Characterization of two-qubit perfect entanglers

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Here we consider perfect entanglers from another perspective. It is shown that there are some special perfect entanglers which can maximally entangle a full product basis. We have explicitly constructed a one-parameter family of such entanglers together with the proper product basis that they maximally entangle. This special family of perfect entanglers contains some well-known operators such as CNOT and DCNOT, but not $\sqrt{\text{SWAP}}$. In addition, it is shown that all perfect entanglers with entangling power equal to the maximal value, $\frac{1}{2}$, are also special perfect entanglers. It is proved that the one-parameter family is the only possible set of special perfect entanglers. Also we provide an analytic way to implement any arbitrary two-qubit gate, given a proper special perfect entangler supplemented with single-qubit gates. Such these gates are shown to provide a minimum universal gate construction in that just two of them are necessary and sufficient in implementation of a generic two-qubit gate.

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I. INTRODUCTION

Entanglement has been proved to be a crucial ingredient in many quantum information processing (QIP) tasks, such as quantum computation and quantum communication [1]. In this respect, entanglement is a unique quantum mechanical resource which its production, quantification, and manipulation are of paramount importance in QIP. A fundamental relevant question here is how to characterize entangling capabilities of quantum operations. In fact, in this regard a lot of investigation have been done from many different aspects [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18].

In this paper we investigate the problem of characterization of perfect entanglers [17] from a new perspective. Perfect entanglers are defined as unitary operators that can generate maximally entangled states from some suitably chosen separable states. These operators are, in some sense, half of all nonlocal two-qubit unitary operators. Thus characterization of their (geometric and algebraic) structure(s) will be important. Fortunately, there are some well-defined (and relatively easy to calculate) tools to measure entangling properties of quantum operators, and also entanglement properties of two-qubit states [2, 13, 19]. By using these tools we show that one can analyze perfect entanglers and find that some of them have the unique property of maximally entangling a complete set of orthonormal product vectors. We explicitly construct such operators and show that they have the maximal entangling power, $\frac{1}{2}$. It is proved that these are the only unitary operators which have this property. However this investigation has its own importance, we provide a probable application for them. An analytic way to use such special perfect entanglers as the building blocks of the most efficient universal gate simulation is put forward. This assigns another remarkable role for such special entanglers in universality issues and the related topics.

The structure of this paper is as follows. In Sec. II we review some necessary definitions and some important facts about nonlocal two-qubit operators. This section is supplemented with appendices at the end the paper. In Sec. III we explicitly construct a one-parameter family of such special perfect entanglers and some relevant examples are provided. Also we go further and show that the family we have found is exactly the family of perfect entanglers with maximal entangling power, $\frac{1}{2}$, and no other perfect entangler except these ones have the mentioned property. In Sec. IV we discuss applications of these special perfect entanglers in universal gate simulation. We show that they can be used as elementary building blocks in minimum universal construction of two-qubit gates. The paper is concluded in Sec. V.

II. PRELIMINARIES

In this section we want to review briefly some facts on nonlocal two-qubit unitary operators. More discussion on this matter can be found in the appendices and references therein. It is known that [5, 17, 20] any two-qubit unitary operator $U \in \text{SU}(4)$ can be written in the following form

$$U = (A_1 \otimes B_1)e^{-i(c_1\sigma_1 \otimes \sigma_1 + c_2\sigma_2 \otimes \sigma_2 + c_3\sigma_3 \otimes \sigma_3)}(A_2 \otimes B_2),$$

(1)

where $\sigma_i$’s are the Pauli spin matrices, and $A_1$, $B_1 \in \text{SU}(2)$ are some single-qubit unitary operators. By using this decomposition for $U$, called the canonical decomposition, one can define local equivalence of two unitary operators. Two operators $U, U' \in \text{SU}(4)$ are considered locally equivalent, $U \cong U'$, if there exist some single-qubit unitary operators $u_1, u_2, v_1, v_2 \in \text{SU}(2)$, such that

$$U' = u_1 \otimes v_1 U u_2 \otimes v_2.$$  

(2)

It has been shown that using the concept of local equivalence one can find some freedoms in $c_i$’s such that one can always restrict oneself to the region $\frac{1}{3} \geq c_1 \geq c_2 \geq |c_3|$ in the $(c_1, c_2, c_3)$ space (Appendix A). This is the so-called Weyl chamber [1]. Hereafter, whenever we write $[c_1, c_2, c_3]$ we will assume using these freedoms. So when we want to deal...
with local equivalence we can always consider $U \equiv \mathcal{U} \equiv [c_1, c_2, c_3]$, up to the freedoms. For the following uses it is helpful to present the explicit form of $\mathcal{U}$. In the standard computational basis (where $\sigma_3|0\rangle = |0\rangle$, $\sigma_3|1\rangle = |-1\rangle$), we have

$$\mathcal{U} = \begin{pmatrix} e^{-ic_3}c^- & e^{ic_3}c^+ & -ie^{-ic_3}s^- \\ e^{ic_3}c^+ & e^{-ic_3}c^- & ie^{ic_3}s^+ \\ -ie^{-ic_3}s^+ & ie^{ic_3}s^- & e^{ic_3}c^- \end{pmatrix},$$

(3)

where $c^\pm = \cos(c_1 \pm c_2)$ and $s^\pm = \sin(c_1 \pm c_2)$. Consider the usual Bell basis, $\{|\Phi^\pm\rangle = \frac{|00\rangle \pm |11\rangle}{\sqrt{2}}\}$. Then, it is easily seen that in the basis $^1$

$$|\Phi_1\rangle = |\Phi^+\rangle, \quad |\Phi_2\rangle = -i|\Phi^-\rangle,$$

(4)

$$|\Phi_3\rangle = |\Psi^-\rangle, \quad |\Phi_4\rangle = -i|\Psi^+\rangle,$$

(5)

