Characterization of non-universal two-qubit Hamiltonians

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1 Introduction

Let I_N be the $N \times N$ identity matrix (we will abbreviate I_2 as I). Here are some commonly used notation that will be very handy:

- $\mathrm{M}_N(\mathbb{R}) \subset \mathrm{M}_N(\mathbb{C})$ – the set of all $N \times N$ real (complex) matrices.
- $\mathrm{U}(N) := \left\{U \in \mathrm{M}_N(\mathbb{C}) \mid U^\dagger U = I_N\right\}$ – the *unitary group*.
- $\mathrm{SU}(N) := \{U \in \mathrm{U}(N) \mid \det U = 1\} \subset \mathrm{U}(N)$ – the *special unitary group*.
- $\mathrm{O}(N) := \left\{O \in \mathrm{M}_N(\mathbb{R}) \mid O^\mathsf{T} O = I_N\right\} \subset \mathrm{M}_N(\mathbb{R}) \cap \mathrm{U}(N)$ – the *orthogonal group*.
- $\mathrm{SO}(N) := \{O \in \mathrm{O}(N) \mid \det O = 1\} \subset \mathrm{O}(N)$ – the *special orthogonal group*.
- $\mathfrak{u}(N) := \left\{H \in \mathrm{M}_N(\mathbb{C}) \mid H = H^\dagger\right\}$ – the *Lie algebra* of $\mathrm{U}(N)$ or the set of all $N \times N$ *Hermitian matrices*.

- S_n – the *symmetric group* or the set of all n-element permutations.
- $\mathcal{S}_n \subset \mathrm{M}_{2^n}(\{0,1\}) \cap \mathrm{O}(2^n)$ – the group of all n-qubit permutation matrices. To every permutation $\pi \in S_n$ we assign the corresponding n-qubit permutation matrix $P_\pi \in \mathcal{S}_n$ that acts in the standard basis as follows:

$$\forall s \in \{0,1\}^n : P_\pi\big(|s_1\rangle\,|s_2\rangle \ldots |s_n\rangle\big) = \big|s_{\pi^{-1}(1)}\big\rangle\,\big|s_{\pi^{-1}(2)}\big\rangle \ldots \big|s_{\pi^{-1}(n)}\big\rangle. \quad (1)$$

- $[n] := \{1,\ldots,n\}$, the set of natural numbers from 1 to n.

Definition 1. We say that a matrix $M \in \mathrm{M}_N(\mathbb{C})$ is *normal* if $MM^\dagger = M^\dagger M$.

Theorem 1. Let A and B be normal matrices. Then A and B are simultaneously diagonal in some orthonormal basis if and only if $[A,B]=0$.

1.1 The problem

Definition 2. We say that H is an *n-qubit Hamiltonian* if $H \in \mathfrak{u}(2^n)$, i.e., H is $2^n \times 2^n$ complex matrix that is Hermitian ($H^\dagger = H$).

In this paper we deal mainly with 2-qubit Hamiltonians, i.e., 4×4 Hermitian matrices. Usually we simply say "a Hamiltonian H", without explicitly mentioning that it is a 2-qubit Hamiltonian.

Definition 3. We say that we can *simulate* unitary $U \in \mathrm{U}(N)$ using Hamiltonians $H_1,\ldots,H_k \in \mathfrak{u}(N)$, if for all $\varepsilon > 0$ there exist $l \in \mathbb{N}$, $j_1,\ldots,j_l \in \{1,\ldots,k\}$, and $t_1,\ldots,t_l \geq 0$ such that:

$$\left\| U - e^{-iH_{j_1}t_1} e^{-iH_{j_2}t_2} \ldots e^{-iH_{j_l}t_l} \right\| < \varepsilon.$$

Definition 4. We say that an m-qubit Hamiltonian H is *n-universal*, if we can simulate all unitaries in $\mathrm{U}(2^n)$ using Hamiltonians from the set

$$\left\{ P(H \otimes I^{\otimes n-m})P^\dagger \mid P \in \mathcal{S}_n \right\},$$

i.e., we can apply H to any ordered subset of m qubits (out of n qubits in total).

To characterize the 2-qubit Hamiltonians that are 2-universal, we will classify those 2-qubit Hamiltonians that are *not* 2-universal. Note that a 2-qubit Hamiltonian H is 2-universal if we can simulate all unitaries in $\mathrm{U}(4)$ using H and THT, where T is the gate that swaps the two qubits.

2 Proving universality

It is not obvious at all how to check if a given Hamiltonian is universal according to the above definition, i.e., can be used to simulate any unitary matrix. Thus we would like to have an equivalent but simpler universality condition that would be more practical. In other words, we are looking for an efficient algorithm for deciding if a given Hamiltonian is universal.

First, we need to understand which evolutions we can simulate using a given Hamiltonian H. In order to do that, we introduce the notion of Lie algebra.

Definition 5. We say that $\mathcal{L}(H_1, \ldots, H_k)$ is the *Lie algebra generated by Hamiltonians* $H_1, \ldots, H_k$. It is defined inductively by the following three rules:

1. $H_1, \ldots, H_k \in \mathcal{L}(H_1, \ldots, H_k)$,
2. If $A, B \in \mathcal{L}(H_1, \ldots, H_k)$ then $\alpha A + \beta B \in \mathcal{L}(H_1, \ldots, H_k)$ for all $\alpha, \beta \in \mathbb{R}$,
3. If $A, B \in \mathcal{L}(H_1, \ldots, H_k)$ then $i[A, B] = i(AB - BA) \in \mathcal{L}(H_1, \ldots, H_k)$.

One can think of $\mathcal{L}(H_1, \ldots, H_k)$ as a real vector space equipped with a way of combining any two vectors to obtain the third. Note that if A, B are Hermitian, then $i[A, B]$ is also Hermitian, since we have

$$(i[A, B])^\dagger = -i(B^\dagger A^\dagger - A^\dagger B^\dagger) = i[A, B].$$

Therefore, $\mathcal{L}(H_1, \ldots, H_k)$ is a real subspace of Hermitian matrices. It consists of all those Hermitian matrices that can be expressed using finite number of nested commutators and linear combinations of $H_1, \ldots, H_k$.

We are about to prove a lemma that will help to understand the set of evolutions that we are able to simulate using some given set of Hamiltonians. However, first we need a claim that will be used in the proof of the above mentioned lemma. The essence of the claim is that although we cannot physically evolve our system according to a Hamiltonian H for *negative* time, it turns out that we can approximate the effect by evolving our system according to H for some positive amount of time instead.

Claim 1. Let H be a Hamiltonian and $\tau < 0$. Then for all $\varepsilon > 0$ there exists $t \geq 0$ such that $\left\| e^{-iH\tau} - e^{-iHt} \right\| < \varepsilon$.

Proof. sagfg □

Lemma 1. Assume that we are allowed to evolve according to Hamiltonians $H_1, \ldots, H_k$ for any desired amount of time. Then we can simulate unitary U if and only if it can be expressed as $U = e^{-iL}$ for some $L \in \mathcal{L}(H_1, \ldots, H_k)$.

