we call exact universality.

**Definition 1.2.** A collection of 1-qudit gates $A_i$ and 2-qudit gates $B_j$ is called exactly universal if, for each $n \geq 2$, every $n$-qudit gate can be obtained exactly by a circuit made up of the $n$-qudit gates produced by the $A_i$ and $B_j$.

In mathematical terms, universality means that the $n$-qudit gates produced by the $A_i$ and $B_j$ generate a dense subgroup of $U(d^n)$, while exact universality means that these gates generate the full group $U(d^n)$.

Note that a finite collection of 1-qudit and 2-qudit gates can be universal, but it can never be exactly universal, as the group it generates is countable, while $U(d^n)$ is uncountable.

We now state our main result. We introduce the following terminology. A 2-qudit gate $V$ is primitive if $V$ maps decomposables to decomposables, i.e. if $|x\rangle$ and $|y\rangle$ are qudits then we can find qudits $|u\rangle$ and $|v\rangle$ such that $V|x\rangle = |uv\rangle$. We say $V$ is imprimitive when $V$ is not primitive. Let $P : (\mathbb{C}^d)^{\otimes 2} \to (\mathbb{C}^d)^{\otimes 2}$ denote the 2-qudit gate such that $P|xy\rangle = |yx\rangle$.

**Theorem 1.3.** Suppose we are given a 2-qudit gate $V$. Then the following are equivalent:

(i) the collection of all 1-qudit gates $A$ together with $V$ is universal

(ii) the collection of all 1-qudit gates $A$ together with $V$ is exactly universal

(iii) $V$ is imprimitive

We prove Theorem 1.3 in \S\S 7. The implications (ii) ⇒ (i) ⇒ (iii) are easy. The hard part is showing (iii) ⇒ (ii). In \S 8 we give a variant of Theorem 1.3.

In \S 8 we characterize primitive gates in the following way.

**Theorem 1.4.** $V$ is primitive if and only if $V = S \otimes T$ or $V = (S \otimes T)P$ for some 1-qudit gates $S$ and $T$. Thus $V$ acts by $V|xy\rangle = S|x\rangle \otimes T|y\rangle$ or by $V|xy\rangle = S|y\rangle \otimes T|x\rangle$.

**Corollary 1.5.** Almost every 2-qudit gate is imprimitive. In fact the imprimitive gates form a connected open dense subset of $U(d^2)$.

For the proofs, we use Lie group theory, including some representation theory for compact groups. For exact universality, we also use some real algebraic geometry (in proving
Lemma 4.1). Our methods can be used to prove a variety of results on universality and exact universality. We illustrate this is in §9.

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2. Examples and relations to works of other authors

In this section, we give examples of primitive and non-primitive gates.

Proposition 2.1. Suppose a 2-qudit gate \( V \) is diagonal in the computational basis with \( V|jk\rangle = e^{i\theta_{jk}}|jk\rangle \). Then \( V \) is primitive iff for all \( j, k, p, q \) we have

\[
\theta_{jk} + \theta_{pq} \equiv \theta_{jq} + \theta_{pk} \pmod{2\pi} \tag{2.1}
\]

Proof. We apply \( V \) to the decomposable tensor \( |\psi\rangle = (|j\rangle + |p\rangle) \otimes (|k\rangle + |q\rangle) \). If \( V \) is primitive then the result \( V|\psi\rangle = \alpha_{jk}|jk\rangle + \alpha_{jq}|jq\rangle + \alpha_{pk}|pk\rangle + \alpha_{pq}|pq\rangle \) must be decomposable, where we put \( \alpha_{jk} = e^{i\theta_{jk}} \). Thus \( \alpha_{jk} - \alpha_{jq}\alpha_{pk} \) vanishes, which amounts to (2.1). Conversely, if (2.1) holds, we can solve for scalars \( \beta_j \) and \( \gamma_k \) such that \( \alpha_{jk} = \beta_j\gamma_k \). Then \( V = B \otimes C \) where \( B|j\rangle = \beta_j|j\rangle \) and \( C|j\rangle = \gamma_j|j\rangle \).

For example, if all \( \theta_{jk} \) are zero except that \( \theta_{00} \not\equiv 0 \pmod{2\pi} \), then \( V \) is imprimitive. In the case \( d = 2 \), (2.1) reduces to the condition \( \theta_{00} + \theta_{11} \equiv \theta_{01} + \theta_{10} \pmod{2\pi} \) found in §9.