$\mathcal{U}$ is diagonal

$$\mathcal{U} = \sum_{k=1}^{4} e^{-i\lambda_k} |\Phi_k\rangle \langle \Phi_k|,$$

(6)

where

$$\lambda_1 = c_1 - c_2 + c_3, \quad \lambda_2 = -c_1 + c_2 + c_3, \quad \lambda_3 = -(c_1 + c_2 + c_3), \quad \lambda_4 = c_1 + c_2 - c_3.$$

Makhlin $^2$ and Zhang et al. $^7$ have shown that the local equivalence classes can be characterized uniquely by the two local invariants $G_1[U]$ and $G_2[U]$ which are as follows

$$G_1 = \frac{1}{4} [e^{-2ic_3} \cos 2(c_1 - c_2) + e^{2ic_3} \cos 2(c_1 + c_2)]^2,$$

(7)

$$G_2 = \cos(4c_1) + \cos(4c_2) + \cos(4c_3),$$

(8)

Moreover, in $^3$ the important notion of a perfect entangler has been defined. Strictly speaking, a two-qubit unitary operator is called a perfect entangler if it can produce a maximally entangled state from a suitable unentangled (separable) one. It is not hard to see that [cnot], [dcnot]$^2$, and [sqrtswap] classes are all perfect entanglers. For example, for [cnot] a choice can be $[\text{cnot}]|00\rangle = \frac{|00\rangle - i|11\rangle}{\sqrt{2}}$.

To characterize entangling capabilities of unitary operators entangling power has been introduced $^2$. This measure is defined to be the average entanglement that the unitary operator can produce when acting on separable states. It can be shown that entangling power of a unitary operator $U$, $e_p(U)$, has the following simple form

$$e_p(U) = e_p(\mathcal{U}) = \frac{1}{18} \left[3 - \cos 4c_1 \cos 4c_2 + \cos 4c_2 \cos 4c_3 + \cos 4c_3 \cos 4c_1\right],$$

(9)

which only depends on the nonlocal part $[c_1, c_2, c_3]$ (Appendix $^3$).

Other important points that are helpful in our next discussions are separability and maximally entanglement conditions in the magic basis. It has been shown in $^5$ that a state $|\Psi\rangle = \sum_k \mu_k |\Phi_k\rangle$ is separable iff $\sum_k \mu_k^2 = 0$. As well, $|\Psi\rangle$ is maximally entangled iff $\mu_k^2 = e^{-i\delta} |\mu_k|^2$ ($k = 1, \ldots, 4$). This means that a state is maximally entangled iff its coefficients in the magic basis are real, up to a global phase.

III. SPECIAL PERFECT ENTANGLERS

In this section, we are going to study some special members of the space of perfect entanglers. As we see below this turns out to be useful in characterization of structure of the space of perfect entanglers. In this regard, we pose the following question:

Does there exist any perfect entangler which can maximally entangle a full separable basis?

This question is motivated by the following observation which was firstly reported in $^6$. To be complete in our discussion we reproduce it here. It can be seen that for the [cnot] class one can find four orthonormal product states which are transformed to some maximally entangled states. For example, we have

$$[\text{cnot}]|00\rangle = \frac{|00\rangle - i|11\rangle}{\sqrt{2}}, \quad [\text{cnot}]|01\rangle = \frac{|01\rangle - i|10\rangle}{\sqrt{2}},$$

$$[\text{cnot}]|10\rangle = \frac{|10\rangle - i|01\rangle}{\sqrt{2}}, \quad [\text{cnot}]|11\rangle = \frac{|11\rangle - i|00\rangle}{\sqrt{2}}.$$

(10)

This property may not seem so important at this stage. But if we want to find such a separable basis for the [sqrtswap] class the result, as is shown below, is a failure. To see this, we note that the most general separable basis (up to general phase factors for each vector) that can be considered is as follows

$$|\Psi_1\rangle = (a|0\rangle + b|1\rangle) \otimes (c|0\rangle + d|1\rangle),$$

$$|\Psi_2\rangle = (-b|0\rangle + a|1\rangle) \otimes (c|0\rangle + d|1\rangle),$$

$$|\Psi_3\rangle = (e|0\rangle + f|1\rangle) \otimes (-d|0\rangle + c|1\rangle),$$

$$|\Psi_4\rangle = (-f|0\rangle + e|1\rangle) \otimes (-d|0\rangle + c|1\rangle),$$

(11)

in which bar means complex conjugation and $|a|^2 + |b|^2 = |c|^2 + |d|^2 = |e|^2 + |f|^2 = 1$. Now if we act on one of these states, say $|\Psi_1\rangle$, by the [swap] class we obtain

$$[\text{sqrtswap}]|\Psi_1\rangle = e^{-i\bar{f}ac} |00\rangle + \frac{e^{i\bar{f}}}{\sqrt{2}} (ad - ibc)|01\rangle$$

$$-i\frac{e^{i\bar{f}}}{\sqrt{2}} (ad + ibc)|10\rangle + e^{-i\bar{f}bd}|11\rangle.$$

(12)

This state is maximally entangled if its concurrence $^9$, $C = |ad - bc|^2$, is equal to 1 (Appendix $^3$). Thus the [sqrtswap] class turns these orthonormal states into maximally entangled ones if the following conditions are fulfilled simultaneously

$$|ad - bc|^2 = 1, \quad |\bar{a}c + \bar{b}d|^2 = 1,$$

(13)

$$|\bar{c}f - \bar{d}e|^2 = 1, \quad |\bar{e}c + \bar{d}f|^2 = 1.$$

(14)

However, by side by side addition of the equations in $^3$, we get $|a|^2 + |b|^2(|c|^2 + |d|^2) = 2$ which in the light of

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$^1$ There are different conventions about the magic basis $^3$. We follow the definition in $^3$.

