The Canonical Coset Decomposition of
Unitary Matrices Through Householder
Transformations

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Abstract

This paper reveals the relation between the canonical coset decomposition of unitary matrices and the corresponding decomposition via Householder reflections. These results can be used to parametrize unitary matrices via Householder reflections.

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1 Introduction

The parametrization of unitary matrices is important in many fields of physics such as quantum computation [1, 2], particle physics [3] and quantum interferometry [4]. Several methods for the parametrization of $SU(N)$ have been developed, including one that uses Euler angles [5] to find explicit expressions for the Haar measure. Another form was given by Reck et al., who explicitly constructed arbitrary unitary operators in terms of two-state pivots [1]. Dita proposed a parametrization through diagonal unitary matrices interlaced with real orthogonal
matrices \[6\] and Rowe et al. developed another method studying the Wigner functions for $SU(3)$ \[4\], which were also used in a formulation of coherent states for $SU(N)$ in the work of Nemoto\[7\]. More recently, a technique resembling the canonical coset parametrization was presented by Jarlskog \[8, 9\].

Matrix decomposition through Householder reflections \[10\] was recently proposed as an efficient method for synthesizing unitary operators\[2, 11\]. This technique can be implemented in certain quantum systems using $N$ instead of $N^2$ steps as required in methods applying two-state pivots \[1\] following the logic of the Givens rotation \[12\]. The canonical coset parametrization \[13, 14\] of unitary matrices is a general method that may be used to calculate explicit expressions of the Haar \[13, 14, 15\] and Bures measures \[16, 17\], which are known to be important in Bayesian quantum estimation \[18\]. The main purpose of this paper is to establish the connection between the Householder decomposition and the canonical coset parametrization of unitary operators, which could have practical significance in a number of physical applications.

## 2 Householder Decomposition

A unitary operator can be seen as a basis of orthonormal vectors and the Householder decomposition of unitary operators serves to align the original basis in terms of a new basis. The Householder decomposition consists of a sequence of transformations, each of which is a reflection with respect to a hyperplane defined by the orthonormal vector $|n\rangle$, such that

$$R_{|n\rangle} = 1 - 2|n\rangle\langle n|.$$  \hspace{1cm} (1)

As a proper reflection, $R_{|n\rangle}$ satisfies $\det(R_{|n\rangle}) = -1$ and $R_{|n\rangle}R_{|n\rangle} = 1$. Given a set of orthonormal basis elements $|e_k\rangle$, the unitary matrix $U(N)$ may be decomposed as a product of $N$ factors using Householder reflections that are designed to sequentially align the columns of $U(N)$ along the orthonormal basis elements $|e_k\rangle$.

In order to illustrate the Householder decomposition, let $|W_1\rangle$ be the first column of $U(N)$ and $\phi_1$ the phase of the topmost complex component of $|W_1\rangle$. The first Householder reflection is constructed as

$$R_{|u_1\rangle} = 1 - 2 - \frac{1}{\langle u_1 | u_1 \rangle} |u_1\rangle \langle u_1|.$$  \hspace{1cm} (2)
where $|u_1⟩ = |W_1⟩ + e^{iφ_1} |e_1⟩$, such that $R_{|u_2⟩}|W_1⟩ = −|e_1⟩$. For visualization, the case with two-dimensional real vectors is shown in Figure 1. The most general definition of the vector $|u_1⟩$ requires $|e_1⟩$ to be multiplied by the magnitude of the vector $|W_1⟩$, but as $U(N)$ is unitary, then $|W_1⟩$ has unit norm. Although, the opposite sign choice $e^{iφ_1} → −e^{iφ_1}$ could be utilized, a positive sign is required in order to arrive at the canonical coset decomposition as shown in the proof of Theorem 1 below. Moreover, the positive sign is usually chosen to obtain better numerical stability (see [19], page 225). The above procedure is repeated in recursion, with $|W_2⟩$ as the second column of $R_{|u_1⟩}U(N)$ (instead of $U(n)$) and $|u_2⟩ = |W_2⟩ + e^{iφ_2} |e_2⟩$. In this way, the resulting Householder decomposition becomes

$$U(N) = R_{|u_2⟩}R_{|u_3⟩}...R_{|u_{N-1}⟩} U(1)^N,$$

where $U(1)^N$ is the diagonal matrix with element $e^{iφ_l}$ at the $l$-th position along the diagonal.

