A constructive algorithm for the Cartan decomposition of $SU(2^N)$

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Abstract

We present an explicit numerical method to obtain the Cartan-Khaneja-Glaser decomposition of a general element $G \in SU(2^N)$ in terms of its ‘Cartan’ and ‘non-Cartan’ components. This effectively factors $G$ in terms of group elements that belong in $SU(2^n)$ with $n < N$, a procedure that can be iterated down to $n = 2$. We show that every step reduces to solving the zeros of a matrix polynomial, obtained by truncation of the Baker-Campbell-Hausdorff formula, numerically. All computational tasks involved are straightforward and the overall truncation errors are well under control.

1 Introduction

In their seminal paper [K-G], Khaneja and Glaser presented a generic method to decompose ‘large’ unitary elements in terms of ‘smaller’ ones. The initial unitaries can be viewed as evolution operators of a multipartite system of spin-1/2’s or as quantum algorithms acting on qubits. Experimentally it is only possible to control the interactions between a small number of subsystems at a time. Hence, this decomposition is of particular interest. It allows us to address questions such as how to optimize a dynamical evolution in terms of control procedures applied to a small number of spins or how a certain quantum algorithm can be obtained with the smallest possible number of experimentally feasible one and two qubit gates.

In particular, Khaneja and Glaser show that any element of the Lie group $G = SU(2^N)$ is, up to local unitaries in $SU(2)^\otimes N$, determined by components
generated from certain Abelian subalgebras $\mathfrak{h}_n$ and $\mathfrak{f}_n$, $n = 2, ..., N$, of the Lie algebra $\mathfrak{su}(2^N)$. This is achieved by employing iteratively the Cartan decomposition

$$G = K'HK''$$

where $H$ is generated by $\mathfrak{h}_n$ ($\mathfrak{f}_n$) and the factors $K'$ and $K''$ belong to the subgroup $K \subset G$ generated by a particular subalgebra orthogonal to $\mathfrak{h}_n$ ($\mathfrak{f}_n$). These relevant substructures are specified in terms of a fortunate choice of basis for $\mathfrak{su}(2^n)$ that can be obtained recurrently for $n = 2, ..., N$.

The beauty of this result and its promising applications in quantum algorithms [V-W, S-B-M], control theory, quantum error correction [S] or the quantification of entanglement in multi-partite systems [O-S] have motivated the search for a constructive method to perform the decompositions for any given matrix $G \in SU(2^N)$. Although substantial work has been done on the first non-trivial instance $SU(4)$ [K-C, H-V-C], little seems to be known so far for the higher $N$ case [Bu].

Here we address the decomposition problem for the general group $SU(2^N)$. Employing a convenient truncation of the Baker-Campbell-Hausdorff (BCH) formula, we show that the problem allows for a numerical algorithm to calculate all such KHK decompositions with controlled error. Hence, we can perform the full Khaneja-Glaser decomposition of a general element $G \in SU(2^N)$ with arbitrary computational precision.

This article is organized as follows. In Section 2 we briefly review the Khaneja-Glaser decomposition [K-G] and establish the formalism for our approach. In Section 3 we reinterpret the problem in terms of the BCH formula; we explain how a truncation of the BCH series renders our problem solvable by straightforward numerical tasks. In Section 4 we give a user-friendly summary of the essential steps involved and we finally conclude in Section 5.

2 The Khaneja-Glaser decomposition

We consider the compact semi-simple Lie group $G = SU(2^N)$ and a particular compact closed subgroup $K \subset G$; we denote by $\mathfrak{g} = \mathfrak{su}(2^N)$ the Lie algebra of $G$ and by $\mathfrak{g} = \mathfrak{su}(2^N)$ the Lie algebra of $K$ understood as a subalgebra of $\mathfrak{g}$. Since $G$ is semi-simple, the Killing form $\langle \cdot, \cdot \rangle$ is non-degenerate and defines a bi-invariant metric on $G$. Hence, we can define $\mathfrak{m} = \mathfrak{t}^\perp$ to be the orthogonal complement of $\mathfrak{t}$ with respect to the metric. Notice that, in general, the vector space $\mathfrak{m} \subset \mathfrak{g}$ is not a subalgebra. Since $\mathfrak{m}$ is determined by $\mathfrak{t}$ and the Killing metric, we shall refer to this structure as the Lie algebra pair $(\mathfrak{g}, \mathfrak{t})$.

