The decomposition of an arbitrary $2^w \times 2^w$ unitary matrix into signed permutation matrices

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Abstract

Birkhoff’s theorem tells that any doubly stochastic matrix can be decomposed as a weighted sum of permutation matrices. A similar theorem reveals that any unitary matrix can be decomposed as a weighted sum of complex permutation matrices. Unitary matrices of dimension equal to a power of 2 (say $2^w$) deserve special attention, as they represent quantum qubit circuits. We investigate which subgroup of the signed permutation matrices suffices to decompose an arbitrary such matrix. It turns out to be a matrix group isomorphic to the extraspecial group $E_{2^{2w+1}}^+$ of order $2^{2w+1}$. An associated projective group of order $2^{2w}$ equally suffices.

1 Introduction

Let $D$ be an arbitrary $n \times n$ doubly stochastic matrix. This means that all entries $D_{j,k}$ are real and satisfy $0 \leq D_{j,k} \leq 1$ and that all line sums (i.e. the $n$ row sums and the $n$ column sums) are equal to 1. Let $P(n)$ be the group of all $n \times n$ permutation matrices. Birkhoff \cite{birkhoff} has demonstrated

\textbf{Theorem 1} Any $n \times n$ doubly stochastic matrix $D$ can be written

$$D = \sum_j c_j P_j$$

with all $P_j \in P(n)$ and the weights $c_j$ real, satisfying both $0 \leq c_j \leq 1$ and $\sum_j c_j = 1$. 

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Because unitary matrices describe quantum circuits [2] and permutation matrices describe classical reversible circuits [3], the question arises whether a similar theorem holds for matrices from the unitary group U(n).

It is clear that an arbitrary \( n \times n \) unitary matrix cannot be decomposed as a weighted sum of \( n \times n \) permutation matrices. Indeed, such a sum always results in an \( n \times n \) matrix with \( 2n \) identical line sums. We have shown in previous work [4] that a unitary matrix with the additional feature of equal linesums can be Birkhoff decomposed as a weighted sum of permutation matrices. However, if we loosen the requirement of a decomposition in strictly permutation matrices, we can lift the restriction on the equal line-sum of the unitary matrix. In [5] [6] it is demonstrated that an arbitrary U(\( n \)) matrix can be decomposed as a weighted sum of complex permutation matrices and, in particular, of signed permutation matrices if \( n \) is equal to a power of 2, say \( 2^w \). Because it was demonstrated before by us [7] that prime-powers hold interesting properties, in the present paper, we will focus on the special case of \( n = 2^w \).

The \( 2^w \times 2^w \) signed permutation matrices form a finite group of order \((2^w)!2^{2w}\). In the present paper we investigate a particular subgroup of this group, such that the members of the subgroup suffice to decompose an arbitrary matrix from U(\( 2^w \)). The construction of the subgroup in question involves the dihedral group of order 8, which will be discussed in detail in the next section.

Before investigating the dihedral group, we make a preliminary remark about matrices:

**Remark 1** We number rows and columns of any \( 2^w \times 2^w \) matrix from 0 to \( 2^w - 1 \) (instead of the conventional numbering from 1 to \( 2^w \)) and each such number we represent by the \( w \times 1 \) matrix consisting of the \( w \) bits of the binary notation of the row-or-column number.

E.g. the upper-left entry of an \( 8 \times 8 \) matrix \( A \) is entry \( A_{0,0} = A_{(0,0,0)^T} \), whereas its lower-right entry is denoted \( A_{7,7} = A_{(1,1,1)^T} \).

## 2 The dihedral group \( D \)

Unitary \( 2^w \times 2^w \) matrices are interpreted as quantum circuits acting on \( w \) qubits. The number \( w \) is called either the circuit width or the qubit count. For \( w = 1 \), the single-qubit circuit is called a gate, represented by a matrix from U(2). Below, two gates will be used as building block: the X gate and the Z gate.
The $X$ gate, a.k.a. the $\text{NOT}$ gate, is a classical gate, represented by the matrix \( \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \). In contrast, the $Z$ gate is a truly quantum gate, represented by the matrix \( \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \). Together, the $X$ gate and the $Z$ gate generate a group of order 8, consisting of the eight $2 \times 2$ matrices

\[
M_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} = X^2 = Z^2 = I
\]

\[
M_1 = \begin{pmatrix} -1 \\ -1 \end{pmatrix} = XZXZ = ZXX = -I
\]

\[
M_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} = X
\]

\[
M_3 = \begin{pmatrix} -1 \\ -1 \end{pmatrix} = ZXX = -X
\]

\[
M_4 = \begin{pmatrix} 1 \\ -1 \end{pmatrix} = Z
\]

\[
M_5 = \begin{pmatrix} -1 \\ 1 \end{pmatrix} = XZX = -Z
\]

\[
M_6 = \begin{pmatrix} 1 \\ -1 \end{pmatrix} = ZX
\]

\[
M_7 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} = XZ
\]

where $I$ is the identity gate. The group is isomorphic to the dihedral group $D$ of order 8. The above ordering of the indices $j$ of the $M_j$ matrices will be elucidated later on (see Section 3).

We note that the gates $X$ and $Z$, completed with $iXZ = Y$, are called the Pauli matrices. The matrix set $\{M_0, M_6, M_1, M_7\}$ forms a cyclic subgroup of $D$. The matrix set $\{M_0, M_2, M_4, M_6\}$ does not form a group; it does form a projective group. The decomposition properties of both this projective group and the group $D$ itself have been studied by Allouche et al. [8].