In another direction, consider the generalized CNOT gate \( X \) given by \( X|ij\rangle = |i, i \oplus j\rangle \) where \( i \oplus j \) denotes addition of integers modulo \( d \). For \( d = 2 \), \( X \) is the standard CNOT gate. Then \( X \) is imprimitive because \( X \) transforms the decomposable tensor \( (|0\rangle + |1\rangle) \otimes (|0\rangle + |1\rangle) \) into the indecomposable tensor \( |00\rangle + |11\rangle \). Therefore the collection of all 1-qudit gates together with \( X \) is exactly universal. This was already proven when \( d = 2 \) in §9.

Here is another kind of controlled gate. Take some 1-qudit gate \( U \) and define a 2-qudit gate \( X_U \) by \( X_U|0k\rangle = |0\rangle \otimes U|k\rangle \) and, for \( j \not\equiv 0 \), \( X_U|jk\rangle = |jk\rangle \). Then \( X_U \) is primitive if and only if \( U \) is a scalar operator, i.e., \( U|x\rangle = e^{i\theta}|x\rangle \). Indeed, for any \( j \not\equiv 0 \) we have \( X_U(|j\rangle \otimes |x\rangle + |0\rangle \otimes |x\rangle) = |j\rangle \otimes |x\rangle + |0\rangle \otimes U|x\rangle \). This must be decomposable if \( X_U \) is primitive. This can only happen if \( U|x\rangle = e^{i\theta}|x\rangle \). Since \( |x\rangle \) is arbitrary, we see that \( e^{i\theta} \) is independent of \( |x\rangle \). Thus \( U \) is a scalar operator. This construction yields many non-primitive gates which have finite order.

Another point of view is to consider a 2-qudit gate \( V \) just by itself. This is interesting because almost any \( V \) is universal; we call such gates IU gates (individually universal). This was proven in §9 and (for \( d = 2 \)) in §9. More precisely, these authors found finitely many open conditions on gates (e.g., the closure of the subgroup generated by the gate is a maximal torus in \( U(d^2) \)) which automatically imply the gate is IU. In particular, all their gates have infinite order.

By theorem 1.3, IU gates are imprimitive. There are many gates which are imprimitive but not IU: for instance, imprimitive gates which are diagonal in the computational basis.

3. Proof of Theorem 1.3 (outline)

We will end up focusing on 2-qudits, and so we put \( G = U(d^2) \). We define \( H \) to be the subgroup of \( G \) generated by the 2-qudit gates \( A(1) \) and \( A(2) \) for \( A \in U(d) \). Let \( F \) be the subgroup of \( G \) generated by \( H, V, V(2,1) \).

(ii) \( \Rightarrow \) (i): obvious
(i)⇒(iii): Suppose \( V \) is primitive. We will show that universality fails for \( n = 2 \), i.e., \( F \) is not dense in \( G \). Clearly \( F \) lies in the set \( L \) of primitive gates. But (a) \( L \) is a closed subgroup of \( G \) and (b) \( L \neq G \). Indeed (a) follows easily from the definition of primitive since the decomposable tensors in \( (\mathbb{C}^d)^\otimes 2 \) form a closed subset. Also (b) is true because we already exhibited in \( \mathbb{G} \) some 2-qudit gates which are imprimitive. So \( L \), and hence \( F \), is not dense in \( G \).

(iii)⇒(ii) takes more work. Here is an outline. The details are given in §4 (first step), §5 (second step), §6 (fourth step) and §7 (fifth step).

First step: We give a general abstract result, Lemma 4.1, which says that if \( k \) closed connected subgroups of a compact group \( G \) generate a dense subgroup of \( G \), they must in fact generate \( G \).

Second step: Using Lemma 4.1 we reduce the problem to \( n = 2 \).

