NMR quantum gate factorization through canonical cosets

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Abstract

The block canonical coset decomposition is developed as a universal algorithmic tool to synthesize n-qubit quantum gates out of experimentally realizable NMR elements. The two-, three-, and four-qubit quantum Fourier transformations are worked out as examples. The proposed decomposition bridges the state of the art numerical analysis with NMR quantum gate synthesis.

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Introduction. According to the quantum computing circuit model, a quantum gate is a unitary operator designed to perform a predefined operation. The primary aim is to synthesize unitary operators suitable for experimental implementation. Currently, quantum gate synthesis is achieved either by factorization methods, as in the strategy “divide and conquer,” or by optimal control theory [1–3].

The factorization methods’ development was initiated by utilizing the KAK Cartan decomposition to attain minimal time two-qubit operations [4–6] with subsequent extensions to multi-qubit gates [5, 7]. However, the Cartan decomposition, coming from Lie group theory, was not constructive and actual applications required the independent development of numerical routines [8, 9]. Inspired by numerical analysis, alternative approaches, built upon the cosine-sine matrix factorization [7, 10–14], were employed to constructively decompose an arbitrary quantum operation in terms of single-qubit and CNOT gates as well as to estimate the complexity of such implementations. Since CNOT gates are not most convenient in NMR setups [15], these developments did not find experimental applications. While NMR two-qubit synthesis has been thoroughly explored [4, 16, 17], multi-qubit factorization remains largely an open problem [18–20].

In this Letter, we introduce the canonical coset decomposition as a constructive factorization technique to build quantum gates out of standard single- and two-qubit NMR operations. To illustrate this method’s ability, we present the explicit factorizations of the two-, three-, and four-qubit quantum Fourier transform, which is the basic component of many quantum computing algorithms.

Canonical Coset Decomposition is a general group-theoretic tool originally devised to study the geometric structure of unitary matrices [21, 22]. In particular, this method allowed to obtain analytic expressions for the measure of unitary operators [21, 22] as well as the measure [23] and metric [24] of mixed quantum states.

The canonical coset decomposition of a unitary matrix $U$ is

$$U = \begin{pmatrix} \sqrt{1 - X^\dagger X} & -X^\dagger \\ X & \sqrt{1 - XX^\dagger} \end{pmatrix} \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix},$$  \hspace{1cm} (1)
with
\[
U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix},
\]
(2)
\[
X = U_{21}[1 - U_{21}^\dagger U_{21}]^{1/2}U_{11}^{-1},
\]
(3)
\[
V_1 = [1 - X^\dagger X]^{1/2}U_{11} + X^\dagger U_{21},
\]
(4)
\[
V_2 = [1 - XX^\dagger]^{1/2}U_{22} - XU_{12},
\]
(5)

where \(U_{11}\) and \([1 - U_{21}^\dagger U_{21}]^{1/2}\) are invertible. Throughout the Letter we exclusively employ the block canonical coset decomposition, which is a special case of Eq. (1) with \(U_{ij}, X,\) and \(V_{1,2}\) being square matrices of the same dimension.

The block canonical coset decomposition is a very powerful tool because each term in the r.h.s. of Eq. (1) is simpler than the original matrix \(U\). In particular, the first term can be expressed for \(X = \frac{\sin \sqrt{BB^\dagger} B}{\sqrt{BB^\dagger}}\) [21] as
\[
\begin{pmatrix} \sqrt{1 - X^\dagger X} & -X^\dagger \\ X & \sqrt{1 - XX^\dagger} \end{pmatrix} = \exp \begin{pmatrix} 0 & -B^\dagger \\ B & 0 \end{pmatrix};
\]
(6)

additionally, the second term forms a subgroup. In other words, the Lie algebra \(\mathcal{L}(U)\) of unitary matrices is decomposed into a block diagonal subalgebra \(t\) and its complement \(p\)
\[
\mathcal{L}(U) = p \oplus t \equiv \begin{pmatrix} 0 & -B^\dagger \\ B & 0 \end{pmatrix} \oplus \begin{pmatrix} \log V_1 & 0 \\ 0 & \log V_2 \end{pmatrix}.
\]
(7)

For \(n\)-qubit gates \(U(2^n)\), the factorization (1) reads
\[
U(2^n) = \frac{U(2^n)}{U(2^{n-1}) \otimes U(2^{n-1})}[U(2^{n-1}) \otimes U(2^{n-1})],
\]
(8)

where the right factor corresponds to the block diagonal subgroup.