The above matrices $M_j$ (with $0 \leq j \leq 7$) constitute a group representation of the group $D$ which is irreducible. Indeed, the matrix $M_0$ (i.e. $I$) has trace equal to 2, the matrix $M_1$ (i.e. $-I$) has trace $-2$, whereas the remaining six matrices are traceless. Thus

\[
\sum_{j=0}^{7} |\text{Tr}(M_j)|^2 = |2|^2 + |-2|^2 = 8.
\]
Hence, the irreducibility criterion
\[ \sum_{M_j \in D} |\text{Tr}(M_j)|^2 = \text{Order}(D) \]
is fulfilled. We denote this first irrep by \( R_j^{(1)} \) (with \( 0 \leq j \leq 7 \)). According to Burrow [9], the group \( D \) has, besides this 2-dimensional irreducible representation, four 1-dimensional irreps. We denote these by \( R_j^{(2)} \), \( R_j^{(3)} \), \( R_j^{(4)} \), and \( R_j^{(5)} \). We have \( R_j^{(2)} = 1 \), whereas \( R_j^{(3)} \), \( R_j^{(4)} \), and \( R_j^{(5)} \) equal ±1, the character table of \( D \) looking like

\[
\begin{array}{c|ccccc}
R_j^{(2)} & \{M_0\} & \{M_1\} & \{M_2, M_3\} & \{M_4, M_5\} & \{M_6, M_7\} \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & -1 & 1 & -1 & 1 \\
1 & 1 & 1 & -1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 \\
2 & -2 & 0 & 0 & 0 & 0 \\
\end{array}
\]

**Theorem 2** Any \( U(2) \) matrix \( U \), i.e. any matrix representing a single-qubit gate, can be written

\[ U = \sum_j c_j M_j \]

with all \( M_j \in D \) and the weights \( c_j \) complex numbers, such that both \( \sum c_j = 1 \) and \( \sum |c_j|^2 = 1 \).

In order to find the values of the eight coefficients \( c_j \), it suffices to solve a matrix equation [4]:

\[
\sum_{j=0}^{7} c_j \begin{pmatrix} R_j^{(1)} & R_j^{(2)} & R_j^{(3)} & R_j^{(4)} & R_j^{(5)} \\ R_j^{(1)} & R_j^{(2)} & R_j^{(3)} & R_j^{(4)} & R_j^{(5)} \\ R_j^{(1)} & R_j^{(2)} & R_j^{(3)} & R_j^{(4)} & R_j^{(5)} \\ R_j^{(1)} & R_j^{(2)} & R_j^{(3)} & R_j^{(4)} & R_j^{(5)} \\ R_j^{(1)} & R_j^{(2)} & R_j^{(3)} & R_j^{(4)} & R_j^{(5)} \\ R_j^{(1)} & R_j^{(2)} & R_j^{(3)} & R_j^{(4)} & R_j^{(5)} \\ R_j^{(1)} & R_j^{(2)} & R_j^{(3)} & R_j^{(4)} & R_j^{(5)} \end{pmatrix} = \begin{pmatrix} U \\ u^{(2)} \\ u^{(3)} \\ u^{(4)} \\ u^{(5)} \end{pmatrix},
\]

where \( u^{(2)} \), \( u^{(3)} \), \( u^{(4)} \), and \( u^{(5)} \) are arbitrary complex numbers with unit modulus.
This equality of two $6 \times 6$ matrices constitutes a set of eight scalar equations in the eight unknowns $c_j$:

\[
\begin{align*}
    c_0 - c_1 + c_4 - c_5 &= U_{0,0} \\
    c_2 - c_3 + c_6 - c_7 &= U_{0,1} \\
    c_2 - c_3 - c_6 + c_7 &= U_{1,0} \\
    c_0 - c_1 - c_4 + c_5 &= U_{1,1} \\
    c_0 + c_1 + c_2 + c_3 + c_4 + c_5 + c_6 + c_7 &= v^{(2)} \\
    c_0 + c_1 - c_2 - c_3 + c_4 + c_5 - c_6 - c_7 &= v^{(3)} \\
    c_0 + c_1 + c_2 + c_3 - c_4 - c_5 - c_6 - c_7 &= v^{(4)} \\
    c_0 + c_1 - c_2 - c_3 - c_4 - c_5 + c_6 + c_7 &= v^{(5)} .
\end{align*}
\] (1)

We find the following solution (Appendix A):

\[
\begin{align*}
    c_0 &= (U_{0,0} + U_{1,1})/4 + (u^{(2)} + u^{(3)} + u^{(4)} + u^{(5)})/8 \\
    c_1 &= -(U_{0,0} + U_{1,1})/4 + (u^{(2)} + u^{(3)} + u^{(4)} + u^{(5)})/8 \\
    c_2 &= (U_{0,1} + U_{1,0})/4 + (u^{(2)} - u^{(3)} + u^{(4)} - u^{(5)})/8 \\
    c_3 &= -(U_{0,1} + U_{1,0})/4 + (u^{(2)} - u^{(3)} + u^{(4)} - u^{(5)})/8 \\
    c_4 &= (U_{0,0} - U_{1,1})/4 + (u^{(2)} + u^{(3)} - u^{(4)} - u^{(5)})/8 \\
    c_5 &= -(U_{0,0} - U_{1,1})/4 + (u^{(2)} + u^{(3)} - u^{(4)} - u^{(5)})/8 \\
    c_6 &= (U_{0,1} - U_{1,0})/4 + (u^{(2)} - u^{(3)} - u^{(4)} + u^{(5)})/8 \\
    c_7 &= -(U_{0,1} - U_{1,0})/4 + (u^{(2)} - u^{(3)} - u^{(4)} + u^{(5)})/8 .
\end{align*}
\] (2)