$^2$ DCNOT or double-CNOT is defined as $^3$: DCNOT$\equiv$CNOT$^2$CNOT$^2$, where the subscripts 12 for CNOT mean that the first (second) qubit is the control (target) qubit, and similarly for 21.
normalization conditions is an apparent contradiction! A similar contradiction is obtained from Eq. (14). Therefore the \( \sqrt{\text{SWAP}} \) class cannot maximally entangle any full product basis. However, it must be noted that this fact does not forbid finding a pair of orthonormal states which become maximally entangled by this class. For example, by choosing the following pair of orthonormal product vectors

\[
|\Psi_1\rangle = (a|0\rangle + b|1\rangle) \otimes (c|0\rangle + d|1\rangle), \\
|\Psi_1\rangle = (-b|0\rangle + a|1\rangle) \otimes (-d|0\rangle + c|1\rangle),
\]

in which \(|ad-be|^2 = 1\), no contradiction is turned out. It is interesting to note that \(e_p(\sqrt{\text{SWAP}}) = \frac{1}{\pi}\), which is the minimum entangling power among all perfect entanglers.

In the following we are going to find some other unitary operators having this property. Hereafter, the perfect entangler that can maximally entangle a full product basis are called special perfect entanglers (SPE). We are trying to explicitly construct such operators together with their related product basis.

Since working with a general product basis, Eq. (11), is hard let us, for the time being, restrict ourselves to a rather special case of product basis set. It is seen that by a suitable local unitary operator, \(U_1 \otimes U_2\), it is always possible to transform two of the basis vectors of \(\{|\Psi_i\rangle\}_{i=1}^3\), say \(|\Psi_1\rangle\) and \(|\Psi_2\rangle\), to the separable states \(|00\rangle\) and \(|10\rangle\). If we choose

\[
U_1 = \begin{pmatrix} \bar{a} & \bar{b} \\ -b & a \end{pmatrix}, \quad U_2 = \begin{pmatrix} \bar{c} & \bar{d} \\ -d & c \end{pmatrix},
\]

then \(U_1 \otimes U_2\) acts on the vectors of Eq. (11) as

\[
U_1 \otimes U_2|\Psi_1\rangle = |00\rangle, \\
U_1 \otimes U_2|\Psi_2\rangle = |10\rangle, \\
U_1 \otimes U_2|\Psi_3\rangle = \left[(\bar{a}e + \bar{b}f)|0\rangle + (-be + af)|1\rangle\right]|1\rangle, \\
U_1 \otimes U_2|\Psi_4\rangle = \left[-(\bar{b}e + \bar{a}f)|0\rangle + (bf + ae)|1\rangle\right]|1\rangle.
\]

Thus this separable basis is locally equivalent to the following more simpler set

\[
\{|00\rangle, |10\rangle, (A|0\rangle + B|1\rangle)|1\rangle, -(\bar{B}|0\rangle + \bar{A}|1\rangle)|1\rangle\},
\]

for the specific values of \(A\) and \(B\) as in Eq. (17). Here a point in order. However for any unitary operators \(U_1, U_2 \in SU(2)\) we have \(E(U_1 \otimes U_2|\Psi\rangle) = E(|\Psi\rangle)\), generally it cannot be concluded that \(E(U_1 \otimes U_2|\Psi\rangle) = E(|\Psi\rangle)\). As an example, \(\text{CNOT}|00\rangle = |00\rangle\), but \(\text{CNOT}(H \otimes I)|00\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}\) (\(H\) is the Hadamard matrix). This point hints us that our solution(s) may not be the most general one(s), that is, it is still possible to find other SPE in addition to what we find below. We return to this point a bit later. Anyway, action of a \(U\) on the basis vectors in Eq. (18), respectively, gives the following results

\[
\begin{pmatrix}
e^{-ic_3}c^* & 0 & 0 \\
0 & e^{-i\theta}c_3^* & B \\
-e^{-i\theta}c_3 & e^{i\theta}c A
\end{pmatrix}
\begin{pmatrix}
e^{-ic_3}s^* & 0 & 0 \\
0 & e^{-i\theta}s_3 & B \\
-e^{-i\theta}s_3 & e^{i\theta}s A
\end{pmatrix}
\begin{pmatrix}
e^{-ic_3} \bar{s} & 0 & 0 \\
0 & e^{-i\theta}\bar{s}_3 & \bar{B} \\
e^{-i\theta}\bar{s}_3 & e^{i\theta}\bar{s} \bar{A}
\end{pmatrix}
\]

The maximal entanglement condition for these states requires that

\[
|s^-c^-| = |s^+c^+| = \frac{1}{2}, \\
|e^{2ic_3}c^+A - e^{-2ic_3}c^-B|^2 = |e^{2ic_3}s^-A - e^{-2ic_3}s^+B|^2 = \frac{1}{2}.
\]

As is seen the conditions on \(c_1\) and \(c_2\) are independent of the the last conditions. Combination of this set of equations gives the following results

\[
\sin 2(c_1 - c_2) = \pm 1, \quad \sin 2(c_1 + c_2) = \pm 1,
\]

\[
|e^{2ic_3}(\pm 1)A^2 - e^{-2ic_3}(\pm 1)B^2| = 1.
\]