Proof. First, we show that if we can evolve according to $H_1, \ldots, H_k$, then we can simulate any $U = e^{-iL}$ where $L \in \mathcal{L}(H_1, \ldots, H_k)$. Recall that Lie algebra was defined in an inductive way, i.e., every $L \in \mathcal{L}(H_1, \ldots, H_k)$ can be obtained from $H_1, \ldots, H_k$ by taking linear combinations and commutators. Thus we consider three cases.

1. We can simulate $U = e^{-iLt}$ for all $t \in \mathbb{R}$ if L is one of $H_1, \ldots, H_k$. Note that simulation for $t < 0$ follows from Claim 1.

2. If we are given simulations of e^{-iAt_1} and e^{-iBt_2} for all $t_1, t_2 \in \mathbb{R}$, then we can simulate $e^{-i(\alpha A+\beta B)}$ for arbitrary $\alpha, \beta \in \mathbb{R}$, since

$$e^{-i(\alpha A+\beta B)} = \lim_{n\to\infty} \left(e^{-i\alpha A/n} e^{-i\beta B/n}\right)^n. \tag{2}$$

3. If we are given simulations of e^{-iAt_1} and e^{-iBt_2} for all $t_1, t_2 \in \mathbb{R}$, then we can simulate $e^{-i(i[A,B])t}$ for all $t \in \mathbb{R}$, since

$$e^{-i(i[A,B])t} = \lim_{n\to\infty} \left(e^{iAt/\sqrt{n}} e^{-iB/\sqrt{n}} e^{-iAt/\sqrt{n}} e^{iB/\sqrt{n}}\right)^n. \tag{3}$$

Consult [2] for the proof of (2) and (3).

Now we proceed to show that, if we can simulate unitary U, then $U = e^{-iL}$ for some $L \in \mathcal{L}(H_1, \ldots, H_k)$. Since we can simulate U, we can approximate it to any desired precision using expressions of the form:

$$e^{-iH_{j_1}t_1} e^{-iH_{j_2}t_2} \ldots e^{-iH_{j_l}t_l}, \tag{4}$$

for some $l \in \mathbb{N}$, $j_1, \ldots, j_l \in \{1, \ldots, k\}$, and $t_1, \ldots, t_l \geq 0$. Now we will show that all expressions of the above form can be expressed as e^{-iL} for some $L \in \mathcal{L}(H_1, \ldots, H_k)$.

Consider Baker-Campbell-Hausdorff formula

$$e^{-iAt_1} e^{-iBt_2} = e^{-iH}, \text{ where} \tag{5}$$

$$H = At_1 + Bt_2 - \frac{t_1 t_2}{2} i[A,B] + \frac{t_1^2 t_2}{12} i[A, i[A,B]] + \frac{t_1 t_2^2}{12} i[B, i[B,A]] + \ldots \tag{6}$$

See [3] for the proof of Baker-Campbell-Hausdorff formula. Assume $A, B \in \mathcal{L}(H_1, \ldots, H_k)$. In order to claim that $H \in \mathcal{L}(H_1, \ldots, H_k)$, we have to show that it can be expressed as a *finite* real linear combination of nested commutators of $H_1, \ldots, H_k$. Since there is only finite number of linearly independent nested commutators in expression (6), we can rewrite it as a finite real linear combination of these linearly independent nested commutators. Therefore, $H \in \mathcal{L}(H_1, \ldots, H_k)$.

Using repeated applications of Baker-Campbell-Hausdorff formula to (4), we can argue that all expressions of the form (4) belong to $\mathcal{L}(H_1, \ldots, H_k)$.

From the above discussion it follows that $\mathcal{S} := \left\{e^{-iL} \mid L \in \mathcal{L}(H_1, \ldots, H_k)\right\}$ is a group under multiplication. Since all subgroups of the unitary group are compact, we conclude that $\mathcal{S}$ is a closed set. Since we can approximate U, there exist a sequence $\{U_n\}_{n=1}^{\infty} \subset \mathcal{S}$ such that

ToDo: Reference! Subgroups of unitary group are compact.

$$U = \lim_{n\to\infty} U_n.$$

We conclude that $U \in \mathcal{S}$ as a limit of a sequence within a closed set. Thus, $U = e^{-iL}$ for some $L \in \mathcal{L}(H_1, \ldots, H_k)$. □

Now we can obtain a simpler and more practical condition of n-universality than the original one in Definition 4.

Lemma 2. An m-qubit Hamiltonian H is n-universal if and only if

$$\mathcal{L}\big(\big\{P(H \otimes I^{\otimes n-m})P^\dagger \mid P \in \mathcal{S}_n\big\}\big) = \mathfrak{u}(2^n),$$

where $\mathcal{S}_n$ is the group of matrices that permute n qubits and $\mathfrak{u}(2^n)$ is the set of all $2^n \times 2^n$ Hermitian matrices.

Proof. Let $N := 2^n$ and $\mathcal{L}$ be the above Lie algebra. Assume $\mathcal{L} = \mathfrak{u}(N)$. Since every unitary $U \in \mathrm{U}(N)$ can be expressed as $U = e^{-iL}$ for some $L \in \mathfrak{u}(N) = \mathcal{L}$, then according to Lemma 1 we conclude that it is possible to simulate the whole $\mathrm{U}(N)$ by applying H to different ordered subsets of m qubits. Therefore, H is n-universal.

We proceed to show the other direction. Assume H is n-universal. Let $A \in \mathfrak{u}(N)$ be an arbitrary Hamiltonian and let $V \in \mathrm{U}(N)$ be such that $VAV^\dagger$ is diagonal. We will show that $A \in \mathcal{L}$.

Since H is n-universal, Lemma 1 tells us that every $U \in \mathrm{U}(N)$ can be expressed as $U = e^{-iL}$ for some $L \in \mathcal{L}$. In particular, it holds for any U that is diagonal in the same basis as A and has eigenvalues $(e^{-i\alpha}, 1, \ldots, 1)$, where $\alpha \in \mathbb{R}$. Thus, for each $\alpha \in \mathbb{R}$ there exists $\mathbf{a} = (a_1, \ldots, a_N) \in \mathbb{Z}^N$ such that

$$L_\alpha(\mathbf{a}) := V \begin{pmatrix} \alpha + 2\pi a_1 & 0 & \ldots & 0 \\ 0 & 2\pi a_2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 2\pi a_N \end{pmatrix} V^\dagger \in \mathcal{L}.$$

There are uncountably many different $\alpha \in \mathbb{R}$ and only countably many different N-tuples $\mathbf{a} \in \mathbb{Z}^N$. Thus, there exist $\mathbf{a} \in \mathbb{Z}^N$ and $\alpha_1, \alpha_2 \in \mathbb{R}$ such that $\alpha_1 \neq \alpha_2$ and $VL_{\alpha_1}(\mathbf{a})V^\dagger, VL_{\alpha_2}(\mathbf{a})V^\dagger \in \mathcal{L}$. So, we have

$$\frac{1}{\alpha_1 - \alpha_2} V\big(L_{\alpha_1}(\mathbf{a}) - L_{\alpha_2}(\mathbf{a})\big)V^\dagger = V \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 0 \end{pmatrix} V^\dagger \in \mathcal{L},$$

since $\mathcal{L}$ is a real vector space. Similarly, we can argue that $V |i\rangle \langle i| V^\dagger \in \mathcal{L}$ for all $i \in \{0,1\}^n$. Therefore, also $A \in \mathcal{L}$ as it can be expressed as a real linear combination of $V |i\rangle \langle i| V^\dagger$, $i \in \{0,1\}^n$. □

Corollary. A 2-qubit Hamiltonian H is 2-universal if and only if $\mathcal{L}(H, THT) = \mathfrak{u}(4)$, where $\mathfrak{u}(4)$ is the set of all 4×4 Hermitian matrices.