One easily checks that $\sum_{j=0}^7 |c_j|^2 = 1$. See Appendix A. By choosing $u^{(2)} = 1$, we additionally guarantee that $\sum_{j=0}^7 c_j = 1$. If, moreover, we also choose $u^{(3)} = u^{(4)} = u^{(5)} = 1$, then we have a compact expression for the eight weights $|1|:

\[
c_j = \delta_{j,0} + \frac{1}{4} \text{Tr}(R_j^{(1)}U) - \frac{1}{4} \text{Tr}(R_j^{(1)}) .
\]

Here, $\text{Tr}(R_j^{(1)})$ is the character $\chi_j^{(1)}$, equal to 0, except $\chi_0^{(1)} = 2$ and $\chi_1^{(1)} = -2$.

One might observe that $M_1 = -M_0$, $M_3 = -M_2$, $M_5 = -M_4$, and $M_7 = -M_6$, such that the sum $c_0M_0 + c_1M_1 + c_2M_2 + c_3M_3 + c_4M_4 + c_5M_5 + c_6M_6 + c_7M_7$ leads to a second decomposition (in terms of the projective group):

\[
    (c_0 - c_1)M_0 + (c_2 - c_3)M_2 + (c_4 - c_5)M_4 + (c_6 - c_7)M_6 .
\] (3)

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Appendix A demonstrates that the sum of the squares of the moduli of the four coefficients equals unity. However, we cannot guarantee that the sum of the coefficients, i.e. \((c_0 - c_1) + (c_2 - c_3) + (c_4 - c_5) + (c_6 - c_7)\), equals unity, as eqns (12) impose that this sum is equal to \(U_{0,0} + U_{0,1}\), independent of the values we choose for the parameters \(u^{(2)}\), \(u^{(3)}\), \(u^{(4)}\), and \(u^{(5)}\).

3 The groups DS\((2^w)\)

In the present section, we apply the dihedral group to quantum circuits.

**Definition 1** A single-qubit circuit represented by one of the eight matrices of the group \(D\) is called a \(D\) gate.

**Definition 2** A \(w\)-qubit circuit consisting of a single \(D\) gate on each of the \(w\) wires is called a \(D\) stack.

The group DS\((2^w)\) consists of all possible \(D\) stacks and hence an element of the group is represented by the Kronecker product

\[
D_0 \otimes D_1 \otimes ... \otimes D_{w-1},
\]

where each \(D_j\) is a member of the group \(D\).

**Definition 3** A \(D\) stack with all \(D\) gates either an \(I\) gate or an \(X\) gate is called a \(X\) stack; a \(D\) stack with all \(D\) gates either an \(I\) gate or a \(Z\) gate is called a \(Z\) stack; a \(D\) stack with all \(D\) gates either an \(I\) gate or a \(-I\) gate is called a \(-I\) stack.

**Lemma 1** Any \(D\) stack can be synthesised by a cascade of one \(Z\) stack, one \(X\) stack, and one \(-I\) stack.

To prove this, it suffices to observe that each \(D\) gate of the stack can be decomposed as follows:

\[
\begin{align*}
M_0 &= Z^0 X^0 (-I)^0 \\
M_1 &= Z^0 X^0 (-I)^1 \\
M_2 &= Z^0 X^1 (-I)^0 \\
M_3 &= Z^0 X^1 (-I)^1 \\
M_4 &= Z^1 X^0 (-I)^0 \\
M_5 &= Z^1 X^0 (-I)^1 \\
M_6 &= Z^1 X^1 (-I)^0 \\
M_7 &= Z^1 X^1 (-I)^1.
\end{align*}
\]
We note that the three exponents together form the binary notation of the subscript $j$ of the matrix $M_j$. The sequence $(Z, X, -I)$ is called a transversal of the group $D$. In (4), each $D_j$ is a $2 \times 2$ matrix from the group $D$ and thus we have:

$$D_j = Z^{b_j} X^{a_j} (-I)^{d_j},$$

where $b_j \in \{0, 1\}$, $a_j \in \{0, 1\}$, and $d_j \in \{0, 1\}$. We introduce the column vectors $b = (b_0, b_1, ..., b_{w-1})^T$ and $a = (a_0, a_1, ..., a_{w-1})^T$.

**Lemma 2** The $Z$ stacks form a group of order $2^w$.

The group consists of $2^w \times 2^w$ diagonal matrices $\zeta$. Its diagonal entries $\zeta_{k,k}$ are equal to $(-1)^{b^T \cdot k}$, where $k$ denotes the column vector $(k_0, k_1, ..., k_{w-1})^T$ of the binary representation of the number $k$. For all matrices $\zeta$, we have that the upper-left entry $\zeta_{0,0}$ equals 1. If $b = 0$, then $\zeta$ is the $2^w \times 2^w$ unit matrix $J$. If $b \neq 0$, then half of the diagonal entries of $\zeta$ are equal to 1, the other half being equal to $-1$. Indeed: let $b_p$ be the least-significant non-zero bit of $b$. Then the two diagonal entries $\zeta_{k,k}$ and $\zeta_{k',k'}$ (with $k$ and $k'$ equal numbers except for the bits $k_p$ and $k'_p$) will be different, one being equal to 1, the other to $-1$. It is clear that we have $2^{w-1}$ such pairs $(k, k')$ on the diagonal of $\zeta$.