By using the triangular inequality, \(|z_1 + z_2| \leq |z_1| + |z_2|\), for two complex variables \(z_1 = |z_1|e^{i\phi_1}\), and noting that the equality holds when \(\phi_1 = \phi_2(\mod 2\pi)\), Eq. (21) can be simplified more. If we note that \(|e^{2ic_3}A^2 \pm e^{-2ic_3}B^2| \leq |A|^2 + |B|^2 = 1\), and parameterize \(A = \cos \theta\) and \(B = e^{2i\theta}\sin \theta\), the phase, is chosen for later convenience), then \(|e^{2ic_3}\cos^2 \theta \pm e^{-2ic_3}\cos^2 \theta| \sin \theta| = 1\) requires that

\[
e^{2ic_3} = \pm e^{-2i(c_3 - 2\phi)},
\]

which has the following simple solutions

\[
c_3 = \phi + \frac{k\pi}{4}, \quad c_3 = \phi + \frac{(2k+1)\pi}{4}, \quad k \in \mathbb{Z}.
\]

Now if we use the freedoms in choosing \(c_1\)’s for a class (Appendix A), there only remain the following solutions

\[
c_3 = \phi, \quad \frac{\pi}{4}. \quad (22)
\]

We shall now go back to the condition (20). Apparently four different cases can be obtained from this equation. But again by a simple algebra and using the freedoms in \(c_3\)’s of a class it appears that the two classes

\[
U_1 \equiv \left[0, \frac{\pi}{4}, \phi\right], \quad (23)
\]

\[
U_2 \equiv \left[\frac{\pi}{4}, 0, \frac{\pi}{4} + \phi\right], \quad (24)
\]

are our independent solutions. Furthermore, by a simple re-definition of \(\phi\) in Eq. (24) and another use of the freedom for \(c_3\)’s, it can be inferred that we actually have found a one-parameter family of SPE

\[
\left[\frac{\pi}{4}, \phi, 0\right], \quad 0 \leq \phi \leq \frac{\pi}{4}.
\]

Figure 1 shows the geometrical representation of the SPE family in the \((c_1, c_2, c_3)\) space. It should be noted that in the two-qubit case we are fortunate to have this simple geometrical interpretation, which is relatively absent for higher cases.

3 The SPE line \(A_1A_2\) in Fig. 1 corresponds to the \(A_2L\) line in Fig. 1 of [3].
In addition, orthonormality conditions, can find some suitable separable basis (question, now, is to find unitary operators, orthogonal form of Eq. (25). Now, we consider the problem in a general manner, if we have Eq. (25). In this basis we can maximize entangled basis. So our answer is not. Also the \([\text{DCNOT}]\) gate (for \(\phi = 0\)) and the [\(\text{DCNOT}\)] gate (for \(\phi = \frac{\pi}{2}\)) are both members of this one-parameter family of SPE, however, \([\sqrt{\text{SWAP}}]\) is not. Also the local invariants of the SPE in Eq. (25) are

\[
G_1 = 0, \quad G_2 = \cos 4\phi.
\]

Using the form, for example, in Eq. (24) we can simply find the form of the transformed states (up to local unitary operators), which are as

\[
e^{-i\phi_1} |001\rangle + e^{i\phi_1} |110\rangle,
\]

\[
e^{-i\phi_2} |\sin(\phi)|00\rangle + |\cos(\phi)|11\rangle,
\]

\[
e^{-i\phi_3} |\cos(\phi)|00\rangle + |\sin(\phi)|11\rangle, \quad (26)
\]

and are clearly maximally entangled.

It is interesting to see that the \([\text{CNOT}]\) gate (for \(\phi = 0\)) and the \([\text{DCNOT}]\) gate (for \(\phi = \frac{\pi}{2}\)) are both members of this one-parameter family of SPE, however, \([\sqrt{\text{SWAP}}]\) is not. Also the local invariants of the SPE in Eq. (25) are

\[
G_1 = 0, \quad G_2 = \cos 4\phi.
\]

Up to now, we just have shown that at least there exists a one-parameter family of unitary operators that are SPE, Eq. (25). Now, we consider the problem in a general manner. In fact, we show that the family (25) is the only possible family of operators that are SPE. To this end, we use the diagonal form of \(U\) in the magic basis, Eq. (6). In this basis we can write

\[
|\Psi^{(i)}_{\text{sep}}\rangle = \sum_k \mu_k^{(i)} |\Phi_k\rangle, \quad |\Psi^{(i)}_{\text{me}}\rangle = \sum_k w_k^{(i)} |\Phi_k\rangle,
\]

where \(\{|\Psi^{(i)}_{\text{sep}}\rangle\}_{i=1}^4\) is a general product (separable) basis, and similarly \(\{|\Psi^{(i)}_{\text{me}}\rangle\}_{i=1}^4\) is a maximally entangled basis. So our question, now, is to find unitary operators, \(U\), for which we can find some suitable separable basis \(\mu_k^{(i)}\)s and a maximally entangled basis \(w_k^{(i)}\) such that

\[
U |\Psi^{(i)}_{\text{sep}}\rangle = |\Psi^{(i)}_{\text{me}}\rangle.
\]

By using Eq. (6), the following relation between \(\mu_k^{(i)}\)’s and \(w_k^{(i)}\)’s is obtained

\[
w_k^{(i)} = e^{-i\lambda_k} \mu_k^{(i)} \quad (i, k = 1, \ldots, 4). \quad (29)
\]

In addition, orthonormality conditions, \(\langle \Psi^{(i)}_{\text{sep}} | \Psi^{(j)}_{\text{sep}} \rangle = \langle \Psi^{(i)}_{\text{me}} | \Psi^{(j)}_{\text{me}} \rangle = \delta_{ij}\) read as

\[
\sum_k \mu_k^{(i)} \mu_k^{(j)} = \sum_k w_k^{(i)} w_k^{(j)} = \delta_{ij}. \quad (30)
\]