The canonical coset decomposition is closely related to other techniques. In particular, if \(X\) is diagonal then the first term in the r.h.s. of Eq. (1) is equal to the middle term of the cosine-sine decomposition [10]. When \(X\) is a single column, the decomposition (1) is equivalent to the Householder transformation [25], which is not only one of the most important operations in numerical analysis [26], but also very useful for the generation of \(n\)-level unitary operators [27–29].
Two-qubit gates. According to Eq. (8), the $U(4)$ group associated with two-qubit gates is decomposed as

$$U(4) = \frac{U(4)}{U(2) \otimes U(2)}[U(2) \otimes U(2)].$$

(9)

The reverse form of Eq. (9),

$$U(4) = U(2) \otimes U(2) \frac{U(4)}{U(2) \otimes U(2)},$$

(10)

can be achieved by using the identity $U = (U|^†)|^†$ and performing the decomposition (9) on $U|^†$.

The matrix log of $U(4)$ is spanned by the basis elements listed in Tables I(A) and I(B), where the basis of the subalgebra $t$ is given in Table I(B). Since $t$ includes both single and two-qubit interactions, isolation of single-qubit operations necessitates the following factorization:

$$U(2) \otimes U(2) = \frac{U(2) \otimes U(2)}{U(2)} U(2),$$

(11)

$$U(2) \otimes U(2) = \begin{pmatrix} G_1 & 0 \\ 0 & G_2 \end{pmatrix},$$

(12)

$$U(2) = \begin{pmatrix} S_1 & 0 \\ 0 & S_1 \end{pmatrix},$$

(13)

$$U(2) \otimes U(2) = \begin{pmatrix} S_2 & 0 \\ 0 & S_2^† \end{pmatrix},$$

(14)

where $S_2 = [G_1 G_2^†]|^1/2$ and $S_1 = S_2^† G_1$. Equation (13) accomplishes the desired isolation. Even thought Eq. (14) is not a single-qubit operator, it can be readily transformed into one by employing the standard NMR methods. Thus, making the factorization (11) suitable for NMR experiments.
The first factor in the r.h.s. of Eq. (9) can be further simplified by a recursive factorization (9) and (10)

\[
U(4) = U(2) \otimes U(2) \frac{U(4)}{[U(2) \otimes U(2)]^2} U(2) \otimes U(2),
\]

(15)

where the middle term becomes simple enough for NMR synthesis. Having initiated the unitary operators

\[
V := \exp \left( \frac{i \pi}{4} \sigma_2 \otimes \sigma_0 \right), \quad \widetilde{U}(2) := 1, \quad \widetilde{W}(2) := 1,
\]

(16)

the recursive decomposition is realized by the following algorithm:

1. Perform the factorization (9) of \( U \) and assign \( U^{(1)} := \frac{U(4)}{U(2) \otimes U(2)}, \quad U^{(2)} := U(2) \otimes U(2) \);

2. \( \widetilde{U}^{(2)} := U^{(2)} \widetilde{U}(2), \quad U^{(1)} := V^\dagger U^{(1)} V; \)

3. Perform the decomposition (10) of \( U^{(1)} \) and assign \( W^{(1)} := V[U(2) \otimes U(2)]V^\dagger, \quad W^{(2)} := V \frac{U(4)}{U(2) \otimes U(2)} V^\dagger; \)

4. \( \widetilde{W}^{(1)} := \widetilde{W}(1) W^{(1)}, \quad U := W^{(2)}; \)

5. Return to step 1 if the convergence conditions \( U^{(2)} \approx 1 \) and \( W^{(1)} \approx 1 \) are not met;

6. Finally, the right subgroup in Eq. (15) is stored in \( \widetilde{U}(2) \) and the left subgroup – \( \widetilde{W}(1) \).

The matrix log of the left, middle, and right terms in Eq. (15) are spanned by the elements from Tables II(A), II(B), and II(C), respectively. Since the middle term is made of the elements \( \{ \sigma_2 \otimes \sigma_i \}_{i=0,1,2,3} \), it is well suited for NMR synthesis.