3 Characterization of 2-universal Hamiltonians

In this section we will classify 2-qubit Hamiltonians that are *not* 2-universal. Since we will be talking only about 2-universality, we will simply say that a Hamiltonian is universal (instead of "2-universal") or non-universal (instead of "not 2-universal").

3.1 The T gate

The gate that swaps two qubits is central to our problem of characterizing 2-universal Hamiltonians, since it is the only non-trivial permutation of two qubits. In this section we make a few simple observations revealing some properties of the swap gate that will be relevant to the further discussion. We will use the letter T to refer to the swap gate.

The matrix representation of the T gate is:

$$T := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{7}$$

It has two eigenspaces, namely

$$E_- := \text{span}_{\mathbb{C}} \{|01\rangle - |10\rangle\} \text{ and } E_+ := \text{span}_{\mathbb{C}} \{|00\rangle, |01\rangle + |10\rangle, |11\rangle\}, \tag{8}$$

where E_- corresponds to the eigenvalue -1 and E_+ to the eigenvalue $+1$. We call the vector

$$|s\rangle := \frac{|01\rangle - |10\rangle}{\sqrt{2}} \tag{9}$$

that spans E_- the *singlet* state.

Lemma 3. Let N be a normal matrix. The singlet $|s\rangle$ is an eigenvector of N if and only if $[N, T] = 0$.

Proof. Assume $|s\rangle$ is an eigenvector of N. Then $\mathcal{B} = \{|s\rangle, |n_1\rangle, |n_2\rangle, |n_3\rangle\}$ is an orthonormal eigenbasis of N for some orthonormal vectors $\{|n_i\rangle\}_{i=1}^3 \subset \mathbb{C}^4$. Since $\mathcal{B}$ is orthonormal, $\{|n_i\rangle\}_{i=1}^3 \in E_-^\perp = E_+$. Therefore, $\mathcal{B}$ is also an eigenbasis of T; and both N and T are simultaneously diagonal in this basis. Thus, according to Theorem 1 $[N, T] = 0$.

Assume $[N, T] = 0$. By Theorem 1 we know that N and T are simultaneously diagonal in some orthonormal basis $\mathcal{B}$. Since $|s\rangle$ spans the one-dimensional eigenspace E_- of T, we know that $e^{i\phi} |s\rangle \in \mathcal{B}$ for some $\phi \in \mathbb{R}$. Thus, $|s\rangle$ is an eigenvector of N. □

3.2 Examples of non-universal Hamiltonians

In this section we will consider three families of non-universal Hamiltonians. Later on we will see that these three families capture the essence of what makes a Hamiltonian non-universal.

- *Consider a local Hamiltonian* $H = H_1 \otimes I + I \otimes H_2$. Note that we end up acting independently on both qubits no matter whether we evolve our system according to H or THT, since

$$THT = I \otimes H_1 + H_2 \otimes I.$$

Therefore, any sequence of evolutions according to H and THT will result in action that is independent on both qubits and we will not be able to simulate entangling operations.

- *Consider a Hamiltonian H that shares an eigenvector v with the gate that swaps two qubits, T.* In this case any sequence of evolutions according to H and THT will leave the vector v unchanged. Therefore, we will not be able to simulate unitaries that act non-trivially on this vector.

- *Consider a traceless Hamiltonian H.* Since the trace is basis independent, also $\mathrm{Tr}(THT) = 0$. Now note that by exponentiating a traceless Hamiltonian we get a unitary with determinant one. Any sequence of evolutions according to H and THT corresponds to a product of unitaries from the special unitary group. This shows that using a traceless Hamiltonian we will not be able to simulate anything outside the special unitary group.

We summarize the observations made above in the following lemma.

Lemma 4. A two-qubit Hamiltonian H is non-universal if any of the following conditions holds:

1. H is a local Hamiltonian, i.e., $H = H_1 \otimes I + I \otimes H_2$, for some singe-qubit Hamiltonians H_1, H_2,

2. H shares an eigenvector with T, the gate that swaps two qubits,

3. $\mathrm{Tr}(H) = 0$.

The converse of the above lemma in its present form is not true. However, in the following sections we will generalize the first condition (see Lemma 6). Then we will be able to show that the converse of the generalized lemma holds as well, i.e., if a Hamiltonian does not fall in any of the three categories then it is universal.

3.3 Transformations preserving universality

3.3.1 T-similarity

In this section we look for unitary transformations that conjugate all universal two-qubit Hamiltonians to universal ones and all non-universal two-qubit Hamiltonians to non-universal ones. We say that such transformations *preserve the universality property.*

Let us recall when two matrices are said to be similar.

Definition 6. Matrices A and B are said to be *similar* if there exists an invertible matrix P such that $B = PAP^{-1}$.

Now we are ready to introduce a new notion – we call it T-similarity.

Definition 7. Matrices A and B are said to be T-*similar* if there exists a unitary matrix P such that $B = PAP^\dagger$ and $[P, T] = 0$.

Note that in the case of T-similarity we require the transformation P ensuring the similarity to be unitary instead of just invertible.

Theorem 2. *T-similar Hamiltonians have the same universality property.*

Proof. Assume A and B are T-similar, which means that there is a unitary P such that $B = PAP^\dagger$ and $[P, T] = 0$. Suppose A is universal. We want to show that B is also universal. Since A is universal, we can simulate any $U \in \mathrm{U}(4)$ with any desired precision:

$$U \overset{\varepsilon}{=} e^{-iAt_1} e^{-iTATt_2} e^{-iAt_3} \dots e^{-iTATt_n}, \tag{10}$$

where $\overset{\varepsilon}{=}$ means that the right hand side approximates U with precision ε with respect to the spectral norm. Let us replace the Hamiltonian A in the simulation (10) with B and then use the fact that $TP = PT$:

$$\begin{aligned}
&e^{-iBt_1} e^{-iTBTt_2} e^{-iBt_3} \dots e^{-iTBTt_n} = \\
&= e^{-iPAP^\dagger t_1} e^{-iTPAP^\dagger Tt_2} e^{-iPAP^\dagger t_3} \dots e^{-iTPAP^\dagger Tt_n} = \\
&= e^{-iPAP^\dagger t_1} e^{-iPTATP^\dagger t_2} e^{-iPAP^\dagger t_3} \dots e^{-iPTATP^\dagger t_n} = \\
&= Pe^{-iAt_1} P^\dagger Pe^{-iTATt_2} P^\dagger Pe^{-iAt_3} P^\dagger \dots Pe^{-iTATt_n} P^\dagger = \\
&= Pe^{-iAt_1} e^{-iTATt_2} e^{-iAt_3} \dots e^{-iTATt_n} P^\dagger \overset{\varepsilon}{=} PUP^\dagger
\end{aligned}$$

Note that we have obtained a simulation of $PUP^\dagger$. Since the unitary group $\mathrm{U}(4)$ is invariant under conjugation, we conclude that also Hamiltonian B can be used to simulate any $U \in \mathrm{U}(4)$ with the desired precision (just replace A in the simulation of $P^\dagger UP$ with B). Thus, we have shown that B is also universal.