We shall adopt the following typographic conventions in most cases

- $G$ capital bold: group or subgroup
- $G$ capital: element of $G$
- $\mathfrak{g}$ German fraktur: Lie algebra or subspace
- $g$ normal: element of $\mathfrak{g}$
The only exception to the choice of fonts just stated will be the familiar Pauli matrices, seen as elements of $\mathfrak{su}(2)$, which will be denoted by majuscules

$$X = \frac{i}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \frac{i}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \frac{i}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and the 2×2 identity matrix $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. Finally, we shall use an abbreviated normalized notation for their tensor products given by

$$A_1 A_2 \ldots B_j \ldots A_k = \left( \begin{array}{c} 2 \\ 1 \end{array} \right)^{k-1} A_1 \otimes A_2 \otimes \ldots \otimes B_j \otimes \ldots \otimes A_k, \quad A_i = X, Y, Z.$$

For example, $YXI = \frac{i}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

### 2.1 Cartan decomposition

**Definition 1** A Cartan decomposition of $\mathfrak{g}$ is an orthogonal split of $\mathfrak{g}$

$$\mathfrak{g} = \mathfrak{t} \oplus \mathfrak{m}$$

given by a Lie algebra pair $(\mathfrak{g}, \mathfrak{k})$ satisfying the commutation relations

$$[\mathfrak{t}, \mathfrak{t}] \subset \mathfrak{t}, \quad [\mathfrak{m}, \mathfrak{t}] \subset \mathfrak{m}, \quad [\mathfrak{m}, \mathfrak{m}] \subset \mathfrak{t}.$$  \hfill (1)

In this case $(\mathfrak{g}, \mathfrak{t})$ is called a symmetric Lie algebra pair.

**Remark 2** The apparently artificial conditions in the above definition have an interpretation in Riemannian geometry: $\mathfrak{g} = \mathfrak{t} \oplus \mathfrak{m}$ is a Cartan decomposition if and only if the quotient manifold $G/K = \exp(\mathfrak{m})$ is a globally Riemannian symmetric space [K-N]. Such a space possesses a canonical global involution (i.e., an automorphism $s$ of the space onto itself such that $s^2 = I$) which induces naturally a linear involution $s_*$ on $\mathfrak{g}$ that preserves the Lie algebra structure [..]. Since $s_*$ squares to identity, its eigenvalues must be $\pm 1$, and the subspaces $\mathfrak{t}$ and $\mathfrak{m}$ emerge respectively as the $+1$ and $-1$-eigenspaces of $s_*$.  

We can start exploring the Cartan decomposition $\mathfrak{g} = \mathfrak{t} \oplus \mathfrak{m}$ by noticing that if $\mathfrak{h} \subset \mathfrak{m}$ is a subalgebra of $\mathfrak{g}$ then, by (1), $\mathfrak{h}$ is automatically Abelian. Since $\mathfrak{m}$ itself is not in general a subalgebra of $\mathfrak{g}$, it is natural to look for a maximal (Abelian) subalgebra $\mathfrak{h} \subset \mathfrak{m}$.

**Definition 3** A Cartan subalgebra of the pair $(\mathfrak{g}, \mathfrak{t})$ is a maximal (in $\mathfrak{m}$) Abelian subalgebra $\mathfrak{h} \subset \mathfrak{m}$.

From now on we shall assume that the Cartan subalgebra $\mathfrak{h}$ refers to the pair $(\mathfrak{g}, \mathfrak{t})$ unless stated otherwise. The following Proposition shows that the whole $\mathfrak{m}$ is obtained from $\mathfrak{h}$ by the adjoint action of $K$ and that there is only one such $\mathfrak{h}$ up to this action. In the context of the particular application we have in mind, this means $\mathfrak{h}$ carries the ‘essential’ information about $\mathfrak{m}$.
Proposition 4 Let \( \mathfrak{h} \) and \( \mathfrak{h}' \) be two Cartan subalgebras; then

1. \( \mathfrak{m} = \bigcup_{K \in \mathfrak{K}} \text{Ad}_K(\mathfrak{h}) \);

2. \( \mathfrak{h}' = \text{Ad}_K(\mathfrak{h}) \) for some element \( K \in \mathfrak{K} \).

Proof. Please see Appendix B. \( \blacksquare \)

Denote \( \mathbf{H} = \exp(\mathfrak{h}) \subset \mathbf{G} \) the subgroup generated by \( \mathfrak{h} \). The Cartan decomposition theorem states that any group element \( \mathbf{G} \in \mathbf{G} \) can be written as an element \( H \in \mathbf{H} \) together with left- and right-multiplications by elements of \( \mathfrak{K} \):

**Theorem 5 (Cartan decomposition)** The Cartan decomposition \( \mathfrak{g} = \mathfrak{k} \oplus \mathfrak{m} \) induces a Cartan decomposition of the group \( \mathbf{G} \),

\[
\mathbf{G} = \mathbf{K}\mathbf{H}\mathbf{K}^+, \tag{2}
\]

where \( \mathbf{H} = \exp(\mathfrak{h}) \).

The Cartan decomposition of a given element \( \mathbf{G} \in \mathbf{G} \) has the form

\[
\mathbf{G} = K_0K_1HK_1^+ = K_0M, \tag{3}
\]

where \( K_0, K_1 \in \mathbf{K}, H \in \mathbf{H} \) and \( M = K_1HK_1^+ \in \exp(\mathfrak{m}) \).