The group of $Z$ stacks is isomorphic to the direct product $C_2^w$. We denote it by $ZS(2^w)$. If $w > 1$, then all the members of the group have determinant equal to 1.

**Lemma 3** The $X$ stacks form a group of order $2^w$.

The group consists of $2^w \times 2^w$ permutation matrices $\chi$ with entries $\chi_{k,l}$ equal to $\delta_{l,a+k}$, where $I$ denotes the vector $(l_0, l_1, ..., l_{w-1})^T$ and where the sum is a bitwise addition modulo 2. We denote the group by $XS(2^w)$. It is isomorphic to the direct product $C_2^w$. This is no surprise, realizing that it is isomorphic to $ZS(2^w)$, because we have $H2H = X$, where $H$ is the Hadamard matrix. If $w > 1$, then all the members of the group have determinant equal to 1.

**Lemma 4** The $-I$ stacks form a group of order $2$.

The group consists of the $2^w \times 2^w$ unit matrix $J$ and the $2^w \times 2^w$ diagonal matrix with all diagonal entries equal to $-1$, i.e. matrix $-J$. The non-zero entries thus equal $(-1)^d$, where $d = (d_0 + d_1 + ... + d_{w-1}) \mod 2$. Both members of the group have determinant equal to 1. The group is isomorphic to the cyclic group $C_2$.
Because of Lemma 1 a D stack is a cascade of a Z stack, an X stack, and a −I stack. Hence, each member of DS(2\(^w\)) is a product of a diagonal matrix, a permutation matrix and a ±1 scalar. All \(2^w \times 2^w \times 2\) products yield distinct matrices. Thus:

**Lemma 5** The D stacks form a group DS(2\(^w\)) of order 2 \(\times 4^w\).

These matrices are signed permutation matrices. The fact that the −I stacks reduce to a group of order two, allows us to reduce the −I stack in Lemma 1 to just one −I gate. This −I gate may be located on any of the \(w\) wires of the circuit.

**Lemma 6** The group DS(2\(^w\)) consists of \(4^w\) couples \(\{S_{2j}, S_{2j+1}\}\), such that \(S_{2j+1} = -S_{2j}\).

Indeed: if \(S\) is a member of DS(2\(^w\)), then, because −J is also a member of DS(2\(^w\)), we have that \((-J)S = -S\) belongs to DS(2\(^w\)). The \(4^w\) matrices \(S_{2j}\) constitute a projective group.

**Lemma 7** The group DS(2\(^w\)) consists of signed permutation matrices:

- \(2^w\) matrices with all \(2^w\) non-zero entries equal to 1;
- \(2^w\) matrices with all \(2^w\) non-zero entries equal to −1;
- \(2 \times 2^w(2^w - 1)\) matrices with \(2^w/2\) entries equal to 1 and \(2^w/2\) entries equal to −1.

The group DS(2\(^w\)) is isomorphic to one of the two extraspecial 2-groups \([11]\) of order \(2^{2w+1}\) (i.e. the one of ‘type +’), denoted \(E_{2^{2w+1}}^+\). This group \([12]\) is a subgroup of the Pauli group \([13]\ [14]\), which has order \(2^{2w+2}\).

We note that, as soon as one of the factors \(D_j\) of the Kronecker product \([4]\) is not diagonal (i.e. as soon as one of the factors belongs to the set \(\{M_2, M_3, M_6, M_7\}\)), all diagonal entries of the product are equal to 0. In contrast, if all factors are diagonal (i.e. if all factors belong to the set \(\{M_0, M_1, M_4, M_5\}\)), then all diagonal entries of the product are equal to ±1. Moreover, half of the diagonal entries equals 1 and half of the diagonal entries equals −1, except for two cases: \(J\) has all diagonal entries equal to 1 and −\(J\) has all diagonal entries equal to −1. We conclude that all members of the group DS(2\(^w\)) are traceless, except for Tr(\(J\)) = \(2^w\) and Tr(−\(J\)) = −\(2^w\). Hence

\[
\sum_j |\text{Tr}(S_j)|^2 = |2^w|^2 + |-2^w|^2 = 2 \times 4^w.
\]
This demonstrates the fact that the $2^w \times 2^w$ signed permutation matrices representing the DS($2^w$) circuits form an irreducible representation of $E_{2^{2w+1}}^+$. Indeed, the irreducibility criterion
\[ \sum_j |\text{Tr}(S_j)|^2 = \text{Order}(E_{2^{2w+1}}^+) \]
is fulfilled.

An arbitrary member $S_j$ of the group DS($2^w$) has three parameters:
- the vector $b$,
- the vector $a$, and
- the scalar $d$.

This means that the subscript $j$ is a short-hand notation for $(b, a, d)$. The even subscripts $j$ are used for matrices with $d = 0$ and the odd subscripts $j$ are used for matrices with $d = 1$. The entries of the matrix $S_j$ are
\[ (S_j)_{k,l} = (-1)^{d+b^T \cdot k} \delta_{l,a+k} \],
where the components of the vectors $a$ and $k$ are bitwise added modulo 2. For $w > 1$, the matrix $S_j$ has unit determinant. Indeed, above we have seen that, for $w > 1$, any $Z$ stack, any $X$ stack, and any $-I$ stack are represented by a matrix with determinant equal to 1.