The construct of the canonical coset decomposition from the Householder decomposition is given by the following theorem.

![Figure 1: Graphical representation of a Householder reflection constructed for a real two-dimensional unit-length vector $|W_1⟩$ reflected on the plane perpendicular to $|u_1⟩$. The net result is a reflection that positions $|W_1⟩$ along the direction $−|e_1⟩$. An additional reflection can be performed to position $|W_1⟩$ along $|e_1⟩$.](image-url)
Theorem 1. The factors of the canonical coset decomposition

\[ U(N) = \frac{U(N)}{U(N-1) \otimes U(1)} \frac{U(N-1)}{U(N-2) \otimes U(1)} ... \frac{U(2)}{U(1) \otimes U(1)} U(1)^{\otimes N}, \]

(4)
can be expressed in terms of Householder reflections \( R_{|u_k\rangle} \) as

\[ \frac{U(N)}{U(N-1) \otimes U(1)} = R_{|u_1\rangle} R_{|e_1\rangle}, \]

(5)
\[ \frac{U(N-2)}{U(N-2) \otimes U(1)} = R_{|u_2\rangle} R_{|e_2\rangle}, \]

(6)
\[ \vdots \]
\[ \frac{U(1)^{\otimes N}}{U(1) \otimes U(1)} = R_{|e_1\rangle} R_{|e_2\rangle} ... R_{|e_{N-1}\rangle} U(1)^N, \]

(7)
where the corresponding Householder decomposition is

\[ U(N) = R_{|u_1\rangle} R_{|u_2\rangle} ... R_{|u_{N-1}\rangle} U(1)^N, \]

(8)
such that

\[ |u_1\rangle = |W_1\rangle + e^{i\phi_1} |e_1\rangle, \]

(9)
with \( |W_1\rangle \) being the first column of \( U(N) \) and \( \phi_1 \) the phase of the first component of \( |W_1\rangle \). The remaining vectors \( |u_k\rangle \) are calculated recursively.

Proof. Let us define the normalized vector \( |n_1\rangle \) as

\[ |n_1\rangle = \frac{1}{\sqrt{\langle u_1|u_1\rangle}} |u_1\rangle \]

(10)
The first column of \( U(N) \) can be decomposed into parallel and perpendicular parts with respect to \( |e_1\rangle \) as

\[ |W_1\rangle = |W_{1\parallel}\rangle + |W_{1\perp}\rangle = \rho e^{i\phi_1} |e_1\rangle + |W_{1\perp}\rangle, \]

(11)
where \( \rho e^{i\phi_1} \) is the polar representation of the first component of \( |W_1\rangle \). The normalized vector \( |n_1\rangle \) can be expressed as

\[ |n_1\rangle = \frac{1}{\sqrt{\langle u_1|u_1\rangle}} \left( |W_{1\perp}\rangle + (\rho + 1)e^{i\phi_1} |e_1\rangle \right). \]

(12)
This allows writing \( |n_1\rangle \) as

\[ |n_1\rangle = |n_{\parallel}\rangle + |n_{\perp}\rangle = \gamma |e_1\rangle + |n_{\perp}\rangle, \]

(13)
with \( \gamma = \frac{(\rho + 1)e^{i\phi}}{\sqrt{\langle u_1 | u_1 \rangle}} \) and \( |n_\perp \rangle = \frac{|W_{1 \perp} \rangle}{\sqrt{\langle u_1 | u_1 \rangle}} \). From (11) and (12) we obtain

\[
1 = \rho^2 + \langle W_{1 \perp} | W_{1 \perp} \rangle
\]

(14)

\[
\langle u_1 | u_1 \rangle = \langle W_{1 \perp} | W_{1 \perp} \rangle + (\rho + 1)^2,
\]

(15)

which can be used to extract \( \langle u_1 | u_1 \rangle = 2(1 + \rho) \) and write \( \gamma \) as

\[
\gamma = \sqrt{\frac{(1 + \rho)}{2}} e^{i\phi}.
\]

(16)

The product of the following Householder operators can be expanded as

\[
R_{|n\rangle} R_{|e_1\rangle} = (1 - 2|n\rangle\langle n|)(1 - 2|e_1\rangle\langle e_1|)
\]