If A is non-universal, then B has to be non-universal as well, as otherwise it would contradict what we have showed above. □

Now with our new tool in hand we can return to Lemma 4 and try to generalize it using Theorem 2. We could conjugate all three classes of Hamiltonians in Lemma 4 by unitaries commuting with the T gate and see if we get any new non-universal Hamiltonians.

Let us first consider the local Hamiltonians (condition 1 in Lemma 4). It turns out that by conjugating local Hamiltonians with unitaries that commute with T it is possible to obtain non-universal Hamiltonians that are not mentioned in Lemma 4. For example, consider the following local Hamiltonian H and unitary U which commutes with T:

$$H := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes I + I \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad U := \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

By conjugating the local Hamiltonian H by unitary U, we obtain a non-universal Hamiltonian that is not local:

$$UHU^\dagger = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} = I \otimes I + \frac{1}{2}(X \otimes X - Y \otimes Y)$$

Thus, we conclude that local Hamiltonians are not closed under conjugation by unitaries that commute with the T gate.

We will see that the other two families of non-universal Hamiltonians mentioned in conditions 2 and 3 of Lemma 4 are closed under conjugation with unitaries that commute with the T gate. It is very easy to see this in the case of traceless Hamiltonians (condition 3). Since the trace is basis independent, traceless Hamiltonians are closed under conjugation. In the following lemma we prove that also Hamiltonians in condition 2 are closed under conjugation with unitaries that commute with T.

Lemma 5. The set of two-qubit Hamiltonians sharing an eigenvector with the T gate is closed under conjugation with unitaries that commute with T.

Proof. Let $|v\rangle$ be the eigenvector shared by H and the T gate, i.e., $H|v\rangle = \lambda_H |v\rangle$ and $T|v\rangle = \lambda_T |v\rangle$. We will show that $U|v\rangle$ is an eigenvector shared by the T gate and $UHU^\dagger$, where $[T, U] = 0$. First, note that $UHU^\dagger(U|v\rangle) = UH|v\rangle = \lambda_H U|v\rangle$. We also have $T(U|v\rangle) = UT|v\rangle = \lambda_T U|v\rangle$. Thus, $U|v\rangle$ is an eigenvector shared by the T gate and $UHU^\dagger$.

Note that in the proof we did not make use of the fact that the T gate is the unitary that swaps two qubits. Therefore, the above lemma holds for an arbitrary matrix T. □

The following lemma is a generalization of Lemma 4. It follows directly from the discussion above and Lemma 5.

Lemma 6. A two-qubit Hamiltonian H is non-universal if any of the following conditions holds:

1. H is T-similar to a local Hamiltonian,
2. H shares an eigenvector with T, the gate that swaps two qubits,
3. $\mathrm{Tr}(H) = 0$.

Imagine that we want to determine if a given Hamiltonian is universal. The best we could do at this point would be to check whether it falls into any of the families that are listed as non-universal in Lemma 6. However, it is not straightforward how to check if a given Hamiltonian is T-similar to a local Hamiltonian (condition 1). Thus, in the next section we introduce a new notion that will turn out useful in checking condition 1 in the above lemma.

3.3.2 Pattern

Definition 8. Assume that a two-qubit Hamiltonian H has eigenvalues λ_i with the corresponding orthonormal eigenvectors $|\psi_i\rangle$. Then we define a *pattern* of H to be

$$\begin{Bmatrix} \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 \\ s_1 & s_2 & s_3 & s_4 \end{Bmatrix}, \tag{11}$$

where $s_i := |\langle s|\psi_i\rangle|^2$ and $|s\rangle$ is the singlet state as given in (9). Note that pattern is defined up to a permutation of the columns.

One could wonder why we use exactly $|s\rangle$ for calculating the overlaps. Recall that the T gate has only two eigenspaces: E_+ and E_- given in (8), and E_- is spanned by $|s\rangle$. Therefore, the overlap with the singlet state completely determines the overlap with the $(+1)$-eigenspace E_+.

Definition 9. We say that a Hamiltonian H is *degenerate* if it has a degenerate (i.e., repeated) eigenvalue.

Note that pattern is not well defined for degenerate Hamiltonians. This is because one can choose any orthonormal eigenbasis of the subspace corresponding to the degenerate eigenvalue. In such a case every symbol of the form (11) that fulfills the requirements posed in the definition is considered to be a pattern of the corresponding Hamiltonian.

It turns out that for the purpose of characterizing universal Hamiltonians, we could restrict our attention only to non-degenerate Hamiltonians that have well-defined patterns. Lemma 7 tells us that all degenerate Hamiltonians are non-universal. So the reader might choose to assume that whenever we consider a pattern of a Hamiltonian, it is well defined, since we restrict our attention to non-degenerate Hamiltonians. However, we will take a more general approach and prove all theorems for general (possibly degenerate) Hamiltonians.

Lemma 7. If a two-qubit Hamiltonian H has a degenerate eigenvalue, then it is not universal.

Proof. Assume H has a degenerate eigenvalue. Then the eigenspace E corresponding to the degenerate eigenvalue has dimension at least two. Recall that the T gate has a 3-dimensional $(+1)$-eigenspace E_+. Now note that the intersection $E \cap E_+$ is at least 1-dimensional, since $E, E_+ \subseteq \mathbb{C}^4$ and $\dim(E) \geq 2$, $\dim(E_+) = 3$. Any nonzero $|v\rangle \in E \cap E_+$ is a common eigenvector of H and the T gate. By Lemma 4 we conclude that H is non-universal. □

Now we want to investigate to what extent pattern of a degenerate Hamiltonian is not well defined. The following lemma shows that for degenerate Hamiltonians pattern is defined up to a way we choose to split up the sum of the overlaps corresponding to the degenerate eigenvalue.

Lemma 8. Let H be a degenerate Hamiltonian with a degenerate eigenvalue λ_1. Let E be the k-dimensional eigenspace corresponding to the degenerate eigenvalue λ_1, where $2 \le k \le 4$. Then H has all patterns of the form

$$\begin{Bmatrix} \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 \\ s_1 & s_2 & s_3 & s_4 \end{Bmatrix}, \tag{12}$$

where $\lambda_1 = \lambda_2 = \ldots = \lambda_k$ and $s_1 + s_2 + \ldots + s_k = \|\Pi_E |s\rangle\|^2$ and Π_E is the projection onto the eigenspace E.