Third step: \( H \) is the set of 2-qudit gates of the form \( S \otimes T \). So \( H \) is a closed connected Lie subgroup of \( G \). Lemma 4.1 suggests that we look for a closed connected subgroup \( H' \) of \( G \) such that \( H \) and \( H' \) generate a dense subgroup of \( G \) (3.1)

Fourth step: We will use the Lie algebras \( \mathfrak{g} = \text{Lie } G \), \( \mathfrak{h} = \text{Lie } H \) and \( \mathfrak{h}' = \text{Lie } H' \). Showing (3.1) amounts to showing that \( \mathfrak{h} \) and \( \mathfrak{h}' \) generate \( \mathfrak{g} \) as a Lie algebra. Let \( \mathfrak{z} \) be the Lie subalgebra generated by \( \mathfrak{h} \) and \( \mathfrak{h}' \). Then \( \mathfrak{h} \subseteq \mathfrak{z} \subseteq \mathfrak{g} \). Using some representation theory, we show abstractly in Lemma 6.1 that there is no Lie algebra strictly in between \( \mathfrak{h} \) and \( \mathfrak{g} \). Thus \( \mathfrak{z} = \mathfrak{h} \) or \( \mathfrak{z} = \mathfrak{g} \).

Fifth step: We need to rule out \( \mathfrak{z} = \mathfrak{h} \). Clearly \( \mathfrak{z} = \mathfrak{h} \iff \mathfrak{h} = \mathfrak{h}' \iff H = H' \rightarrow V \) normalizes \( H \). But we prove in Proposition 7.1 that the normalizer of \( H \) is the set of primitive gates. So \( V \) cannot normalize \( H \). Thus \( \mathfrak{z} \neq \mathfrak{h} \).

Sixth step: Thus \( \mathfrak{z} = \mathfrak{g} \). This proves (3.1). Now (3.1) and Lemma 4.1 imply that \( H \) and \( H' \) generate \( G \). So a fortiori, \( H \) and \( V \) generate \( G \).

Remark 3.1. (i) We actually proved something stronger than exact universality, namely that \( H \) and \( V \) generate \( G \).

(ii) To prove (iii)⇒(i) directly, there is no need for \( H' \) or Lemma 4.1. We can simply work with \( F \). The problem is to show that \( F \) is dense in \( G \), which amounts to showing that \( \mathfrak{f} = \mathfrak{g} \) where \( \mathfrak{f} \) is the Lie algebra of the closure \( \overline{F} \) of \( F \) in \( G \). Clearly \( \mathfrak{h} \subseteq \mathfrak{f} \subseteq \mathfrak{g} \) Then we use the same two results, Lemma 6.1 and Proposition 7.1, to show, respectively, that (a) \( \mathfrak{f} = \mathfrak{h} \) or \( \mathfrak{f} = \mathfrak{g} \) and (b) \( \mathfrak{f} = \mathfrak{h} \) does not happen.

4. First step: From universality to exact universality

Our bridge from universality to exact universality is

Lemma 4.1. Let \( \mathcal{G} \) be a compact Lie group. If \( \mathcal{H}_1, \ldots, \mathcal{H}_k \) are closed connected subgroups and they generate a dense subgroup of \( \mathcal{G} \), then in fact they generate \( \mathcal{G} \).

Proof. We can take \( k = 2 \) since the general case easily reduces to this. Consider the subset \( \Sigma = \mathcal{H}_1 \mathcal{H}_2 \) of \( \mathcal{G} \) and its \( n \)-fold products \( \Sigma^n = \Sigma \cdots \Sigma \). Then \( \Sigma, \Sigma^2, \ldots \) is an increasing
Lemma 6.1. There are no Lie algebras strictly in between $\mathfrak{h}$ and $\mathfrak{g}$. We want to show that there exists $m$ such that $\Sigma^m = \mathcal{G}$.

To begin with, we observe that $\Sigma^n$ is compact and connected. This follows as $\Sigma^n$ is the image of the continuous multiplication map $\mu$ from the compact connected set $(\mathcal{H}_1 \times \mathcal{H}_2)^{\times n}$ into $\mathcal{G}$. So $\Sigma^\infty$ is connected. So $G$ is connected.

In fact we can conclude much more using $\mu$. For $G$ has an additional structure compatible with its Lie group structure: $G$ is a smooth irreducible real algebraic variety. (In fact, we can faithfully represent $G$ on some $\mathbb{C}^N$ and then $G$ is an irreducible closed real algebraic subvariety of the space of matrices of size $N$.) The subgroups $\mathcal{H}_1$ and $\mathcal{H}_2$ are closed irreducible subvarieties; here we use the connectedness of $\mathcal{H}_1$ and $\mathcal{H}_2$.