(17)

\[
= 1 - 2|n_\perp\rangle\langle n_\perp| - 2\gamma|e_1\rangle\langle n_\perp| + 2\gamma^*|n_\perp\rangle\langle e_1|
\]

\[
+ 2(|\gamma|^2 - 1)|e_1\rangle\langle e_1|.
\]

The identity matrix can be decomposed as \( 1 = 1_\perp + |e_1\rangle\langle e_1| \) and introduced above to yield

\[
R_{|n\rangle} R_{|e_1\rangle} = 1_\perp - 2|n_\perp\rangle\langle n_\perp| - 2\gamma|e_1\rangle\langle n_\perp| + 2\gamma^*|n_\perp\rangle\langle e_1| + (2|\gamma|^2 - 1)|e_1\rangle\langle e_1|,
\]

(18)

which can be decomposed into four parts expressed in block matrix form as

\[
R_{|n\rangle} R_{|e_1\rangle} = \begin{pmatrix}
2|\gamma|^2 - 1 & -2\gamma|n_\perp| \\
2\gamma^*|n_\perp| & 1_\perp - 2|n_\perp\rangle\langle n_\perp|
\end{pmatrix}.
\]

(19)

Next, the following variable change is applied

\[
|X\rangle = 2\gamma^*|n_\perp\rangle,
\]

(20)

and the variable \( r \) is defined as the magnitude of \( |X\rangle \)

\[
r = \sqrt{\langle X|X \rangle}.
\]

(21)

From (13) we see that

\[
r^2 = 4|\gamma|^2|n_\perp|n_\perp\rangle = 4|\gamma|^2(1 - |\gamma|^2),
\]

(22)

and with some algebra this leads to

\[
\sqrt{1 - r^2} = 2|\gamma|^2 - 1.
\]

(23)
This construction is consistent only if \( 1 \geq 2|\gamma|^2 - 1 \geq 0 \), which is seen to be true by inspecting (16). Moreover, (16) implies that \( 2|\gamma|^2 - 1 = \rho \).

The block matrix (19) can be written in the form of a canonical coset as follows

\[
R_{\{n\}}R_{\{e_1\}} = \begin{pmatrix} \sqrt{1 - r^2} & -\langle X \rangle \\ \langle X \rangle & \mathbf{1}_{\perp} - \frac{1 - \sqrt{1 - r^2}}{r^2} \langle X \rangle \langle X \rangle \end{pmatrix}
\]

\[
= \begin{pmatrix} \sqrt{1 - r^2} & -\langle X \rangle \\ \langle X \rangle & \sqrt{1_{\perp} - \langle X \rangle \langle X \rangle} \end{pmatrix}
\]

\[
= \frac{U(N)}{U(N-1) \otimes U(1)},
\]

which is the form given by Gilmore[13, 14].

The remainder of the cosets can be found recursively with the insertion of reflections of the form \( R_{\{e_k\}} \), which can be constructed by replacing the \( k \)-th element of the identity matrix with \(-1\). There is flexibility in the sequential choice of the reflections \( R_{\{e_k\}} \) because they commute with each other \([R_{\{e_j\}}, R_{\{e_k\}}] = 0\). Additionally, since \( R_{\{u_k\}} \) is a block matrix, the following identity can be verified

\[
[R_{\{e_j\}}, R_{\{u_k\}}] = 0 \quad \text{for} \quad k > j.
\]

Thus, the theorem is proved. \( \blacksquare \)

**Corollary 1** The factors of the reversed canonical coset decomposition,

\[
U(N) = U(1)^{\otimes N} \frac{U(2)}{U(1) \otimes U(1)} \ldots \frac{U(N - 1)}{U(N - 2) \otimes U(1)} \frac{U(N)}{U(N-1) \otimes U(1)^{\dagger}}.
\]

(28)

can be expressed in terms of the reversed Householder reflections \( R_{\{u_k\}} \) as

\[
\frac{U(N)}{U(N-1) \otimes U(1)} = R_{\{e_1\}}R_{\{u_1\}}
\]

(29)

\[
\frac{U(N - 1)}{U(N - 2) \otimes U(1)} = R_{\{e_2\}}R_{\{u_2\}}
\]

(30)

\[\vdots\]

\[
\frac{U(1)}{U(1) \otimes U(1)^{\dagger}} = (U(1)^N R_{\{u_{N-1}\}} \ldots R_{\{e_2\}} R_{\{e_1\}})
\]

(31)

where, the corresponding Householder decomposition is

\[
U(N) = U(1)^N R_{\{u_{N-1}\}} \ldots R_{\{u_2\}} R_{\{u_1\}}.
\]

(32)
such that
\[ \langle u_1 \rangle = \langle W_1 \rangle + e^{i\phi_1} \langle e_1 \rangle, \quad (33) \]
with \( \langle W_1 \rangle \) being the first row of \( W \) and \( \phi_1 \) the phase of the first component of \( \langle W_1 \rangle \). The remainder of the vectors \( \langle u_k \rangle \) are calculated recursively.