Now, taking into account the last points of Sec. III, separability of \(\{|\Psi^{(i)}_{\text{sep}}\rangle\}_{i=1}^4\) and maximally entanglement of \(\{|\Psi^{(i)}_{\text{me}}\rangle\}_{i=1}^4\), respectively, requires that

\[
\sum_k \mu_k^{(i)} = 0, \quad w_k^{(i)} = e^{-i\delta^{(i)}} |w_k^{(i)}|^2, \quad (31)
\]

from which (by using Eq. (29)) one obtains

\[
\sum_k e^{2i\lambda_k} w_k^{(i)} = 0, \quad w_k^{(i)} = \pm e^{-i\delta^{(i)}} |w_k^{(i)}|. \quad (33)
\]

If we replace Eq. (34) in Eq. (33) and multiply it by \(e^{2\epsilon}\), after separating real and imaginary parts we get

\[
\alpha_1 = 4(c_1 + c_2), \quad \alpha_2 = 4(c_1 + c_3), \quad \alpha_3 = 4(c_2 + c_3).
\]

Orthonormality condition, Eq. (30), is equal to unitarity of the matrix \(U_{ik} := w_k^{(i)}\), which instead gives the below results

\[
\sum_k |w_k^{(i)}|^2 = 1, \quad (37)
\]

\[
\sum_k w_k^{(i)} w_j^{(k)} = \delta_{ij} \quad (38)
\]

By using Eq. (34), Eq. (38) can be simplified as

\[
e^{2i\delta} \sum_k |w_k^{(i)}||w_j^{(k)}| = \sum_k |w_k^{(k)}||w_j^{(k)}| = \delta_{ij}. \quad (39)
\]

If we now add the relations in Eq. (35) for different \(i\)’s, and consider Eq. (77), it is obtained that

\[
\cos \alpha_1 + \cos \alpha_2 + \cos \alpha_3 = 0. \quad (40)
\]

In a similar manner, Eq. (36) results into

\[
\sin \alpha_1 + \sin \alpha_2 + \sin \alpha_3 = 0. \quad (41)
\]

By combination of these two equations, the following final condition for a class \([c_1, c_2, c_3]\) being a SPE is obtained

\[
\cos 4c_1 \cos 4c_2 + \cos 4c_2 \cos 4c_3 + \cos 4c_3 \cos 4c_1 = -1. \quad (42)
\]

This, in turn, implies that \(\epsilon_p(\mathcal{U}) = \frac{\pi}{4}\). Therefore, we have proved that if a unitary operator, \(\mathcal{U}\), is a SPE it must have the maximal entangling power. Now, let us investigate all possible solutions of Eq. (42). It is trivial to check that if one of the \(c_i\)’s, say \(c_1\), is equal to \(\frac{\pi}{4}\), then the only choices for the other \(c_i\)’s are \(0(\frac{\pi}{4})\) and \(0 \leq \phi \leq \frac{\pi}{2}\). This is the very family of SPE as in Eq. (25). More generally, the only acceptable solutions of Eq. (42) are also of the form in (25) (and its permutations).

Thus it has been shown that only the unitary operators \([\frac{\pi}{4}, \phi, 0]\) which are the unique family with \(\epsilon_p = \frac{\pi}{4}\) can be SPE. This fact...
stresses that for the SPE entangling power is a sufficient tool which can characterize them uniquely.

Now let us consider the subspace of non-perfect entanglers, especially the \([\text{SWAP}]\) class in the sense that how they act on separable bases. We want to point out a simple property of this class. As has been proved in [22], any nonlocal two-qubit (qudit) unitary operator other than those in the \([\text{SWAP}]\) class can be used as a universal operator (of course together with elementary single-qubit unitary operators). Additionally, it has been known that any unitary operator \(V\) leaves product states product (that is, for any \([x]\) and \([y]\) there exist some \([u]\) and \([v]\) such that \(V[x]y = [u][v]\)) is either a local unitary operator \(A \otimes B\) or \((A \otimes B)S\), for some \(A\) and \(B\). Now, it can be deduced that the only unitary operators that can transform any separable basis to some separable basis are those in the \([\text{SWAP}]\) class. This can be seen as follows. Consider two arbitrary vectors \([a]\) and \([b]\). Suppose that \(V\) is such an operator that transforms any product basis to another one. To see that if \(V[a]|b\rangle\) is a separable state, we can construct another basis set in which \([a]\langle b]\) is one of the basis vectors. For example,

\[
\{ |a\rangle|b\rangle, |a\rangle|c\rangle, |b\rangle|c\rangle, |b\rangle|a\rangle \},
\]

is such a new basis. Thus \(V\) must transform \([a]\langle b]\) to some \([a\rangle]\langle b]\). As mentioned above, this indicates that \(V\) is either local or locally equivalent to the \(\text{SWAP}\) operator. Here we should remark that the above statement is true only if \(V\) leaves any separable basis a separable one. For example, the \(\text{CNOT}\) operator transforms the usual computational basis \(\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}\) to another separable basis, however, it is nonlocal.

Finally, we shall show that by using the spectral decomposition of the nonlocal part, Eq. (6), a simple (yet remarkable) property of \(\mathcal{U}\), which is related to the magic basis, can be deduced.

**Lemma.** There is no separable basis \(\{ |\alpha_i\rangle \otimes |\beta_i\rangle \}_{i=1}^4\) that can be transformed to the magic basis by an operator \(\mathcal{U}\), as in Eq. (3).