Clearly $\mu$ is a morphism of irreducible real algebraic varieties. It follows using the Tarski-Seidenberg theorem that $\Sigma^n$ is a semi-algebraic set in $G$ and its “algebraic closure” $Z_n$ is irreducible. Here $Z_n$ is the unique smallest closed real algebraic subvariety of $G$ which contains $\Sigma^n$. So $Z_1, Z_2, \ldots$ is an increasing sequence of closed irreducible subvarieties whose union is dense in $G$. It follows, by dimension theory in algebraic geometry, that $Z_p = G$ for some $p$. Since $\Sigma^p$ is semi-algebraic, the fact $Z_p = G$ implies that $\Sigma^p$ contains an open neighborhood $\mathcal{O}$ of one of its points $g$. (This is the payoff for introducing real algebraic geometry.) Now it follows that $\Sigma^{2p+1}$ contains an open neighborhood $\mathcal{U}$ of the identity. Indeed, we take $\mathcal{U} = \mathcal{O}g^{-1}$ and notice that that $g^{-1}$ lies in $\Sigma^{p+1}$.

We next claim that $\Sigma^\infty = G$. First, $\Sigma^\infty$ is open in $G$; this follows since $\Sigma^{2p+1+k}$ contains the open neighborhood $\Omega_k = \mathcal{U} \Sigma^k$ of $\Sigma^k$. Second, $\Sigma^\infty$ is clearly a subgroup of $G$. But $G$ is connected and so $G$ has no open subgroup other than itself. So $\Sigma^\infty = G$.

The last paragraph shows that $G$ is the union of the increasing sequence of open sets $\Omega_k$. But $G$ is compact, and so this forces $G = \Omega_q$ for some $q$. Hence $G = \Sigma^{2p+1+q}$. $\square$

5. Second step: Reduction to $n = 2$

**Theorem 5.1.** The set of all $2$-qudit gates is exactly universal.

**Proof.** We will apply Lemma 4.1 to the $\binom{n}{2}$ subgroups $H(p, q) = \{B(p, q) \mid B \in G\}$ of $U(d^n)$, indexed by pairs $(p, q)$ with $p < q$. Each $H(p, q)$ is a connected closed subgroup of $U(d^n)$. We need to show that the $H(p, q)$ generate a dense subgroup of $U(d^n)$; this amounts to showing that the Lie algebras of the $H(p, q)$ generate the Lie algebra of $U(d^n)$. This was done by DiVincenzo in [1]. Although DiVincenzo only worked in the case $d = 2$, his method easily extends to the case $d > 2$. Thus Lemma 4.1 applies and tells us the $H(p, q)$ generate $U(d^n)$. $\square$

For $d = 2$, Theorem 5.1 was already known by rather different methods. It was explained in [2] how to explicitly build any $n$-qudit gate out of the $n$-qudit gates produced by the 1-qubit gates $A$ together with the CNOT gate.

6. Fourth step: Analyzing the Lie algebra $\mathfrak{g}$.

**Lemma 6.1.** There are no Lie algebras strictly in between $\mathfrak{h}$ and $\mathfrak{g}$.

**Proof.** We will write elements of $G = U(d^2)$ and $\mathfrak{g} = \mathfrak{u}(d^2)$ as matrices of size $d^2$, by using the computational basis of $(\mathbb{C}^d)^{\otimes 2}$. Now $H$ is the subgroup of $G$ of matrices of the form $h_{S,T}$ where $h_{S,T} = S \otimes T$ is the Kronecker product of unitary matrices $S$ and $T$ of size $d$. 


The main idea now is to study $\mathfrak{g}$ as a representation $\pi$ of $K = SU(d) \times SU(d)$ where $(S,T)$ acts on $\mathfrak{g}$ by $\pi^{S,T}(\xi) = h_S \xi h_T^{-1}$. This is useful because if $\mathfrak{r}$ is a Lie subalgebra of $\mathfrak{g}$ and $\mathfrak{r}$ contains $\mathfrak{h}$, then the operators $\pi^{S,T}$ preserve $\mathfrak{r}$. So $\mathfrak{h} \subseteq \mathfrak{r} \subseteq \mathfrak{g}$ as representations of $K$. We will show that there is no representation of $K$ strictly in between $\mathfrak{h}$ and $\mathfrak{g}$.

Now $\mathfrak{g}$ decomposes into a direct sum of irreducible representations of $K$. This follows formally since $K$ is a compact Lie group. But also we can write down the decomposition explicitly.