Proof. Pick an arbitrary orthonormal basis $\{|e_1\rangle, |e_2\rangle, \ldots, |e_k\rangle\}$ of E. Let U be any unitary, that sends $\Pi_E |s\rangle$ to $\sqrt{s_1}|e_1\rangle + \sqrt{s_2}|e_2\rangle + \ldots + \sqrt{s_k}|e_k\rangle$ and acts as identity on $E^\perp$. Now note that

$$\left|\langle s| U^\dagger |e_i\rangle\right|^2 = \left|(U|s\rangle)^\dagger |e_i\rangle\right|^2 = s_i, \tag{13}$$

since

$$U|s\rangle = U(I - \Pi_E)|s\rangle + U(\Pi_E |s\rangle) \tag{14}$$

$$= (I - \Pi_E)|s\rangle + (\sqrt{s_1}|e_1\rangle + \sqrt{s_2}|e_2\rangle + \ldots + \sqrt{s_k}|e_k\rangle) \tag{15}$$

and $\langle e_i| (I - \Pi_E)|s\rangle = 0$. This tells us that $\left\{U^\dagger |e_1\rangle, U^\dagger |e_2\rangle, \ldots, U^\dagger |e_k\rangle\right\}$ is an orthonormal basis of E that gives rise to the pattern of the desired form (12). □

Corollary. Assume degenerate Hamiltonians H_1 and H_2 both have a pattern p. Then all patterns of H_1 are also patterns of H_2 and vice versa. In such a case we say that H_1 and H_2 have the *same patterns*.

Lemma 9. Suppose $U \in \mathrm{U}(4)$ and $[U, T] = 0$. Then the singlet state $|s\rangle$ is eigenvector of both U and $U^\dagger$.

Proof. Since $[U, T] = 0$, we know that U and T are simultaneously diagonal in some orthonormal basis (see Theorem 1). The singlet $|s\rangle$ must belong to this basis, since it spans the one-dimensional (-1)-eigenspace of the T gate. Therefore, $|s\rangle$ has to be an eigenvector of U as well. Note that U and $U^\dagger$ have the same eigenvectors. Thus, $|s\rangle$ is also an eigenvector of $U^\dagger$. □

Theorem 3. Hamiltonians H_1 and H_2 are T-similar if and only if they have the same patterns.

Proof. Assume H_1 and H_2 are T-similar, i.e., $H_2 = UH_1U^\dagger$ for some $U \in \mathrm{U}(4)$ such that $[U, T] = 0$. We want to show that H_1 and $UH_1U^\dagger$ have the same patterns. Since $[U, T] = 0$, by Lemma 9 we know that $|s\rangle$ is an eigenvector of $U^\dagger$. Let $|v\rangle$ be an eigenvector of H_1. Then $U|v\rangle$ is the corresponding eigenvector of $UH_1U^\dagger$. Now we have $\langle s|Uv\rangle = \left\langle U^\dagger s|v\right\rangle = \langle s|v\rangle$, i.e., the corresponding eigenvectors of H_1 and $UH_1U^\dagger$ have the same overlaps with the singlet state. Since conjugation does not change the eigenvalues, we have shown that patterns of H_1 and $H_2 = UH_1U^\dagger$ are the same.

Assume that H_1 and H_2 have a pattern p. Then there exists $U \in \mathrm{U}(4)$ such that $H_2 = UH_1U^\dagger$, since H_1 and H_2 have the same eigenvalues. Let $e^{i\varphi_j}$ be the eigenvalues of H_1 and H_2, and $|v_j\rangle$, $|w_j\rangle$ be the eigenvectors that give rise to the pattern p. Let $r_j := |\langle s|v_j\rangle| = |\langle s|w_j\rangle|$. We can express the singlet state $|s\rangle$ in the eigenbasis of H_1:

$$|s\rangle = \sum_{j=1}^{4} r_j e^{i\alpha_j} |v_j\rangle . \tag{16}$$

Since $[U, T] = 0$, by Lemma 9 the singlet state $|s\rangle$ is an eigenvector of $U^\dagger$ and we have $|\langle s|Uv_j\rangle| = \left|\left\langle U^\dagger s|v_j\right\rangle\right| = |\langle s|v_j\rangle| = r_j$ and

$$\langle s| U |v_j\rangle = r_j e^{i\beta_j} \tag{17}$$

for some phase β_j. Define $U' := UA$, where

$$A := \sum_{j=1}^{4} e^{-i(\alpha_j+\beta_j)} |v_j\rangle \langle v_j| . \tag{18}$$

We claim that (a) $U' H_1 {U'}^\dagger = H_2$, (b) $|\langle s| U' |s\rangle| = 1$.

(a) Note that H_1 and A commute, as they have the same eigenvectors. Also note that $AA^\dagger = I$, since A is a unitary. Therefore, we have

$$U' H_1 {U'}^\dagger = UAH_1A^\dagger U^\dagger = UH_1AA^\dagger U^\dagger = UH_1U^\dagger = H_2.$$

(b) We have:

$$\langle s| U' |s\rangle = \sum_{j=1}^{4} e^{i\alpha_j} r_j \langle s| U' |v_j\rangle \tag{19}$$

$$= \sum_{j=1}^{4} e^{i\alpha_j} r_j \langle s| U \sum_{k=1}^{4} e^{-i(\alpha_k+\beta_k)} |v_k\rangle \langle v_k|v_j\rangle \tag{20}$$

$$= \sum_{j=1}^{4} e^{i\alpha_j} r_j \langle s| U e^{-i(\alpha_j+\beta_j)} |v_j\rangle = \sum_{j=1}^{4} e^{-i\beta_j} r_j \langle s| U |v_j\rangle . \tag{21}$$

By applying (17) we get

$$\langle s| U' |s\rangle = \sum_{j=1}^{4} r_j^2 = 1. \tag{22}$$

Part (a) tells us that H_1 and H_2 are similar via U'. From (b) it follows that $|s\rangle$ is an eigenvector of U'. Thus according to Lemma 3, U' commutes with T. Hence, H_1 and H_2 are T-similar. □

The following theorem will allow us to check easily whether a given Hamiltonian is T-similar to a local Hamiltonian. Thus, we will be able to efficiently determine whether a given Hamiltonian falls into any of three families of non-universal Hamiltonians listed in Lemma 6.

Theorem 4. A two-qubit Hamiltonian H is T-similar to a local Hamiltonian if and only if it has a pattern of the form:

$$\begin{Bmatrix} \lambda_{11} & \lambda_{12} & \lambda_{21} & \lambda_{22} \\ s & t & t & s \end{Bmatrix}, \text{ where } \lambda_{11}+\lambda_{22}=\lambda_{12}+\lambda_{21}. \tag{23}$$

Proof. Assume H is T-similar to some local Hamiltonian $H' = H_1 \otimes I + I \otimes H_2$. According to Theorem 3, H and H' have the same patterns. Thus, in order to show that H has a pattern of the form (23), it suffices to prove that H' has the required pattern.