**Proof:** (By contradiction) Suppose that for a given operator \(\mathcal{U}\) there exists such a basis, \(\mathcal{U}|\alpha_i\rangle \otimes |\beta_i\rangle = |\Phi_i\rangle\). This is equivalent to \(\mathcal{U}|\Phi_i\rangle = |\alpha_i\rangle \otimes |\beta_i\rangle\). By using the form in Eq. (6), this gives rise to \(e^{i\lambda}|\Phi_i\rangle = |\alpha_i\rangle \otimes |\beta_i\rangle\) which is an evident contradiction! □

It should be emphasized that, for example, for the \([\text{CNOT}]\) class we have

\[
\begin{align*}
\frac{|0\rangle + |1\rangle}{\sqrt{2}} |0\rangle & \rightarrow \frac{|0\rangle + |1\rangle}{\sqrt{2}}, \\
\frac{|0\rangle + |1\rangle}{\sqrt{2}} |1\rangle & \rightarrow \frac{|1\rangle + |0\rangle}{\sqrt{2}}.
\end{align*}
\]

The right hand side is the usual Bell basis. However, this does not violate the above lemma. In fact, the point is the difference between the usual Bell basis and the magic basis. The two sets of basis vectors are not locally related. This can be seen by examining, for example, the following operator

\[U = |\Phi_1\rangle\langle \Phi^+| + |\Phi_2\rangle\langle \Phi^-| + |\Phi_3\rangle\langle \Psi^-| + |\Phi_4\rangle\langle \Psi^+|.
\]

This operator is diagonal in the magic basis, and thus is nonlocal. Actually, for this specific operator \(G_1[U] = 0\) and \(G_2[U] = -1\) which indicate \(U \in [\text{DCNOT}]\).

### IV. APPLICATIONS TO EFFICIENT TWO-QUBIT GATE SIMULATION

In this section, we are going to present a remarkable importance of the SPE, which can put forward special theoretical and experimental interests in them.

From theoretical and experimental viewpoints, efficient quantum gate synthesis is of high interest. In fact, there is a vast literature on this topic with many remarkable findings [23, 24, 25, 26, 27, 28, 29, 31, 32, 33, 34, 35]. It has been known that a general (multi-qubit) quantum gate can be simulated using a quantum circuit built of elementary gates which operate on single and two qubits [23]. For instance, Barenco et al. [23] have shown that a combination of the CNOT and single-qubit gates is universal, in the sense that any unitary operation can be simulated by them. This is the commonly adopted universal set in paradigm of quantum computation. However, there has been a lot of interest in universal sets which are highly (or the most) efficient. Actually, there is a practical reason behind this demand. In present day experiments, two-qubit gates as the CNOT gate can only be implemented imperfectly due to today technological limitations (the so-called decoherence). Therefore, in order to reduce the probability that an error occurs in performing a certain unitary operation on several qubits, instrumentally it is highly demanded that the number of the building block gates (i.e., the number of times that the qubits interact) be as small as possible. Furthermore, it is clear that these attempts can be of advantage in analyzing the algorithmic complexity of a given quantum computation and other QIP related tasks [13].

Very recently, it has been shown that in order to implement an arbitrary two-qubit unitary operator not more than three applications of the CNOT or the DCNOT gates are necessary [31, 33]. In this sense, the CNOT and the DCNOT gates are highly efficient elementary gates. However, remarkably, it has also recently been shown that the \(B = e^{-i(\pi/4 \otimes \sigma_2)}\) gate is the most efficient one, in that any arbitrary two-qubit unitary operator can be constructed only by two applications of such gate [34]. The fact we would like to stress on is that all of these three gates; the CNOT, the DCNOT, and the \(B\) gates, are SPE. This can raise the question that if other SPE gates also can give rise to a minimum universal gate construction. To this end, we follow the method proposed in [33, 34]. We need to remind that the \(B\) gate as the most efficient known universal gate can simulate a generic nonlocal two-qubit operator with the following circuit

\[
\begin{array}{cccc}
B & \epsilon^{-i\alpha_3} & \epsilon^{-i\alpha_4} \\
-\epsilon^{-i\alpha_4} & \epsilon^{-i\alpha_3} & \epsilon^{-i\alpha_2} \\
-\epsilon^{-i\alpha_4} & \epsilon^{-i\alpha_2} & \epsilon^{-i\alpha_1}
\end{array}
\]

where the parameters \(a\) and \(b\) satisfy

\[
\begin{align*}
\sin 2a &= \sqrt{\frac{\cos 2c_2 \cos 2c_3}{1 - 2 \sin^2 c_2 \cos^2 c_3}}, \\
\cos 2b &= 1 - 4 \sin^2 c_2 \cos^2 c_3.
\end{align*}
\]

Equivalence of these two circuits can be proved simply by showing that the nonlocal invariants \((G_1\) and \(G_2\)) of the both
circuits are the same. For our study, we choose an arbitrary SPE, which we call $C[\phi] = e^{-i\phi (\sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2)}$. We are looking for some SPE gates other than the $B = C[\frac{\pi}{2}]$ gate that give rise to a minimum construction of two-qubit unitary operators universally. Following [31, 33], we consider the circuit below which is similar to the one in Eq. (43).

$$C[\phi]$$

(45)

and try to find the parameters $a$ and $b$ such that this circuit can simulate a generic nonlocal gate $U(c_1, c_2, c_3)$, as in Eq. (3). After computing the local invariants of this circuit and comparing them with the invariants of $[c_1, c_2, c_3]$, it is seen that the following equations must be satisfied

$$\cos 2a \sin 2b \sin 4\phi = \sin 2c_2 \sin 2c_3$$

(1 + \cos 4\phi) \cos 4a + (1 + \cos 4\phi) \cos 4a \cos 2b + (3 \cos 4\phi - 1) \cos 2b + 4 \cos 2c_2 \cos 2c_3 - (1 + \cos 4\phi) = 0$$

(46)

(47)

In fact, there is another (relatively long) equation which also must be satisfied as the consistency check for the possible solutions, which we have not written here. By the way, it is easy to see that the following two solutions can be found

$$\cos 2b = 1 - \frac{(1 - \cos 2c_2)(1 + \cos 2c_2)}{1 - \cos 4\phi}$$

$$\cos^2 2a = \frac{(1 + \cos 2c_2)(1 - \cos 2c_2) \tan^2 2\phi}{1 + \cos 2c_2 - \cos 2c_2 \cos 2c_3}$$