To do this, we observe that each element of $\mathfrak{g}$ is a finite sum of Kronecker products $X \otimes Y$ where $X$ lies in $\mathfrak{u}(d)$ and $Y$ lies in $i\mathfrak{u}(d)$. Here $\mathfrak{u}(d) = \text{Lie } U(d)$ is the space of skew-hermitian matrices of size $d$. Moreover $\pi^{S,T}(X \otimes Y) = (SXS^{-1}) \otimes (TYT^{-1})$. Thus $\mathfrak{g}$ identifies naturally with the tensor product $\mathfrak{u}(d) \otimes (i\mathfrak{u}(d))$, where Kronecker product corresponds to tensor product. The representation $\pi$ then corresponds to the obvious tensor product representation of $K$ on $\mathfrak{u}(d) \otimes (i\mathfrak{u}(d))$. As a representation of $U(d)$ under conjugation, $\mathfrak{u}(d)$ decomposes into the direct sum of two irreducible representations: $\mathfrak{u}(d) = i\mathbb{R} I \oplus \mathfrak{su}(d)$, where $I$ is the identity matrix and $\mathfrak{su}(d) = \text{Lie } SU(d)$ is the space of skew-hermitian matrices of trace 0. Thus we obtain the decomposition

$$\mathfrak{g} = (i\mathbb{R} I \oplus \mathfrak{su}(d)) \otimes (\mathbb{R} I \oplus i\mathfrak{su}(d)) = p_0 \oplus p_1 \oplus p_2 \oplus p_3$$

into four irreducible representations of $K$, where $p_0 = i\mathbb{R} I \otimes I$, $p_1 = \mathfrak{su}(d) \otimes I$, $p_2 = I \otimes \mathfrak{su}(d)$, and $p_3 = i\mathfrak{su}(d) \otimes \mathfrak{su}(d)$.

We recognize $\mathfrak{h} = p_0 \oplus p_1 \oplus p_2$; this follows since $\mathfrak{h}$ consists of matrices of the form $X \otimes I + I \otimes Y$ where $X$ and $Y$ lie in $\mathfrak{u}(d)$. Thus $\mathfrak{g} = \mathfrak{h} \oplus p_3$ and so there is no representation of $K$ strictly in between $\mathfrak{h}$ and $\mathfrak{g}$.

7. Fifth Step: The normalizer of $H$

We can now show

**Proposition 7.1.** The normalizer of $H$ in $G$ is the group $L$ of primitive gates.

**Proof.** We showed in §5 in proving (i)$\Rightarrow$(iii) that $L$ is a closed subgroup of $G$ with $L$ lying strictly in between $H$ and $G$. It follows by Lemma 6.1 that the Lie algebra of $L$ is $\mathfrak{h}$. Now, since $H$ is a connected Lie group, it follows that $L$ normalizes $H$.

For the converse, we return to our setup in the proof of Lemma 6.1. Let us write $X(1) = X \otimes I$ and $Y(2) = I \otimes Y$ for any matrices $X$ and $Y$ of size $d$. We identified $\mathfrak{h}$ as the set of matrices $X(1) + Y(2)$ of size $d^2$ where $X$ and $Y$ lie in $\mathfrak{u}(d)$.

Suppose $R \in G$ normalizes $H$. Then the conjugation action of $R$ on $\mathfrak{g}$ preserves $\mathfrak{h}$. So given any $X,Y \in \mathfrak{u}(d)$, we have

$$R(X(1) + Y(2))R^{-1} = X'(1) + Y'(2)$$

(7.1)