Importantly, the developed algorithm is applicable to an arbitrary n-qubit system after adjusting the definition of \( V \) according to

\[
V := \exp \left( \frac{i \pi}{4} \sigma_2 \otimes \sigma_0 \otimes \cdots \otimes \sigma_0 \right)_{(n-1) \text{ times}}.
\]

(17)

The two-qubit quantum Fourier transform \( F \) is used to illustrate the proposed algorithm.
As shown in Sec. I of Ref. [30], the recursive decomposition \((15)\) leads to

\[
F = \exp\left( -\frac{i\pi}{4} \sigma_1 \otimes \sigma_0 \right) \exp\left( -\frac{i\pi}{4} \sigma_3 \otimes \sigma_3 \right) \times F_1 \exp\left( \frac{i\pi}{4} \sigma_3 \otimes \sigma_3 \right) \exp\left( \frac{i\pi}{4} \sigma_1 \otimes \sigma_0 \right) \times \exp\left( -\frac{i\pi}{4} \sigma_3 \otimes \sigma_3 \right) F_2 F_{31} \exp\left( \frac{i\pi}{4} \sigma_3 \otimes \sigma_3 \right) U_{32},
\]

(18)

with

\[
i \log(F_1) = 0.55536 \sigma_0 \otimes (\sigma_1 + \sigma_2),
\]

\[
i \log(F_2) = -0.392699 \sigma_2 \otimes \sigma_0,
\]

\[
i \log(F_{31}) = 0.55536 \sigma_0 \otimes (\sigma_1 - \sigma_2),
\]

\[
i \log(U_{32}) = \sigma_0 \otimes (-1.1781\sigma_0 + 0.785398\sigma_3).
\]

(19)

The pictorial representation of this factorization is shown in Fig. 1.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
(A) & $\sigma_0 \otimes \sigma_1$ & $\sigma_0 \otimes \sigma_2$ & $\sigma_0 \otimes \sigma_3$ \\
& $\sigma_2 \otimes \sigma_0$ & $\sigma_2 \otimes \sigma_1$ & $\sigma_2 \otimes \sigma_2$ \\
\hline
(B) & $\sigma_2 \otimes \sigma_0$ & $\sigma_2 \otimes \sigma_1$ & $\sigma_2 \otimes \sigma_2$ \\
& $\sigma_2 \otimes \sigma_0$ & $\sigma_2 \otimes \sigma_1$ & $\sigma_2 \otimes \sigma_2$ \\
\hline
(C) & $\sigma_0 \otimes \sigma_0$ & $\sigma_0 \otimes \sigma_1$ & $\sigma_0 \otimes \sigma_2$ & $\sigma_0 \otimes \sigma_3$ \\
& $\sigma_3 \otimes \sigma_0$ & $\sigma_3 \otimes \sigma_1$ & $\sigma_3 \otimes \sigma_2$ & $\sigma_3 \otimes \sigma_3$ \\
\hline
\end{tabular}
\caption{Basis elements for the Lie algebra $u(4)$ corresponding to (A) left, (B) middle, (C) right terms in Eq. (15).}
\end{table}

FIG. 1: The schematic representation of the two-qubit Fourier matrix factorization \((18)\). Black boxes represent single-qubit $\pi/4$ rotations; gray boxes – taylored single-qubit operators specified by Eq. \((19)\).

Three-qubit gates. According to Eq. \((8)\), a three-qubit gate is decomposed as

\[
U(8) = \frac{U(8)}{U(4) \otimes U(4)} [U(4) \otimes U(4)],
\]

(20)
where $U(4) \otimes U(4)$ is block diagonal. The two-qubit decomposition (15) is extended to three-qubit gates

$$U(8) = U(4) \otimes U(4) \frac{U(8)}{[U(4) \otimes U(4)]^2} U(4) \otimes U(4),$$  \hspace{1cm} (21)

where the central factor’s matrix log is spanned by $\{\sigma_{2ij}\}_{i,j=0,1,2,3}$, where $\sigma_{ijk} = \sigma_i \otimes \sigma_j \otimes \sigma_k$.

According to Eq. (17), the factorization algorithm is applicable in the three-qubit case once the definition of $V$ in Eq. (16) is replaced by $V := \exp(i\pi\sigma_{200}/4)$. The decomposition (11) is naturally generalized to isolate the subgroup $U(4)$ associated with two-qubits

$$U(4) \otimes U(4) = \frac{U(4) \otimes U(4)}{U(4)} U(4).$$  \hspace{1cm} (22)

where the matrix logarithms of $U(4)$ and $U(4) \otimes U(4)/U(4)$ are linear combinations of $\{\sigma_{0ij}\}_{i,j=0,1,2,3}$ and $\{\sigma_{3ij}\}_{i,j=0,1,2,3}$, respectively.