(48)

and

$$\cos 2b = 1 - \frac{(1 + \cos 2c_2)(1 - \cos 2c_2)}{1 - \cos 4\phi}$$

$$\cos^2 2a = \frac{(1 - \cos 2c_2)(1 - \cos 2c_2) \tan^2 2\phi}{1 - \cos 2c_2 - \cos 2c_2 \cos 2c_3}$$

(49)

Both of these solutions satisfy the mentioned consistency check relation, for any $\phi$. However, from these solutions it immediately can be deduced that we must have $\phi \neq 0, \frac{\pi}{2}$. This means that the CNOT and the DCNOT gates cannot be among these gates. This fact is in accordance to the results of [31, 33] which indicate that except some special cases at least three applications of the CNOT and the DCNOT gates are necessary and sufficient for generic gate simulations. In addition, after checking that the solutions must satisfy the relations $-1 \leq \cos 2b \leq 1$ and $0 \leq \cos^2 2a \leq 1$, it is found that if we want to have at least one solution we must choose the value of $\phi$ by considering the values of $c_2$ and $c_3$ of $U(c_1, c_2, c_3)$ operator which is to be simulated. That is, not any $\phi$ (and hence $C[\phi]$) is proper for simulation of an arbitrary nonlocal gate. It can directly be checked that the only value of $\phi$ which is applicable in simulation of all two-qubit unitary operators is $\phi = \frac{\pi}{4}$. Thus, in this way, we argue that the most efficient gate that can be used in universal two-qubit gate construction is the $B = C[\frac{\pi}{4}]$ gate. This fact gives a unique and special role to the $B$ gate among other SPE [34].

To complete our discussion, in the following we show how one can simulate some well-known gates, such as the CNOT and the DCNOT, using our method. For the case of the CNOT gate, we have the following equivalent circuit

$$C[\phi]$$

(45)

which is valid for $0 < \phi < \frac{\pi}{4}$. Similarly, for the DCNOT gate, the following circuit gives an equivalent construction

$$C[\phi]$$

where

$$\cos 2b = - \cos^2 2\phi, \quad \frac{\pi}{8} \leq \phi < \frac{\pi}{4}.$$
power has appeared as a useful tool in characterization of special perfect entanglers. The perfect entanglers with maximum value of entangling power, $\frac{\pi}{8}$, have turned out to be the only possible special perfect entanglers.

As a possible application of these special gates their importance in universal two-qubit gate construction has been emphasized. We have provided a more general (analytic) result for optimality. In this regard, it has been proved that if we have the SPE gates at our disposal we can simulate any generic two-qubit gate by only two applications of the same gates. In fact, in this manner we have a vast possibility for universal gate construction. Although not any SPE gate may be applicable in simulation of a specific two-qubit gate, it is always possible to find some proper SPE for this mean. Specially, the unique role of the $B$ gate, namely, its usage in all two-qubit gate simulations, has been pointed out. In this sense, these results can shed new light on theoretical and experimental investigations to characterize the rich structure of the space of nonlocal unitary operators and using them as the most efficient universal elementary gates.

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APPENDIX A: POSSIBLE FREEDOMS IN NONLOCAL PARTS

It can be simply checked that in a triplet $[c_1, c_2, c_3]$, which represents nonlocal part of an operator, one can easily add any integer multiple of $\frac{\pi}{2}$ to every $c_i$. This can be verified by multiplication of the local operators $\pm i\sigma_i \otimes \sigma_i = e^{\pm \frac{i\pi}{2} \sigma_i \otimes \sigma_i}$. Also $[c_1, c_2, c_3] = [c_1, c_2, c_3]$, where $(ijk)$ is an arbitrary permutation of $(123)$. This can be verified as follows. If in the identity $e_{u_1 \otimes v_1} e_{u_1} v_1 = u_1 \otimes v_1 e_{u_1} v_1$, where all operators are unitary, we take $u_1 \otimes v_1 = e^{-i\Sigma \sigma_1} e^{-i\Sigma \sigma_1}$, it is obtained that $[c_1, c_2, c_3] = [c_1, c_2, c_2]$. A similar procedure can be used to prove the general statement. The other fact about $[c_1, c_2, c_3]$ is that one can always make at least two of $c_i$’s positive (or negative). This can be verified by taking $u_1 \otimes v_1 = \pm i\sigma_k \otimes 1$ in the above mentioned identity. To see more on the freedoms refer, for example, to [13].

APPENDIX B: THE LOCAL INVARIANTS

Consider the matrix $Q$ which is

$$Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & i \\ 0 & i & 0 & 1 \\ 0 & 0 & 1 & -i \\ 1 & 0 & 0 & -i \end{pmatrix}. \quad (B1)$$

| Operator | $[c_1, c_2, c_3]$ | $G_1$ | $G_2$ | $c_{vis}$ |
|----------|-----------------|------|------|---------|
| CNOT     | $[\frac{\pi}{4}, 0, 0]$ | 0    | 1    | $\frac{\pi}{8}$ |
| DCNOT    | $[\frac{\pi}{4}, \frac{\pi}{4}, 0]$ | 0    | -1   | $\frac{\pi}{8}$ |
| B        | $[\frac{\pi}{4}, \frac{\pi}{4}, 0]$ | 0    | 0    | $\frac{\pi}{8}$ |
| SWAP     | $[\frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}]$ | -1   | -3   | 0       |
| $\sqrt{SWAP}$ | $[\frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}]$ | $\frac{1}{2}$ | 0    | $\frac{1}{4}$ |
| controlled-$U$ | $[x, 0, 0]$ | $G_1$ | $2G_1 + 1$ | $1 - \cos 4x$ |
| $A \otimes B$ | $[0, 0, 0]$ | 1    | 3    | 0       |

*This is entangling power which is defined in Eq. [C7].