for some $X',Y' \in \mathfrak{u}(d)$. Then $\text{tr } X + \text{tr } Y = \text{tr } X' + \text{tr } Y'$ where $\text{tr } X$ is the trace of $X$. Consequently we can make $X'$ and $Y'$ unique by requiring $\text{tr } X = \text{tr } X'$ and $\text{tr } Y = \text{tr } Y'$. In particular, if $X,Y \in \mathfrak{su}(d)$, then $X',Y' \in \mathfrak{su}(d)$. In this way, $R$ defines a linear endomorphism $\gamma_R$ of $\mathfrak{su}(d) \oplus \mathfrak{su}(d)$ where $\gamma_R(X,Y) = (X',Y')$. Clearly $\gamma_R$ is invertible. Moreover $\gamma_R$ preserves the Lie algebra bracket — this follows using $[X(1) + Y(2),U(1) + V(2)] = [X,U](1) + [Y,V](2)$. Thus $\gamma_R$ is a Lie algebra automorphism.
Any Lie algebra automorphism of $\mathfrak{su}(d) \oplus \mathfrak{su}(d)$ either preserves the two summands or permutes them. This is forced because $\mathfrak{su}(d)$ is a simple Lie algebra. So we have two cases: either $\gamma_R$ preserves the summands so that $\gamma_R(X, 0) = (X', 0)$ and $\gamma_R(0, Y) = (0, Y')$, or $\gamma_R$ permutes the summands so that $\gamma_R(X, 0) = (0, Y')$ and $\gamma_R(0, Y) = (X', 0)$. In the latter case, notice that $RP$ normalizes $H$ (since $P$ normalizes $H$) and $\gamma_{RP} = \gamma_R \gamma_P$ preserves the summands (since $\gamma_P$ permutes them). So either $\gamma_R$ or $\gamma_{RP}$ preserves the summands. It is enough to show that $R$ or $RP$ is primitive, since $P$ itself is primitive. So we will assume that $\gamma_R$ preserves the summands. Then

$$RX(1)R^{-1} = X'(1) \quad \text{and} \quad RY(2)R^{-1} = Y'(2) \quad (7.2)$$

We want to show (7.2) implies that $R$ is primitive. Suppose we have a decomposable 2-qudit $|xy\rangle$. We want to show $R|xy\rangle$ is also decomposable. To do this, we introduce matrices $X$ and $Y$ in $u(d)$ as follows: $X = ip_x$ and $Y = ip_y$ where $p_x$ is the matrix which orthogonally projects $\mathbb{C}^d$ onto the line $\mathbb{C}x$. Now (7.2) produces two matrices $X'$ and $Y'$ in $u(d)$. (Clearly (7.2) extends automatically to the case where $X, Y, X', Y'$ lie in $u(d)$, since $u(d) = i\mathbb{R}I \oplus \mathfrak{su}(d)$.)

We claim that $X'$ and $Y'$ are also of the form $X' = ip_{x'}$ and $Y' = ip_{y'}$ for some qudits $|x'\rangle$ and $|y'\rangle$. This is true for $X'$ because $X'$ is skew-hermitian, $\text{tr} X' = i$ and rank $X' = 1$. We computed the rank of $X'$ in the following way: (7.2) implies $X(1)$ and $X'(1)$ have the same rank. But rank $X(1) = d(\text{rank } X) = d$ and rank $X'(1) = d(\text{rank } X')$. Then

$$RX(1)Y(2)R^{-1} = RX(1)R^{-1}RY(2)R^{-1} = X'(1)Y'(2) = -p_{x'}(1)p_{y'}(2) \quad (7.3)$$

Let us apply both sides of (7.3) to $R|xy\rangle$. The left hand side gives $R|xy\rangle$. The right hand side must be of the form $e^{i\theta}|x'y'\rangle$. So $R|xy\rangle = e^{i\theta}|x'y'\rangle$ is decomposable. \qed

8. Proof of Theorem 1.4

In this section, we use only the work from 6-7. The following result combined with Proposition 7.1 gives Theorem 1.4.

**Proposition 8.1.** The normalizer of $H$ in $G$ is the union of $H$ and $HP$.

**Proof.** We return to the last phase in the proof of Proposition 7.1. We showed not only $R|xy\rangle = e^{i\theta}|x'y\rangle$ (where $\theta$ depends on $x, y, x', y'$) but also $x'$ depends only on $x$ while $y'$ depends only on $y$. Furthermore $x$ and $y$ determined $x'$ and $y'$ uniquely up to phase factors.

We now construct a 1-qudit gate $S$ as follows: we fix choices of $y$ and $y'$ and then define $S$ by $R|xy\rangle = S|x\rangle \otimes |y\rangle$. If we change our choices of $y$ and $y'$, then this changes $S$ only by an overall phase factor. Similarly, we construct a 1-qudit gate $T$ by $R|xy\rangle = |x'\rangle \otimes T|y\rangle$ where this time we fixed choices of $x$ and $x'$. Now, for each $|xy\rangle$, $R|xy\rangle$ coincides with $S|x\rangle \otimes T|y\rangle$ up to a phase factor which depends on $|xy\rangle$. It is easy to see that these phase factors are in fact all the same. Thus $R = e^{i\theta}S(1)T(2)$. So $R$ belongs to $H$.