First, let us diagonalize H_1 and H_2:

$$H_1 = \alpha_1 |v_1\rangle\langle v_1| + \alpha_2 |v_2\rangle\langle v_2|, \quad H_2 = \beta_1 |w_1\rangle\langle w_1| + \beta_2 |w_2\rangle\langle w_2|. \tag{24}$$

Let the first eigenvectors of H_1 and H_2 be

$$|v_1\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \quad |w_1\rangle = \begin{pmatrix} c \\ d \end{pmatrix}. \tag{25}$$

Since we can ignore the global phase, we may assume that

$$|v_2\rangle = \begin{pmatrix} -b^* \\ a^* \end{pmatrix}, \quad |w_2\rangle = \begin{pmatrix} -d^* \\ c^* \end{pmatrix}. \tag{26}$$

Then

$$|v_1\rangle \otimes |w_1\rangle, \quad |v_1\rangle \otimes |w_2\rangle, \quad |v_2\rangle \otimes |w_1\rangle, \quad |v_2\rangle \otimes |w_2\rangle \tag{27}$$

are eigenvectors of H'. If we calculate the overlaps with $|s\rangle$ we get:

$$|\langle s|v_1, w_1\rangle|^2 = \tfrac{1}{2}|ad - bc|^2 =: s, \tag{28}$$

$$|\langle s|v_1, w_2\rangle|^2 = \tfrac{1}{2}|ac^* + bd^*|^2 =: t, \tag{29}$$

$$|\langle s|v_2, w_1\rangle|^2 = \tfrac{1}{2}|-a^*c - b^*d|^2 = \tfrac{1}{2}|ac^* + bd^*|^2 = t, \tag{30}$$

$$|\langle s|v_2, w_2\rangle|^2 = \tfrac{1}{2}|a^*d^* - b^*c^*|^2 = \tfrac{1}{2}|ad - bc|^2 = s. \tag{31}$$

The eigenvalues corresponding to vectors in (27) are

$$\lambda_{11} = \alpha_1 + \beta_1, \quad \lambda_{12} = \alpha_1 + \beta_2, \quad \lambda_{21} = \alpha_2 + \beta_1, \quad \lambda_{22} = \alpha_2 + \beta_2 \tag{32}$$

and they satisfy $\lambda_{11} + \lambda_{22} = \lambda_{12} + \lambda_{21}$. So we conclude that H' has a pattern of the form (23).

Now let us prove the other direction. We want to show that for any H that has a pattern of the form (23) we can find a local Hamiltonian H' such that H and H' are T-similar. By Theorem 3 we know that if H and H' have the same patterns, then they are T-similar. Therefore, it suffices to show that we can construct a local Hamiltonian $H' = H_1 \otimes I + I \otimes H_2$ with any given pattern of the form (23).

As before, we use α_i and $|v_i\rangle$ to refer to corresponding eigenvalues and eigenvectors of H_1. Similarly, we use β_i and $|w_i\rangle$ for H_2. First, given λ_{ij} from (23), we choose the eigenvalues of H_1 and H_2 as follows: $\alpha_1 = 0$, $\alpha_2 = \lambda_{21} - \lambda_{11}$, $\beta_1 = \lambda_{11}$, and $\beta_2 = \lambda_{12}$. Note that after this choice the eigenvalues of H' are

$$\alpha_1 + \beta_1 = \lambda_{11}, \quad \alpha_1 + \beta_2 = \lambda_{12}, \quad \alpha_2 + \beta_1 = \lambda_{21}, \quad \alpha_2 + \beta_2 = \lambda_{22}, \tag{33}$$

where the last equality holds, since $\lambda_{11} + \lambda_{22} = \lambda_{12} + \lambda_{21}$. Then we have to choose the corresponding eigenvectors of H_1 and H_2 so that they have the required overlaps. It suffices to make the right choice just for $|v_1\rangle$ and $|w_1\rangle$, since they completely determine the overlaps. In fact, it is always possible to choose $|v_1\rangle, |w_1\rangle \in \mathbb{R}^2$. If the angle between real unit vectors $|v_1\rangle = \binom{a}{b}$ and $|w_1\rangle = \binom{c}{d}$ is θ, then $ad - bc = \sin\theta$ (pseudo-scalar product) and $ac + bd = \cos\theta$ (scalar product). Thus, the overlaps (28) and (29) become $\frac{1}{2}\sin^2\theta = s$ and $\frac{1}{2}\cos^2\theta = t$, respectively (recall that $2s + 2t = 1$). So we can take any two real unit vectors having angle

$$\theta = \arcsin\sqrt{2s}. \tag{34}$$

□

Definition 10. We say that H is an *antisymmetric Hamiltonian* if $H = H^\dagger$ (H is Hermitian) and $H^T = -H$ (H is antisymmetric).

If H is an antisymmetric Hamiltonian, then $H^* = -H$. This means that all entries of H are purely imaginary. In fact two-qubit antisymmetric Hamiltonians correspond exactly to real linear combinations of Pauli basis elements containing exactly one Y, i.e., $\text{span}_\mathbb{R}\{I \otimes Y, X \otimes Y, Z \otimes Y, Y \otimes I, Y \otimes X, Y \otimes Z\}$.

Note that if H is an antisymmetric Hamiltonian, then e^{-iHt} and e^{-iTHTt} are real matrices for all $t \geq 0$. This can easily be seen if you think of Taylor expansion of e^x. Also note that $\det(e^{-iHt}) = e^{-i\,\mathrm{Tr}(H)t} = 1$. Therefore, we can simulate only some subset of SO(4) using H and H is clearly non-universal. Moreover, even $rI + H$ is non-universal for all $r \in \mathbb{R}$. This is because $e^{-i(rI+H)t} = e^{-irt}e^{-iHt}$ and so every unitary that can be simulated is of the form $e^{i\varphi}O$, where $O \in \mathrm{SO}(4)$ and $\varphi \in \mathbb{R}$. Now by Theorem 2 we conclude that all Hamiltonians that are T-similar to $rI + H$ are non-universal as well.

However, it turns out that we don't need to add any new family of non-universal Hamiltonians to the list in Lemma 6. The following theorem tells us that the above described family of non-universal Hamiltonians coincides with the family of Hamiltonians T-similar to some local Hamiltonian (first item in Lemma 6).

Theorem 5. Let H be a two-qubit Hamiltonian. Then the following are equivalent:

(1) H is T-similar to a local Hamiltonian,

(2) H has pattern of the form (23),

(3) H is T-similar to $rI + A$ for some $r \in \mathbb{R}$ and some antisymmetric Hamiltonian A.

Proof. From Theorem 4 we know that (1) and (2) are equivalent. We will show that (2) and (3) are equivalent.

Assume (2) holds. Theorem 3 tells us that T-similar matrices have the same overlaps. Therefore, it suffices to show that given a pattern

$$p = \begin{Bmatrix} \lambda_{11} & \lambda_{12} & \lambda_{21} & \lambda_{22} \\ s & \frac{1-2s}{2} & \frac{1-2s}{2} & s \end{Bmatrix}, \text{ with } \lambda_{11} + \lambda_{22} = \lambda_{12} + \lambda_{21} \tag{35}$$

it is possible to choose $r \in \mathbb{R}$ and antisymmetric Hamiltonian A so that $rI + A$ has pattern p. First, take $r := \frac{1}{2}(\lambda_{11} + \lambda_{22})$. Now let

$$A' := \begin{pmatrix} \varphi_1 & 0 \\ 0 & \varphi_2 \end{pmatrix} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{36}$$

where $\varphi_1 := \lambda_{11} - r$ and $\varphi_2 := \lambda_{12} - r$. Eigenvalues of A' are $\varphi_1, \varphi_2, -\varphi_1, -\varphi_2$ with the corresponding eigenvectors

$$\begin{aligned} |v'_{11}\rangle &:= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad |v'_{12}\rangle := \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \\ |v'_{21}\rangle &:= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}, \quad |v'_{22}\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}. \end{aligned} \tag{37}$$