If $Z_j$ is the $Z$ gate acting on the $j$th qubit, if $X_j$ is the $X$ gate acting on the $j$th qubit, and if $-I_0$ is the $-I$ gate acting on the 0th qubit, then the sequence $(Z_0, Z_1, ..., Z_{w-1}, X_0, X_1, ..., X_{w-1}, -I_0)$ is a transversal of DS($2^w$). The sequence $(b_0, b_1, ..., b_{w-1}, a_0, a_1, ..., a_{w-1}, d)$ is a binary number addressing unambiguously a particular member of DS($2^w$). In the following, we will present two decompositions of a unitary matrix $U$ using the dihedral group, one (Section 4) where the sum of the weights will not necessarily equal 1, and a second, related, one (Section 5) where the sum of the weights is constrained to 1.

4 First decomposition of the unitary matrix

The $2^{2w+1}$ matrices $S_j$ of the group DS($2^w$) are linearly dependent, as e.g. we have $S_0 + S_1 = J + (-J) = 0$. In contrast, we have

**Lemma 8** The $2^{2w}$ matrices $S_{2j}$ of the projective group are linearly independent.
We prove this by contradiction. Indeed, assume that a list \((\alpha_0, \alpha_2, \alpha_4, \ldots, \alpha_{2w+1-2})\), different from the zero list \((0, 0, 0, \ldots, 0)\), exists, such that
\[
\sum_{j=0}^{2^{2w}-1} \alpha_j S_{2j} = 0 .
\]
We multiply both sides of this equation to the left with \(S_{2k}^T\), where \(k\) is any integer from \((0, 1, 2, \ldots, 2^w - 1)\). Subsequently, we take the trace of both sides of the equation. According to Appendix B, we find \(\alpha_{2k} 2^w = 0\) for all \(k\), and thus all \(\alpha_{2k} = 0\). Hence, the list \((\alpha_0, \alpha_2, \alpha_4, \ldots, \alpha_{2w+1-2})\) is the zero list, in contradiction with the assumption. This proof is reminiscent of the proof by Veltman \[15\] \[16\] of a similar property of \(4 \times 4\) gamma matrices.

Because the \(2^w\) matrices \(S_{2j}\) thus form a complete set of \(2^w \times 2^w\) matrices, we have:

**Theorem 3** Any \(U(2^w)\) matrix \(U\), i.e. any matrix representing a \(w\)-qubit quantum circuit, can be written
\[
U = \sum_j g_{2j} S_{2j} \tag{5}
\]
with all \(S_{2j}\) member of the projective group associated to \(DS(2^w)\) and the weights \(g_{2j}\) complex numbers.

Multiplying \(5\) to the left by \(S_{2k}^T\) and taking traces, leads to \(\text{Tr}(S_{2k}^T U) = g_{2k} 2^w\) and thus to the value of the weights:
\[
g_{2k} = 2^{-w} \text{Tr}(S_{2k}^T U) . \tag{6}
\]

According to Appendix C, we have
\[
\sum_j g_{2j} = 2^{-w} \sum_j \text{Tr}(S_{2k}^T U) = 2^{-w} 2^w \sum_l U_{0,l} = \sum_l U_{0,l} .
\]
Thus the sum of the weights equals the uppermost row sum of the matrix \(U\), a number not necessarily equal to 1. Using the short-hand notation \(n = 2^w\), we note that
\[
|g_{2j}|^2 = \frac{1}{n^2} |\text{Tr}(S_{2j}^T U)|^2
\]
\[
= 1 - \left(1 - \frac{|\text{Tr}(S_{2j}^T U)|^2}{n^2}\right)
\]
\[
= 1 - D(S_{2j}, U) ,
\]

where

\[ D(A, B) = 1 - \frac{|\text{Tr}(A^\dagger B)|^2}{n^2} \]

is the distance between the \( n \times n \) unitary matrices \( A \) and \( B \), according to Khatri et al. [17], the trace \( \text{Tr}(A^\dagger B) \) being known as the Hilbert–Schmidt inner product of \( A \) and \( B \). Hence, the nearer the \( S_{2j} \) matrix is to the given matrix \( U \), the more it contributes to the decomposition of \( U \). Finally, we have

\[ \sum_j |g_{2j}|^2 = 1. \]

Proof is in the Appendix C.

As an example, we decompose the unitary transformation

\[ U = \frac{1}{12} \begin{pmatrix} 8 & 4 + 8i & 0 & 0 \\ 2 + i & -2i & 3 - 9i & -3 - 6i \\ 1 - 7i & -6 + 2i & 6 & -3 + 3i \\ 3 + 4i & 2 - 4i & 3 - 3i & 9i \end{pmatrix}. \]  \hfill (7)

Its decomposition according to Theorem 3 and eqn (6) is

\[ g_0S_0 + g_2S_2 + g_4S_4 + \ldots + g_{30}S_{30} = \]

\[ \frac{14 + 7i}{48} \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} + \frac{2 - 11i}{48} \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} + \]

\[ \frac{14 - 7i}{48} \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} + \ldots + \frac{6 + 11i}{48} \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}. \]

In this particular example, the 16 distances \( D(U, S_{2j}) \) vary from \( 2015/2304 \approx 0.876 \) to \( 2291/2304 \approx 0.994 \).