This finishes the case where (7.2) holds. In the other case, where $RX(1)R^{-1} = Y'(2)$ and $RY(2)R^{-1} = X'(1)$, we conclude that $RP$ lies in $H$. Thus every $R$ normalizing $H$ belongs to either $H$ or $HP$. The converse is clear. \qed

We note that $HP = PH$ since $P$ normalizes $H$.

Using Theorem 1.4 we can derive explicit equations characterizing primitive gates. Let $V_{ij,ki}$ be the matrix coefficients of $V$ in the computational basis.
Corollary 8.2. Let $V$ be a 2-qudit gate. Then $V$ is primitive if and only if $V$ satisfies one of the following two conditions:

(i) $V_{ij,kl}V_{ij,k'l'} = V_{ij,kl}V_{ij,k'l'}$
(ii) $V_{ij,kl}V_{ij,k'l'} = V_{ij,kl}V_{ij,k'l'}$

Proof. We will show that $V$ belongs to $H$ if and only if (i) holds, while $V$ belongs to $HP$ if and only if (ii) holds.

We can view $V$ as an element of $M(d) \otimes M(d)$ where $M(d)$ is the space of matrices of size $d$. Now $V$ is decomposable in this setting if and only if we can find $A$ and $B$ in $M(d)$ such that $V = A \otimes B$ (so that $V |xy⟩ = A |x⟩ \otimes B |y⟩$). Now we recognize (i) as the classical set of quadratic equations which characterize when $V$ is decomposable. The point is that $V$ is decomposable only if $V$ belongs to $H$ (the converse is obvious). Indeed, if $V = A \otimes B$ then, since $V$ is unitary, it follows easily that $A = \lambda S$ and $B = \lambda^{-1} T$ where $\lambda$ is a positive number and $S$ and $T$ are unitary. So $V = S \otimes T$.

On the other hand, $V$ belongs to $HP$ if and only if $VP$ belongs to $H$. But (i) holds for $VP$ if and only if (ii) holds for $V$.

Remark 8.3. We have a different (and more direct) way of proving Theorem 1.4 using some projective complex algebraic geometry. The starting point is to observe that a primitive gate $V$ induces a holomorphic automorphism of $\mathbb{CP}^{d-1} \times \mathbb{CP}^{d-1}$.

Finally, we prove Corollary 1.5. The set of imprimitive gates is $G \setminus L$. This is open in $G$ since we proved $L$ is closed. The rest requires using results on the topology of smooth manifolds. Since $L$ is a closed submanifold of $G$ with $L \neq G$, it follows that $G \setminus L$ is dense in $G$. Now connectedness of $G \setminus L$ follows as soon as we check that $L$ has codimension at least two in $G$. This is the case because $\dim G = d^4$ and $\dim L = \dim H = 2d^2 - 1$ and so the codimension is $d^4 - 2d^2 + 1 \geq 9$.

9. A variant of Theorem 1.3

In this section we consider, in response to a question of G. Chen, what happens to Theorem 1.3 when we require that the 1-qudit gates $A$ are special, i.e., satisfy $\det A = 1$. We can prove an analog of (i)$\iff$(iii): given a 2-qudit gate $V$, the following are equivalent:

(i') The collection of all special 1-qudit gates $A$ together with $V$ is universal.

(ii') $V$ is imprimitive and $\det V$ is not a root of unity.

We cannot get exact universality here because the determinants of the gates generated by $A(1), A(2), V, V(2,1)$ are constrained to all be powers of $\det V$. But these powers form only a dense subset of $U(1)$. So a certain set of determinants never appears.

We can get a full analog of Theorem 1.3 in the following way:

Theorem 9.1. Suppose we are given a family $X$ of 2-qudit gates $Q_\phi$, indexed by angles $\phi$ modulo $2\pi$, such that $\det Q_\phi = e^{i\phi}$. Then the following are equivalent:

(i) the collection of all special 1-qudit gates $A$ together with $X$ is universal
(ii) the collection of all special 1-qudit gates $A$ together with $X$ is exactly universal
(iii) at least one $Q_\phi$ is imprimitive
Proof. Each part runs parallel to the proof of Theorem \[\text{1.3}\]. We define $H^z$ to be the subgroup of $SU(d^2)$ generated by the gates $A(1)$ and $A(2)$ for $A$ special; then $H^z$ is the set of gates of the form $S \otimes T$ where $S$ and $T$ belong to $SU(d)$. Let $F^z$ be the subgroup of $U(d^2)$ generated by $H^z$ and all the gates $Q_\phi$ and $Q_\phi(2,1)$.