Table I summarizes the results for some examples. As is seen, the $[\text{CNOT}], [\text{DCNOT}]$, and $[\sqrt{\text{SWAP}}]$ all belong to different equivalence classes. There is a powerful theorem which exactly determines which unitary operators are perfect entangler [13, 17].

**Theorem:** A two-qubit unitary operator is a perfect entangler iff the convex hull of the eigenvalues of $m(U)$ contains zero.

An immediate result of this theorem is that among controlled-$U$ operators only the $[\text{CNOT}]$ class is perfect entangler (Table I).

APPENDIX C: ENTANGLING POWER

Entangling power, $e_p(U)$, is a widely accepted measure for quantifying entangling capabilities of a unitary quantum operator $U$ [2]. Consider a bipartite quantum system with state space of $\mathcal{H}_A \otimes \mathcal{H}_B$ (in qubit case $\mathcal{H}_A = \mathcal{H}_B = \mathbb{C}^2$). If $E$ is an entanglement measure over $\mathcal{H}_A \otimes \mathcal{H}_B$, the entangling power of $U$ (with respect to $E$) is defined as

$$e_p(U) := E(U|\psi\rangle \otimes |\phi\rangle) \langle \psi, \phi |,$$

where the bar denotes the average over all the product states $|\psi\rangle \otimes |\phi\rangle$ distributed according to some probability density.
$p(\psi, \phi)$ over the manifold of product states. To ensure local invariance for $e_p(U)$ the measure of integration, $p$, must be taken locally invariant. A simple and proper distribution which satisfies this requirement is the uniform distribution. In $E$ has been taken to be linear entropy, which is defined as
\[ E(|\Psi\rangle_{AB}) := 1 - \text{tr}(\rho^2_{A(B)}), \tag{C2} \]
where $\rho_{A(B)} = \text{tr}_{B(A)}(|\Psi\rangle_{A(B)}\langle\Psi|)$ is the reduced density matrix of the system $A(B)$. Now it is in order to mention the relation of $E$ and the other (rather more well-known) measure of entanglement, concurrence $[19]$. Concurrence of any two-qubit density matrix, $\rho_{AB}$, is defined as
\[ C(\rho_{AB}) := \max \{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{C3} \]
in which $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ are square roots of eigenvalues of the matrix $\rho_{AB}\sigma_2 \otimes \sigma_2 \rho_{AB}\sigma_2 \otimes \sigma_2$ (* means complex conjugation in the standard computational basis). For a pure state of two qubits, $|\Psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$, this reduces to $C(\Psi) = 2|ad - bc|$. In this case, one can see that eigenvalues of the reduced density matrices are $\lambda_{\pm} = \sqrt{1 \pm \frac{1}{4} C^2(\Psi)}$, from which
\[ E(\Psi) = \frac{1}{2} C^2(\Psi). \tag{C4} \]
Since $C$ ranges from $0$ (for separable states) to $1$ (for maximally entangled states), we have $0 \leq E \leq \frac{1}{2}$.

Some important properties of $e_p(U)$ are listed below.

(i) For every $U \in \text{SU}(4)$ we have $0 \leq e_p(U) \leq \frac{1}{2}$.
(ii) For every $A, B \in \text{SU}(2)$, $e_p(A \otimes B) = 0$. This is clear from the fact that $E(|\psi\rangle \otimes |\phi\rangle) = 0$.
(iii) $e_p(U)$ is locally invariant, that is, for every $A, B \in \text{SU}(2)$, $e_p(A \otimes BU) = e_p(UA \otimes B) = e_p(U)$. This property is also simple to verify by noting that
\[ E(U|\psi\rangle \otimes |B|\phi\rangle) = E(U|\psi\rangle \otimes |\phi\rangle) = E(U'|\psi'\rangle \otimes |\phi'\rangle). \]
(iv) For every $U \in \text{SU}(4)$, $e_p(U\dagger) = e_p(U)$. The equality holds because of $E(|\Psi\rangle^*|\Psi\rangle) = E(|\Psi\rangle|\Psi\rangle)$.
(v) If $S$ is the usual swap operator $(S|\psi\rangle \otimes |\phi\rangle = |\phi\rangle \otimes |\psi\rangle)$, for every $|\psi\rangle$ and $|\phi\rangle$, then $e_p(SU) = e_p(U\dagger S) = e_p(U)$. These are immediate consequences of $E(S\Psi) = E(\Psi)$, for all $|\Psi\rangle$.
(vi) Another trivial property is that $e_p(S) = 0$.
To see more about the entangling power, its properties, and generalizations refer to $[2, 14, 15]$.

By using the above facts, one can find an analytical form for entangling power of a unitary operator as in Eq. (9). The last equality follows from Eq. (9) and using the parametrization $|\psi\rangle = \left(\cos \frac{\theta}{2}, e^{i\phi}\sin \frac{\theta}{2}\right)$ ($0 \leq \theta \leq \pi, 0 \leq \phi < 2\pi$) for a single-qubit state vector. Then a simple integration as $e_p(U) = \frac{1}{(4\pi)^2} \int d\theta d\theta' d\phi d\phi' \sin \theta \sin \theta' d\phi d\phi'$, gives the result. This form for $e_p$ is clearly locally invariant, and shows that all unitary operators in the same equivalence class possess an equal entangling power, however the converse is not true generally. It is simple to check that this expression respects all the freedoms mentioned earlier for $c_i$’s of a class. The last column in Table I gives $e_p$ for some well-known equivalence classes. It is important to note that the single parameter $e_p$ cannot replace the two local invariants $G_1$ and $G_2$ to uniquely characterize equivalence classes.

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