The factorization (21) of the three-qubit quantum Fourier transform results in $F =$
Each of these factors are further decomposed in Sec. II of [30]

\[ U_1 = \exp \left( \frac{i\pi}{4} \sigma_{303} \right) \exp \left( \frac{i\pi}{4} \sigma_{100} \right) \exp \left( \frac{i\pi}{4} \sigma_{330} \right) F_{11} \]
\[ \times \exp \left( -\frac{i\pi}{4} \sigma_{330} \right) \exp \left( -\frac{i\pi}{4} \sigma_{100} \right) \exp \left( -\frac{i\pi}{4} \sigma_{303} \right) \]
\[ \times \exp \left( \frac{i\pi}{4} \sigma_{033} \right) F_{12} \exp \left( -\frac{i\pi}{4} \sigma_{033} \right) \]
\[ \times \exp \left( \frac{i\pi}{4} \sigma_{330} \right) F_{13} \exp \left( -\frac{i\pi}{4} \sigma_{330} \right), \quad (23) \]

\[ U_2 = \exp \left( \frac{i\pi}{4} \sigma_{100} \right) \exp \left( \frac{i\pi}{4} \sigma_{330} \right) \exp \left( -\frac{i\pi}{4} \sigma_{100} \right) \]
\[ \times \exp \left( \frac{i\pi}{4} \sigma_{020} \right) \exp \left( \frac{i\pi}{4} \sigma_{033} \right) F_{21} \exp \left( -\frac{i\pi}{4} \sigma_{033} \right) \]
\[ \times \exp \left( -\frac{i\pi}{4} \sigma_{020} \right) \exp \left( \frac{i\pi}{4} \sigma_{010} \right) \exp \left( \frac{i\pi}{4} \sigma_{033} \right) F_{22} \]
\[ \times \exp \left( -\frac{i\pi}{4} \sigma_{033} \right) \exp \left( -\frac{i\pi}{4} \sigma_{010} \right) W_{23} \exp \left( \frac{i\pi}{4} \sigma_{100} \right) \]
\[ \times \exp \left( -\frac{i\pi}{4} \sigma_{330} \right) \exp \left( -\frac{i\pi}{4} \sigma_{100} \right), \quad (24) \]

\[ U_3 = \exp \left( \frac{i\pi}{4} \sigma_{330} \right) \exp \left( \frac{i\pi}{4} \sigma_{020} \right) \exp \left( \frac{i\pi}{4} \sigma_{033} \right) F_{311} \]
\[ \times \exp \left( -\frac{i\pi}{4} \sigma_{033} \right) \exp \left( -\frac{i\pi}{4} \sigma_{020} \right) \exp \left( \frac{i\pi}{4} \sigma_{010} \right) \]
\[ \times \exp \left( \frac{i\pi}{4} \sigma_{033} \right) F_{312} \exp \left( -\frac{i\pi}{4} \sigma_{033} \right) \exp \left( -\frac{i\pi}{4} \sigma_{010} \right) \]
\[ \times W_{313} \exp \left( -\frac{i\pi}{4} \sigma_{330} \right) \exp \left( \frac{i\pi}{4} \sigma_{033} \right) \]
\[ \times F_{323} \exp \left( -\frac{i\pi}{4} \sigma_{033} \right) U_{324}, \quad (25) \]

where \( F_{j...}, W_{j...} \) and \( U_{jk...} \) are single-qubit operators. This factorization is also depicted in Fig. 2

Finally, the four-qubit Fourier transform is elaborated in Sec. III of Ref. [30].

Conclusions. The block canonical coset decomposition is introduced as an algorithmic procedure to synthesize an arbitrary n-qubit quantum gate out of one- and two-qubit NMR operations. In particular, we worked out the implementations of the two-, three-, and four-qubit quantum Fourier transform given by a dense matrix (i.e., without zero entries), therefore presenting a convincing illustration of our method’s capability. Moreover, a highly optimized numerical implementation of the developed algorithm can be carried out through
FIG. 2: The schematic representation of the three-qubit Fourier matrix factorization from Eqs. (23), (24), and (25). Black boxes represent single-qubit $\pi/4$ rotations; gray boxes – taylored single-qubit operators.

the block Householder decomposition [31][34]. Thus, the current work provides an important bridge between the state of the art numerical analysis and NMR quantum gate synthesis.

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