### 5 Second decomposition of the unitary matrix

After Klappenecker and Rötteler [10] and De Baerdemacker et al. [4] and taking into account that any finite group has the trivial 1-dimensional irreducible representation, we have
Theorem 4  If a unitary matrix $U$ can be written
\[ U = \sum_j g_j G_j \]
with all $G_j$ member of some finite group $G$, then there exists a decomposition
\[ U = \sum_j h_j G_j \]
such that both $\sum_j h_j = 1$ and $\sum_j |h_j|^2 = 1$.

Together, Theorems 3 and 4 lead to the final result:

Theorem 5  Any $U(2^w)$ matrix $U$, i.e. any matrix representing a $w$-qubit quantum circuit, can be written
\[ U = \sum_j h_j S_j \]
with all $S_j \in DS(2^w)$ and the weights $h_j$ complex numbers, such that both $\sum_j h_j = 1$ and $\sum_j |h_j|^2 = 1$.

From [4] we have a closed form for the weights appearing in (8):
\[ h_j = \frac{1}{N} \sum_{\nu=1}^{\mu} n_\nu \text{Tr} \left( R_j^{(\nu)^\dagger} U_0^{(\nu)} \right), \]
where $\mu$ is the number of irreducible representations of $S_j$, where $n_\nu$ is the dimension of the particular irrep $R_j^{(\nu)}$, and where $N$ is the order of the group $G$.

If, for $U(j)\nu$ we choose the given matrix $U$ and for each matrix $U_j^{(\nu)}$ with $2 \leq \nu \leq \mu$ we choose the $n_\nu \times n_\nu$ unit matrix, then (9) becomes
\[ h_j = \frac{1}{N} \left[ n_1 \text{Tr} \left( R_j^{(1)^\dagger} U \right) + \sum_{\nu=2}^{\mu} n_\nu \text{Tr} \left( R_j^{(\nu)^\dagger} \right) \right]. \]

We take advantage of Schur’s orthogonality relation:
\[ \sum_\nu n_\nu \text{Tr} \left( R_j^{(\nu)^\dagger} \right) = \sum_\nu n_\nu \text{Tr} \left( R_j^{(\nu)^\dagger} R_0^{(\nu)} \right) = \delta_{0,j} N. \]
Because moreover \( n_1 = 2^w \) and \( N = 2^{2w+1} \), we obtain the explicit expression for the weight:

\[
h_j = \delta_{0,j} + \frac{1}{2^{w+1}} \text{Tr} \left( R_j^{(1)\dagger} U \right) - \frac{1}{2^{w+1}} \text{Tr} \left( R_j^{(1)} \dagger \right)
\]

\[
= \delta_{0,j} + \frac{1}{2^{w+1}} \text{Tr}(S_j^T U) - \frac{1}{2^{w+1}} \text{Tr}(S_j).
\]

As demonstrated in Appendix B, we have \( \text{Tr}(S_0) = 2^w \), \( \text{Tr}(S_1) = -2^w \), and \( \text{Tr}(S_j) = 0 \) for \( j > 1 \). Hence:

\[
h_0 = \frac{1}{2^{w+1}} \text{Tr}(U) + \frac{1}{2}
\]

\[
h_1 = -\frac{1}{2^{w+1}} \text{Tr}(U) + \frac{1}{2}
\]

\[
h_j = \frac{1}{2^{w+1}} \text{Tr}(S_j^T U) \quad \text{for } j > 1.
\]

(11)

Matrix example (7), according to Theorem 5 and eqn (11), has decomposition

\[
h_0 S_0 + h_1 S_1 + h_2 S_2 + \ldots + h_{31} S_{31} =
\]

\[
\frac{62 + 7i}{96} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{34 - 7i}{96} \begin{pmatrix} -1 & -1 \\ -1 & -1 \end{pmatrix}
\]

\[
+ \frac{2 - 11i}{96} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} + \ldots + \frac{-6 - 11i}{96} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.
\]

6 Generalization

The above conclusions for arbitrary \( U(2^w) \) matrices can easily be generalized to arbitrary \( U(p^w) \) matrices, where \( p \) is an arbitrary prime. Indeed, let \( \omega \) be the \( p \)th root of 1. We define the X gate and Z gate by their respective \( p \times p \) matrices:

\[
X = \begin{pmatrix} 1 & 1 & \ldots & 1 \\ 1 & 1 & \ldots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \ldots & 1 \end{pmatrix}
\]

\[
\text{and} \quad Z = \begin{pmatrix} 1 & \omega & \omega^2 & \ldots & \omega^{p-2} & \omega^{p-1} \\ \omega & 1 & \omega & \ldots & \omega^{p-3} & \omega^{p-2} \\ \omega^2 & \omega & 1 & \ldots & \omega^{p-4} & \omega^{p-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \omega^{p-2} & \omega^{p-3} & \omega^{p-4} & \ldots & 1 & \omega^{p-1} \\ \omega^{p-1} & \omega^{p-2} & \omega^{p-3} & \ldots & \omega & 1 \end{pmatrix}.
\]
We have

\[ X^p = Z^p = I, \]

where \( I \) is the \( p \times p \) unit matrix. Moreover, we have

\[ XZ = \omega ZX. \]

As a result, any matrix generated by the two generators \( X \) and \( Z \) can be written as \( Z^b X^a \omega^d \) with \( b \in \{0, 1, 2, \ldots, p - 1\} \), \( a \in \{0, 1, 2, \ldots, p - 1\} \), and \( d \in \{0, 1, 2, \ldots, p - 1\} \). Therefore, the group generated by \( X \) and \( Z \) is the extraspecial group \( \mathbf{E}_{p^3}^+ \) of order \( p^3 \). This group takes over the role of the dihedral group \( D_{p^3} \).