One important consequence of Theorem 1 is the opportunity it affords to parametrize the Householder reflections. This can be accomplished with the use of (20), as described in the following corollary.

**Corollary 2** The normal Householder vector \( \langle n \rangle \) can be parametrized in terms of the canonical coset vector \( \langle X \rangle \) as
\[ \langle n \rangle = \gamma \langle e_1 \rangle + \frac{1}{2\gamma^*} \langle X \rangle, \quad (34) \]
where
\[ |\gamma| = \sqrt{1 - \langle X |X \rangle + \frac{1}{2}}, \quad (35) \]
with the phase of \( \gamma \) extracted from the phase of the first diagonal element of \( U(1)^N \).

The parametrization of unitary matrices is essential in order to calculate the Haar metric and Haar measure [15] of unitary matrices, and for this purpose using Householder reflections is more efficient than other alternatives such as the parametrization in terms of Euler angles [5]. In the same spirit, the parametrization of the Householder normal vectors \( \langle n \rangle \) (34) can be exploited to generate random unitary matrices with the Haar measure as suggested by Ivanov [20]. This can be accomplished by homogeneously distributing \( \langle X \rangle \) within Euclidean balls [21] while uniformly distributing the phase of \( \gamma \) in the range \( \text{arg}(\gamma) \in [-\pi, \pi] \). For example, the generation of random unitary matrices \( U(3) \) with the Haar measure requires the following parametrization
\[ U(3) = (1 - 2|n_1\rangle\langle n_1|)(1 - 2|n_2\rangle\langle n_2|)\text{diag}(e^{i\phi_1}, e^{i\phi_2}, e^{i\phi_3}), \quad (36) \]
where the phases \( \phi_k \) are drawn from a uniform distribution over the range \( [-\pi, \pi] \) and where \( |n_1\rangle \) and \( |n_2\rangle \) are parametrized within balls \( B^1 \) and \( B^2 \), respectively.
As an illustrative example for the calculation of the canonical coset decomposition, consider

\[ U_0 = \begin{pmatrix} \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix}. \]  

(37)

The Householder decomposition is

\[ U_0 = |R\rangle|u_1\rangle |R\rangle |u_2\rangle U(1)^3, \]

where

\[ |R\rangle|u_1\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{2} & \frac{i(2+\sqrt{2})}{4} & -\frac{i}{4+2\sqrt{2}} \\ 1 & 0 & 0 & 0 \\ -\frac{i}{2} & \frac{i}{4+2\sqrt{2}} & 0 \\ 0 & \frac{i}{2+\sqrt{2}} & \frac{i(1+\sqrt{2})}{2+\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \]

(38)

\[ |R\rangle|u_2\rangle = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & \frac{i}{2+\sqrt{2}} \\ 0 & \frac{1}{2+\sqrt{2}} & \frac{i(1+\sqrt{2})}{\sqrt{2}} \\ 0 & \frac{i}{2+\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \]

(39)

\[ U(1)^3 = \begin{pmatrix} -i & 0 & 0 \\ 0 & -i & 0 \\ 0 & 0 & -1 \end{pmatrix}. \]

(40)

This leads to the corresponding canonical coset decomposition

\[ \frac{U(3)}{U(2) \otimes U(1)} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{2} & \frac{i}{2} \\ -\frac{1}{2} & \frac{(2+\sqrt{2})}{4} & -\frac{i}{4+2\sqrt{2}} \\ \frac{i}{2} & \frac{i}{4+2\sqrt{2}} & \frac{i}{2+\sqrt{2}} \end{pmatrix} \]

(41)

\[ \frac{U(2)}{U(1) \otimes U(1)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{i(1+\sqrt{2})}{2+\sqrt{2}} \\ 0 & -\frac{i(1+\sqrt{2})}{2+\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \]

(42)

\[ U(1)^3 = \begin{pmatrix} i & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & -1 \end{pmatrix}. \]