(ii) $\Rightarrow$ (i) is obvious.

(i) $\Rightarrow$ (iii): if (iii) fails, then $F^z$ lies in the group of $L$ of primitive gates. But $L$ is not dense in $G$.

(iii)$\Rightarrow$(ii): We can take $n = 2$ as in the proof of Theorem \[\text{1.3}\]. Pick some $Q_\phi$ which is not primitive, and put $V = Q_\phi$. Our aim is to show $F^z = U(d^2)$.

We claim that $H^z$ and $H^b$ generate $SU(d^2)$, where we put $H^b = VH^zV^{-1}$. Clearly, $H^z$ and $H^b$ are closed connected subgroups of $SU(d^2)$. So, by Lemma \[\text{4.1}\], proving the claim reduces to showing that $H^z$ and $H^b$ generate a dense subgroup of $SU(d^2)$. This amounts to showing that the Lie algebras $h^z = \text{Lie } H^z$ and $h^b = \text{Lie } H^b$ generate $g$.

Let $\mathfrak{g}^z$ be the Lie algebra generated by $h^z$ and $h^b$; then $\mathfrak{g}^z \subseteq \mathfrak{g} \subseteq \mathfrak{su}(d^2)$. As in the proof of Lemma \[\text{6.1}\], $\mathfrak{g}^z$ must be a representation of $K$. So we return to the decomposition \[\text{6.1}\]. We recognize that $\mathfrak{su}(d^2) = \mathfrak{p}_1 \oplus \mathfrak{p}_2 \oplus \mathfrak{p}_3$ while $h^z = \mathfrak{p}_1 \oplus \mathfrak{p}_2$. Therefore $\mathfrak{su}(d^2) = h^z \oplus \mathfrak{p}_3$.

We conclude $\mathfrak{g}^z = h^z$ or $\mathfrak{g}^z = \mathfrak{su}(d^2)$.

We want to rule out $\mathfrak{g}^z = h^z$. Clearly $\mathfrak{g}^z = h^z \iff h^z = h^b \iff H^z = H^b \iff V$ normalizes $H^b$. But $H^z$ and $H$ have the same normalizer: this follows since $H$ is the product of $H^z$ with the scalar 2-qudit gates, and also $H^z$ is the set of gates in $H$ with determinant equal to 1. So Proposition \[\text{7.1}\] tells us that that $V$ cannot normalize $H^b$. Thus $\mathfrak{g}^z \neq h^z$.

This proves our claim that $H^z$ and $H^b$ generate $SU(d^2)$. Therefore $F^z$ contains $SU(d^2)$. But also $F^z$ contains a gate of each determinant $e^{i\phi}$. So $F^z = U(d^2)$.

Here is a concrete illustration which was suggested to us by G. Chen. We take $d = 2$ and consider the gates (written in the computational basis)

$$U_{\theta,\phi} = \begin{pmatrix} \cos \theta & -ie^{i\phi} \sin \theta \\ -ie^{-i\phi} \sin \theta & \cos \theta \end{pmatrix}, \quad Q_\phi = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix} \quad (9.1)$$

Corollary 9.2. The collection of gates $U_{\theta,\phi}$ and $Q_\phi$ (where $\theta$ and $\phi$ run through $\mathbb{R}$) is exactly universal.

Proof. It is known that the gates $U_{\theta,\phi}$ generate $SU(2)$. We can also see this directly using Lemma \[\text{4.1}\]. Indeed, for each value of $\phi$, the $U_{\theta,\phi}$ form a closed connected subgroup $S_\phi$ of $SU(2)$. Consider the two subgroups $S_0$ and $S_{\pi/2}$. It is easy to see that their Lie algebras generate $\mathfrak{su}(2)$. This means $S_0$ and $S_{\pi/2}$ generate a dense subgroup of $SU(2)$. So by Lemma \[\text{4.1}\], $S_0$ and $S_{\pi/2}$ generate $SU(2)$.

Obviously $\det Q_\phi = e^{i\phi}$, and so we get exact universality from Theorem \[\text{9.1}\] as soon as we check that some $Q_\phi$ is imprimitive. In fact, we saw in \[\text{2}\] that $Q_\phi$ is always imprimitive, except of course if $Q_\phi$ is the identity. \[\square\]

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