Any gate generated by \( X \) and \( Z \), we call an E gate. A circuit acting on \( w \) qudits and consisting of a single E gate on each of the \( w \) wires, we call an E stack. The E stacks form a group isomorphic to \( \mathbf{E}_{p^{2w+1}}^+ \) of order \( p^{2w+1} \). An arbitrary E stack is represented by a \( p^w \times p^w \) complex permutation matrix \( C_j \) with entries

\[ (C_j)_{k,l} = \omega^{d+bT_{k,l}} \delta_{a+k}, \]

where + stands for addition modulo \( p \). The Hilbert–Schmidt inner product \( T_{j,k} = \text{Tr}(C_j^T C_k) \) of two such matrices equals \( \omega^q p^w \) if \( C_k = \omega^q C_j \) for some \( q \in \{0, 1, 2, \ldots, p - 1\} \) and equals zero otherwise. This fact leads to a decomposition of an arbitrary \( U(p^w) \) matrix:

\[ U = \sum_j g_{pj} C_{pj}, \]

with all \( C_{pj} \) member of the projective group of order \( p^{2w} \), associated to \( \mathbf{E}_{p^{2w+1}}^+ \), and with the weights \( g_{pj} \) being equal to \( p^{-w} \text{Tr}(C_j^T U) \) and having the property \( \sum_j |g_{pj}|^2 = 1 \). Finally, this leads to a second decomposition:

\[ U = \sum_j h_j C_j, \]

with all \( C_j \) member of the group \( \mathbf{E}_{p^{2w+1}}^+ \) of order \( p^{2w+1} \) and with the weights \( h_j \) having the two properties \( \sum_j |h_j|^2 = 1 \) and \( \sum_j h_j = 1 \).

7 Conclusion

We conclude that a unitary matrix, describing an arbitrary \( w \)-qubit quantum circuit, i.e. a member of the matrix group \( U(2^w) \), can be decomposed as
a weighted sum of a finite number of signed permutation matrices, each
describing a stack of \( w \) gates, each a single-qubit dihedral gate. The weights
of the sum add up to 1, just like the squares of the moduli of these weights.
The signed permutation matrices belong to a subgroup isomorphic to the
e extraspecial group \( E_{2^{2w+1}}^+ \). The order of this group is \( 2^{2w+1} \). A projective
group of order \( 2^{2w} \) suffices for the decomposition if we do not impose that
the sum of the weights is equal to 1, i.e. if we only impose that the sum
of squared moduli of the weights equals unity. Similar conclusions hold for
members of the unitary matrix group \( U(p^w) \), with \( p \) an arbitrary prime.

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A Detailed calculations for $\text{U}(2)$

The former four equations of (11) yield

\[
\begin{align*}
c_0 - c_1 &= \left( U_{0,0} + U_{1,1} \right) / 2 \\
c_2 - c_3 &= \left( U_{0,1} + U_{1,0} \right) / 2 \\
c_4 - c_5 &= \left( U_{0,0} - U_{1,1} \right) / 2 \\
c_6 - c_7 &= \left( U_{0,1} - U_{1,0} \right) / 2 ;
\end{align*}
\]

(12)

the latter four equations yield

\[
\begin{align*}
c_0 + c_1 &= \left( u^{(2)} + u^{(3)} + u^{(4)} + u^{(5)} \right) / 4 \\
c_2 + c_3 &= \left( u^{(2)} - u^{(3)} + u^{(4)} - u^{(5)} \right) / 4 \\
c_4 + c_5 &= \left( u^{(2)} + u^{(3)} - u^{(4)} - u^{(5)} \right) / 4 \\
c_6 + c_7 &= \left( u^{(2)} - u^{(3)} - u^{(4)} + u^{(5)} \right) / 4 .
\end{align*}
\]

(13)

These results immediately lead to the solution (2).

Additionally, the four eqns (12) lead to

\[
|c_0 - c_1|^2 + |c_2 - c_3|^2 + |c_4 - c_5|^2 + |c_6 - c_7|^2 = \frac{1}{2} ( |U_{0,0}|^2 + |U_{0,1}|^2 + |U_{1,0}|^2 + |U_{1,1}|^2 ) = 1 ,
\]

while the four eqns (13) lead to

\[
|c_0 + c_1|^2 + |c_2 + c_3|^2 + |c_4 + c_5|^2 + |c_6 + c_7|^2 = \frac{1}{4} ( |u^{(2)}|^2 + |u^{(3)}|^2 + |u^{(4)}|^2 + |u^{(5)}|^2 ) = 1 .
\]

The identities

\[
\begin{align*}
|c_0|^2 + |c_1|^2 &= |c_0 - c_1|^2 / 2 + |c_0 + c_1|^2 / 2 \\
|c_2|^2 + |c_3|^2 &= |c_2 - c_3|^2 / 2 + |c_2 + c_3|^2 / 2 \\
|c_4|^2 + |c_5|^2 &= |c_4 - c_5|^2 / 2 + |c_4 + c_5|^2 / 2 \\
|c_6|^2 + |c_7|^2 &= |c_6 - c_7|^2 / 2 + |c_6 + c_7|^2 / 2
\end{align*}
\]

thus yield

\[
\sum_{j=0}^{7} |c_j|^2 = 1/2 + 1/2 = 1 .
\]
B Trace of signed permutation matrix