(43)

The reversed canonical coset decomposition \([28]\) can be obtained
using the reversed Householder reflections with the following results

\[
\frac{U(3)}{U(2) \otimes U(1)} = \begin{pmatrix}
\frac{1}{\sqrt{2}} & \frac{1}{2} & 0 \\
-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 1
\end{pmatrix}
\] (44)

\[
\frac{U(2)}{U(1) \otimes U(1)} = \begin{pmatrix}
1 & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}
\end{pmatrix}
\] (45)

\[
U(1)^3 = \begin{pmatrix}
i & 0 & 0 \\
i & 0 & 0 \\
0 & i & 0 \\
0 & 0 & -1
\end{pmatrix}.
\] (46)

3 Conclusions

We formally proved the connection between the Householder and canonical coset decompositions of unitary matrices. This result allows for performing the canonical coset decomposition of unitary matrices very efficiently. Furthermore, the Householder decomposition is now fully parametrized in terms of the canonical coset vectors \(|X\rangle\).

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Appendix

The following exponential involving the complex vector \(B\) can be written in terms of the Cartesian coordinates \(x^j\) as

\[
\exp \begin{pmatrix}
0 & B \\
-B^\dagger & 0
\end{pmatrix} = \begin{pmatrix}
[1 - XX^\dagger]^{1/2} & X \\
-X^\dagger & [1 - X^\dagger X]^{1/2}
\end{pmatrix}
\] (47)

such that

\[
X = \frac{\sin \sqrt{B^\dagger B}}{\sqrt{B^\dagger B}} B = \begin{pmatrix}
x^1 + ix^2 \\
x^3 + ix^4 \\
\vdots \\
x^{2N-3} + ix^{2N-2}
\end{pmatrix}
\] (48)
The Cartesian coordinates range inside an even ball $B^{2k}$, where the radial coordinate is $r^2 = X^\dagger X$. This exponential is important because it provides a parametrization of the coset $U(N)_{U(N-1) \otimes U(1)}$ as a $N \times N$ matrix, which can be used to parametrize the unitary operator $\Omega$ as

$$\Omega \in \frac{U(N)}{U(1)} = \frac{U(N)}{U(N - 1) \otimes U(1)} \frac{U(N - 1)}{U(N - 2) \otimes U(1)} \ldots \frac{U(2)}{U(1) \otimes U(1)}.$$  \hspace{1cm} (49)

In the current paper we are interested in the representation of $U(3)$, which are generated from two cosets. The left coset is

$$\frac{U(2)}{U(1) \otimes U(1)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{1 - (x^1)^2 - (x^2)^2} & 0 \\ 0 & \frac{x^1 + ix^2}{\sqrt{1 - (x^1)^2 - (x^2)^2}} & \frac{-x^1 + ix^2}{\sqrt{1 - (x^1)^2 - (x^2)^2}} \end{pmatrix},$$  \hspace{1cm} (50)

with the variables inside a disk $(x^1)^2 + (x^2)^2 \leq 1$. The right coset is

$$\frac{U(3)}{U(2) \otimes U(1)} = \begin{pmatrix} \sqrt{1 - \xi^2} & -x^5 + ix^6 & -x^3 + ix^4 \\ x^5 + ix^6 & V_{22} & V_{23} \\ x^3 + ix^4 & V_{23}^* & V_{33} \end{pmatrix},$$  \hspace{1cm} (51)

with

$$V_{22} = \frac{(x^3)^2 + (x^4)^2 + \sqrt{1 - \xi^2((x^5)^2 + (x^6)^2)}}{\xi^2},$$  \hspace{1cm} (52)

$$V_{23} = \frac{\sqrt{1 - \xi^2} - 1}{\xi^2}(x^3 - ix^4)(x^5 + ix^6),$$  \hspace{1cm} (53)

$$V_{33} = \frac{\sqrt{1 - \xi^2}}{\xi^2}[(x^3 + x^4) + \frac{1}{\xi^2}(x^5 + x^6)],$$  \hspace{1cm} (54)

$$\xi^2 = (x^3)^2 + (x^4)^2 + (x^5)^2 + (x^6)^2,$$  \hspace{1cm} (55)

and the variables in the following range

$$(x^3)^2 + (x^4)^2 + (x^5)^2 + (x^6)^2 \leq 1.$$  \hspace{1cm} (56)

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