Note that the eigenvalues of $rI + A'$ are $\lambda_{11}, \lambda_{12}, \lambda_{21}, \lambda_{22}$ with corresponding eigenvectors $\left|v'_{ij}\right\rangle$ as in (37). So the matrix $rI + A'$ has the correct eigenvalues but not necessarily the correct overlaps. Thus, we conjugate $rI + A'$ with an orthogonal matrix

$$O := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta & 0 \\ 0 & \sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{38}$$

to get matrix A with eigenvectors that give rise to the desired overlaps. Consider the following eigenbasis of $A := O(rI + A')O^\dagger$:

$$\begin{aligned} |v_{11}\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i\cos\theta \\ i\sin\theta \\ 0 \end{pmatrix}, |v_{12}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -\sin\theta \\ \cos\theta \\ i \end{pmatrix}, \\ |v_{21}\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -\sin\theta \\ \cos\theta \\ -i \end{pmatrix}, |v_{22}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i\cos\theta \\ -i\sin\theta \\ 0 \end{pmatrix}, \end{aligned} \tag{39}$$

where $|v_{ij}\rangle = O\left|v'_{ij}\right\rangle$ corresponds to the eigenvalue λ_{ij}. The overlaps of these eigenvectors are

$$|\langle s|v_{11}\rangle|^2 = |\langle s|v_{22}\rangle|^2 = \frac{1}{4}(\cos\theta - \sin\theta)^2 = \frac{1-\sin(2\theta)}{4} \tag{40}$$

$$|\langle s|v_{21}\rangle|^2 = |\langle s|v_{21}\rangle|^2 = \frac{1}{4}(\cos\theta + \sin\theta)^2 = \frac{1+\sin(2\theta)}{4}. \tag{41}$$

Therefore, if we choose $\theta := \frac{1}{2}\arcsin(1-4s)$, we get overlap s in (40) and $\frac{1-2s}{2}$ in (41). So we have constructed matrix $A = O(rI + A')O^\dagger = rI + OA'O^\dagger$ that has pattern p. Note that $OA'O^\dagger$ is indeed antisymmetric Hamiltonian, since $(OA'O^\dagger)^\dagger = OA'O^\dagger$ and $(OA'O^\dagger)^* = -OA'O^\dagger$ as A' is an antisymmetric Hamiltonian and O is an orthogonal matrix.

We proceed to show the other direction. Assume (3) holds. Again, due to Theorem 3, it suffices to show that $rI + A$ has a pattern of the form (23). Assume A has an eigenvector $|v\rangle$ with eigenvalue λ. Since A is antisymmetric Hamiltonian and $A = -A^*$, we get that

$$A\,|v^*\rangle = -(A\,|v\rangle)^* = -(\lambda\,|v\rangle)^* = -\lambda\,|v^*\rangle\,,$$

where $|v^*\rangle$ is obtained from $|v\rangle$ by taking complex conjugate of each of its components. So A has also eigenvector $|v^*\rangle$ with eigenvalue $-\lambda$.

We consider two cases – when A has only non-zero eigenvalues and when it has 0 as its eigenvalue.

- Assume A has only non-zero eigenvalues. Then $rI + A$ has eigenvalues $r+\lambda_1, r-\lambda_1, r+\lambda_2, r-\lambda_2$ with corresponding eigenvectors $|v_1\rangle, |v_1^*\rangle, |v_2\rangle$, $|v_2^*\rangle$. Since, the singlet is real vector, we have $|\langle s|v_i\rangle|^2 = |\langle s|v_i^*\rangle|^2$. So $rI+A$ has a pattern

$$p = \begin{Bmatrix} r+\lambda_1 & r+\lambda_2 & r-\lambda_2 & r-\lambda_1 \\ s & \frac{1-2s}{2} & \frac{1-2s}{2} & s \end{Bmatrix}, \tag{42}$$

  where $s := |\langle s|v_1\rangle|^2$. Note that $(r+\lambda_1)+(r-\lambda_1) = 2r = (r+\lambda_2)+(r-\lambda_2)$. Therefore, pattern p is of the desired form (23).

- Assume A has eigenvalue 0. If $A = 0$, then $rI + A = rI$. Since all eigenvalues of rI are the same, according to Lemma 8, we can choose an eigenbasis of rI to obtain any desired overlaps. For instance, $rI + A$ has a pattern

$$p = \begin{Bmatrix} r & r & r & r \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{Bmatrix}, \tag{43}$$

  which is of the form (23).

  Now assume $A \neq 0$. Then A has non-zero eigenvalues $\pm\lambda$ with corresponding eigenvectors $|v\rangle$ and $|v^*\rangle$. Thus, eigenvalue 0 has multiplicity 2. Accordingly, $rI+A$ has eigenvalues $r\pm\lambda$ with corresponding eigenvectors $|v\rangle$ and $|v^*\rangle$ and eigenvalue r with multiplicity 2. According to Lemma 8, we can choose two orthonormal eigenvectors in (r)-eigenspace so that they have the same overlaps with $|s\rangle$. Therefore, $rI + A$ has a pattern

$$p = \begin{Bmatrix} r+\lambda & r & r & r-\lambda \\ s & \frac{1-2s}{2} & \frac{1-2s}{2} & s \end{Bmatrix}, \tag{44}$$

where $s := |\langle s|v\rangle|^2 = |\langle s|v^*\rangle|^2$. It remains to note that the pattern p is of the desired form (23).

□

3.4 Proving the converse

In this section we show that the list of non-universal families of Hamiltonians in Lemma 6 is in fact complete. That is, we prove that any two-qubit Hamiltonian that does not fall in any of the three categories in Lemma 6 is universal.

3.4.1 Tridiagonal form

Theorem 6 (Construction 2)**.** Any Hamiltonian H is T-similar to a real symmetric *tridiagonal* matrix

$$\begin{pmatrix} a & b & 0 & 0 \\ b & c & d & 0 \\ 0 & d & e & f \\ 0 & 0 & f & g \end{pmatrix}, \tag{45}$$

where $a, b, c, d, e, f, g \in \mathbb{R}$ and $b, d, f \geq 0$.