We compute the Hilbert–Schmidt inner product $T_{j,k}$ of two signed permutation matrices $S_j$ and $S_k$:

$$T_{j,k} = \text{Tr}(S_j^T S_k) = \sum_u (S_j^T S_k)_{u,u} = \sum_u \sum_p (S_j^T)_{u,p} (S_k)_{p,u}$$

$$= \sum_u \sum_p (S_j)_{p,u} (S_k)_{p,u}$$

$$= \sum_{u} \sum_{p} (-1)^{d_j + b_j^T \cdot p} \ delta_{u,a_j+p} (-1)^{d_k + b_k^T \cdot p} \ delta_{u,a_k+p}$$

$$= \sum_{p} (-1)^{d_j + d_k + (b_j^T + b_k^T) \cdot p} \sum_{u} \ delta_{u,a_j+p} \ delta_{u,a_k+p} .$$

If the eqns

$$u = a_j + p$$

$$u = a_k + p$$

are fulfilled, then the corresponding number $u$ points to a ±1 entry in position $(u, u)$ of the matrix $S_j^T S_k$. A necessary condition for a solution is $a_j = a_k$. Therefore $T_{j,k} = 0$ if $a_j \neq a_k$. If instead $a_j = a_k$, then

$$\sum_{u} \ delta_{u,a_j+p} \ delta_{u,a_k+p} = 1$$

and

$$T_{j,k} = (-1)^{d_j + d_k} \sum_{p} (-1)^{(b_j^T + b_k^T) \cdot p} .$$

If $b_j = b_k$, then $\sum_{p} (-1)^{(b_j^T + b_k^T) \cdot p} = 2^w$. If instead $b_j \neq b_k$, then

$\sum_{p} (-1)^{(b_j^T + b_k^T) \cdot p} = 0$. Thus, iff both $a_j = a_k$ and $b_j = b_k$, then $T_{j,k} = \pm 2^w$. We conclude:

- $T_{j,k} = 2^w$ if $S_k = S_j$,
- $T_{j,k} = -2^w$ if $S_k = -S_j$, and
- else $T_{j,k} = 0$.

In order to calculate the trace of an arbitrary $S_k$, it suffices to apply the above results with $S_j$ equal to $S_0 = J$, the $n \times n$ unit matrix: $\text{Tr}(S_k) = T_{0,k}$. Thus: $\text{Tr}(S_0) = 2^w$ and $\text{Tr}(S_1) = -2^w$; all other $\text{Tr}(S_j) = 0$. 

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C Detailed calculations for \( U(2^w) \)

Confronting the two decompositions of \( U \) (Sections 4 and 5, respectively) reveals the following relationship between the \( 2^w \) weights \( g_{2j} \) and the \( 2^{w+1} \) weights \( h_j \):

\[
\begin{align*}
g_0 &= 2h_0 - 1 \\
g_{2j} &= 2h_{2j} \quad \text{for } j > 0 .
\end{align*}
\]

Together with \( h_1 = -h_0 + 1 \) and \( h_{2j+1} = -h_{2j} \) for \( j > 0 \), this yields the inverse relationship:

\[
\begin{align*}
h_0 &= (1 + g_0)/2 \\
h_1 &= (1 - g_0)/2 \\
h_{2j} &= g_{2j}/2 \quad \text{for } j > 0 \\
h_{2j+1} &= -g_{2j}/2 \quad \text{for } j > 0 .
\end{align*}
\]

This allows us to compute the sum \( \sum |g_j|^2 \) from the known \( \sum |h_j|^2 = 1 \):

\[
1 = \sum |h_j|^2 = |h_0|^2 + |h_1|^2 + \sum_{j>0} |h_{2j}|^2 + \sum_{j>0} |h_{2j+1}|^2 \\
= \frac{1}{4} |1 + g_0|^2 + \frac{1}{4} |1 - g_0|^2 + \frac{1}{4} \sum_{j>0} |g_j|^2 + \frac{1}{4} \sum_{j>0} |g_j|^2 \\
= \frac{1}{2}(1 + |g_0|^2) + \frac{1}{2} \sum_{j>0} |g_{2j}|^2 .
\]

Hence:

\[
|g_0|^2 + \sum_{j>0} |g_{2j}|^2 = 1
\]

and thus \( \sum_j |g_{2j}|^2 = 1 \).

For the sum of the weights \( g_j \), we compute

\[
\sum_j \text{Tr}(S_{2j}^T U) = \sum_{k,l} \sum_j (S_{2j})_{k,l} U_{k,l} \\
= \sum_{k,l} U_{k,l} \sum_j (-1)^{0+b^T_k} \delta_{l,a+k} .
\]

Whereas until here \( \sum_j \) means summing over the parameters \( a \) and \( b \), from now on, we can restrict the value of \( a \) to \( 1-k \). Thus summing only happens
over the parameter $b$:

$$\sum_j \text{Tr}(S_{2j}^T U) = \sum_{k,l} U_{k,l} \sum_b (-1)^{b^T \cdot k}$$

$$= \sum_{k \neq 0, l} U_{k,l} \sum_b (-1)^{b^T \cdot k} + \sum_l U_{0,l} \sum_b (-1)^{b^T \cdot 0}$$

$$= \sum_{k \neq 0, l} U_{k,l} 0 + \sum_l U_{0,l} \sum_b 1$$

$$= \sum_l U_{0,l} 2^w = 2^w \sum_l U_{0,l}.$$ 

So, finally, (6) becomes

$$\sum_j g_{2j} = \frac{1}{2^w} 2^w \sum_l U_{0,l} = \sum_l U_{0,l}.$$