Proof. Let us again work in the basis where T is diagonal (denoted by $\tilde{T}$). Then all matrices that commute with $\tilde{T}$ are block matrices of the form $\mathrm{U}(1) \oplus \mathrm{U}(3)$. We will use only the matrices that look as follows:

[This is probably called Jacobi or Householder method.]

$$\begin{pmatrix} 1 & 0 \\ 0 & \mathrm{U}(3) \end{pmatrix}. \tag{46}$$

Let the first column of H be $(h_1, h_2, h_3, h_4)^T$, where $\|(h_2, h_3, h_4)^T\| = b$. Then we can find P_1 in the form (46), such that the first column of $H_1 := P_1 H P_1^\dagger$ is $(h_1, b, 0, 0)^T$, where $b \geq 0$. Next, we consider the matrices of the form

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \mathrm{U}(2) \end{pmatrix}. \tag{47}$$

Again, let the second column of H_1 be $(h_1, h_2, h_3, h_4)^T$, where $\|(h_3, h_4)^T\| = d$. Then there is P_2 in the form (47), such that the second column of $H_2 := P_2 H_1 P_2^\dagger$ is $(h_1, h_2, d, 0)^T$, where $d \geq 0$. Note that the first column of H_2 remains the same as for H_1. Finally, we can find P_3 of the form

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \mathrm{U}(1) \end{pmatrix}, \tag{48}$$

such that the last entry f of the third column of $H_3 := P_3 H_2 P_3^\dagger$ is real and non-negative. Since H_3 is Hermitian, its diagonal entries are real. Hence it is of the form (45). □

Theorem 7. Hamiltonian in the tridiagonal form (45) has an eigenvector orthogonal to the singlet $|\tilde{s}\rangle$ if and only if $b = 0$ or $d = 0$ or $f = 0$.

Proof. If $b = 0$ or $d = 0$ or $f = 0$, then the Hamiltonian has an invariant subspace orthogonal to the singlet $|\tilde{s}\rangle$. It has dimension 3 or 2 or 1, respectively.

These conditions are also necessary. If $|v\rangle$ is an eigenvector of Hamiltonian H orthogonal to singlet $|\tilde{s}\rangle$, then $|v\rangle = (0, v_2, v_3, v_4)^T$. Let $|w\rangle := H|v\rangle$, then $|w\rangle = (0, w_2, w_3, w_4)^T$. Thus either $b = 0$ (one of our conditions) or $v_2 = 0$. If $b \neq 0$, then $v_2 = 0$ and we consider w_2. Since it must be zero, either $d = 0$ or $v_3 = 0$. If $d \neq 0$, we repeat the same argument and show that $f = 0$. □

Theorem 8. Hamiltonian in the tridiagonal form (45) corresponds to a unitary that is T-similar to a tensor product if and only if $a = c = e = g$.

Proof. Let us first show that these conditions are sufficient. If they hold, the Hamiltonian has the following eigenvalues and overlaps:

$$\lambda = a \pm_1 \sqrt{\frac{b^2 + d^2 + f^2 \pm_2 z}{2}}, \quad s = \frac{z \pm_2 (b^2 - d^2 - f^2)}{4z}. \tag{49}$$

Here subscripts indicate the correspondence between the signs and

$$z = \sqrt{b^4 + d^4 + f^4 + 2(b^2 d^2 + d^2 f^2 - b^2 f^2)}. \tag{50}$$

Eigenvalues with opposite first sign sum to $2a$ and the corresponding overlaps are equal. Therefore the unitary operation associated with this Hamiltonian will satisfy the conditions of Theorem 4 and hence is T-similar to a tensor product.

Let us show that these conditions are also necessary. It is enough to consider unitaries that are tensor products. Note that we need 4 real parameters to specify any 2×2 Hermitian matrix, since it can be written as a real linear combination of

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{51}$$

where σ_i are Pauli matrices. Note also that a 2-qubit unitary that is a tensor product has a Hamiltonian of the following form:

$$H = H_1 \otimes I + I \otimes H_2, \tag{52}$$

where H_1 and H_2 are 1-qubit Hamiltonians. We need 8 real parameters to specify a matrix of the form (52). However, we can use symmetry to reduce it to 4 real parameters.

First, observe that there is no need to specify the global phase for both qubits, since if unitary is a tensor product, the global phases of both qubits factor out. Hence we specify the global phase just for the first qubit. We can write any 1-qubit Hamiltonian in the following form:

$$\frac{\varphi}{2}I + \frac{\theta}{2}(x\sigma_x + y\sigma_y + z\sigma_z), \tag{53}$$

where σ_i are Pauli matrices, (x, y, z) is a unit vector in $\mathbb{R}^3$, and $\varphi, \theta \in \mathbb{R}$. It corresponds to a rotation about axis (x, y, z) by angle θ and global phase φ. We can change the basis of both qubits with the same local unitary, so that the second qubit is rotated around z axis. Thus we need just one parameter for the second qubit – the angle of rotation. However, there is still some freedom left – we can change the basis for both qubits by conjugating with a unitary that rotates around z axis. This does not affect the second qubit, but we can change the axis of rotation for the first qubit so that it has no y component. Thus we have reduced our Hamiltonian (52) to one with just 4 parameters:

[How is the global phase defined?]

$$H = (\alpha_1 I + x_1\sigma_x + z_1\sigma_z) \otimes I + I \otimes (z_2\sigma_z) \tag{54}$$

Recall that the (-1)-eigenspace of T is spaned by the singlet state $|s\rangle$ defined in equation (9) and the $(+1)$-eigenspace of T is spaned by three vectors defined in (8). However, since the $(+1)$-eigenspace is 3-dimensional, there are many ways how T can be diagonalized to obtain $\tilde{T}$. We can choose a different basis for the $(+1)$-eigenspace and diagonalize T by conjugating with the following matrix:

$$P := \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}. \tag{55}$$

If we conjugate our Hamiltonian (54) with $P^\dagger$, we get:

$$H' = P^\dagger H P = \alpha_1(I \otimes I) + x_1(\sigma_y \otimes \sigma_y) + z_1(I \otimes \sigma_x) - z_2(\sigma_z \otimes \sigma_x). \tag{56}$$

In matrix form H' looks as follows:

$$H' = \begin{pmatrix} \alpha_1 & z_1 - z_2 & 0 & -x_1 \\ z_1 - z_2 & \alpha_1 & x_1 & 0 \\ 0 & x_1 & \alpha_1 & z_1 + z_2 \\ -x_1 & 0 & z_1 + z_2 & \alpha_1 \end{pmatrix}. \tag{57}$$

Observe that H' is almost tridiagonal, therefore it is sufficient to do just one more conjugation. As in the proof of Theorem 6, we can find Q that commutes with $\tilde{T}$, such that $Q^\dagger H' Q$ is tridiagonal. We choose Q as follows:

$$Q := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{z_1 - z_2}{l} & 0 & \frac{x_1}{l} \\ 0 & 0 & 1 & 0 \\ 0 & \frac{-x_1}{l} & 0 & \frac{z_1 - z_2}{l} \end{pmatrix}, \tag{58}$$

where $l = \sqrt{x_1^2 + (z_1 - z_2)^2}$. Then we have

$$H'' = Q^\dagger H' Q = \begin{pmatrix} \alpha_1 & l & 0 & 0 \\ l & \alpha_1 & \frac{-2x_1 z_2}{l} & 0 \\ 0 & \frac{-2x_1 z_2}{l} & \alpha_1 & \frac{x_1^2 + z_1^2 - z_2^2}{l} \\ 0 & 0 & \frac{x_1^2 + z_1^2 - z_2^2}{l} & \alpha_1 \end{pmatrix}. \tag{59}$$

Depending on the values of x_1, z_1, and z_2 we may have to multiply the third or the fourth row and column of H'' by -1 to get the entries above and below the main diagonal non-negative. In any case, the diagonal entries does not change. Hence any Hamiltonian of the form (52) is T-similar to one whose diagonal entries are all equal (in our case they are equal to α_1). □

References

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