Proof. Since \( \mathbf{G}/\mathbf{K} = \exp(\mathfrak{m}) \), there exist \( K_0 \in \mathbf{K} \) and \( M \in \exp(\mathfrak{m}) \) such that \( \mathbf{G} = K_0M \). Let \( m = \log(M) \in \mathfrak{m} \); from Proposition 4, item 1, there exists \( K_1 \in \mathbf{K} \) such that \( \text{Ad}_{K_1}m = \mathfrak{h} \in \mathfrak{h} \), so

\[
\mathbf{G} = K_0 \exp(m) = K_0 \exp\left(\text{Ad}_{K_1^+}\mathfrak{h}\right) = K_0K_1\exp(h)K_1^+. \tag{3}
\]

\( \blacksquare \)

2.2 The Khaneja-Glaser basis

The Khaneja-Glaser basis \([\text{K-G}]\) for arbitrary \( \mathfrak{su}(2^n) \) makes explicit all the structures which concern us. In particular, the splitting \( \mathfrak{g} = \mathfrak{k} \oplus \mathfrak{m} \) and the Cartan subalgebras \( \mathfrak{h}_n \) and \( \mathfrak{j}_n \) are manifest.

We start with a familiar example:

**Example 6** For \( n = 2 \), we propose basis elements for the Lie algebra \( \mathfrak{su}(4) \) and organize them into subspaces \( \mathfrak{m}_2 \) and \( \mathfrak{k}_2 \) as follows:
Now we obtain the Khaneja-Glaser basis for $\mathfrak{su}(2^n)$ by a relatively simple iteration process starting from $\mathfrak{su}(4)$, as summarized in the following diagram:

\[ I_{n-1} = I \otimes (n-1) = I \otimes \ldots \otimes I \]

NB.: Terms of the form $\mathfrak{su}(2^{n-1}) \otimes A$ denote the set obtained by tensoring each element of $\mathfrak{su}(2^{n-1})$ with the matrix $A = X, Y, X, I$; in all cases we consider the span of the basis elements over $\mathbb{R}$.

Notice that for $n > 2$ two successive Cartan decompositions can be performed. First, the expected one referring to the pair $(\mathfrak{su}(2^n), \mathfrak{h}_n)$, with Cartan subalgebra $\mathfrak{h}_n$. In the terms of Theorem 5, this means we can write $G \in SU(2^n)$ as $G = K'HK''$ with $H \in \exp(\mathfrak{h}_n)$ and $K', K'' \in \exp(\mathfrak{k}_n)$. However, the decomposition of $\mathfrak{k}_n$ given by diagram (4) is

\[ \mathfrak{k}_n = \mathfrak{k}_{n,1} \oplus \mathfrak{k}_{n,0} \oplus \text{span}\left\{ I^{n-1}Z \right\} \simeq \mathfrak{su}(2^{n-1}) \oplus \mathfrak{su}(2^{n-1}) \oplus \mathfrak{u}(1), \]

where both $\mathfrak{k}_{n,1}$ and $\mathfrak{k}_{n,0}$ are canonically isomorphic to $\mathfrak{su}(2^{n-1})$. Since our aim is to iteratively decompose the factors $K^{(j)}$ until they eventually reduce to ‘local’ unitaries in $SU(2)^{\otimes N}$ and non-local ‘Cartan’ factors, we would expect
\( \mathfrak{k}_n \) to generate something of the form \( SU(2^{n-1}) \otimes SU(2) \). Thus, there is a \( su(2^{n-1}) \) component too many in \( \mathfrak{k}_n \) that we need to factor away in order to define the complete recurrence step.

A closer look at \( \mathfrak{k}_n \) reveals another Lie Algebra pair, thereby clearing the way for a second Cartan decomposition: we just have to leave aside the ‘complex phase’ generated by \( I^{n-1}Z \) (see diagram (4)) that can be seen as a ‘local’ transformation under the inclusion \( U(1) \hookrightarrow SU(2) \). Let \( \mathfrak{k}_n = \mathfrak{t}_{n,1} \oplus \mathfrak{t}_{n,0} \) denote the subalgebra obtained from \( \mathfrak{k}_n \) in this manner, so that \( \mathfrak{k}_n = \mathfrak{t}_n \oplus u(1) \hookrightarrow \mathfrak{k}_n \oplus su(2) \).

Accordingly, given a group element \( K = \exp(k) \in K \), let us write \( \hat{K} = \exp(\hat{k}) \), where \( \hat{k} \in \mathfrak{k}_n \) is obtained from \( k \in \mathfrak{k} \) by eliminating the component spanned by \( I^{n-1}Z \). This is well defined as \( I^{n-1}Z \) commutes with every element in \( \mathfrak{k}_n \).

It is now straightforward to check that \( (\hat{\mathfrak{k}}_n, \mathfrak{k}_n, 0) \) is also a Lie algebra pair \([K-G]\), whose Cartan subalgebra we call \( \mathfrak{f}_n \). Hence, we can apply Theorem 5 again to decompose the factors \( \hat{K} \) and \( K'' \) into elements of \( \exp(\mathfrak{f}_n) \) together with left and right multiplication by some new factors generated by \( \mathfrak{k}_n, 0 \). This time the orthogonal subalgebra \( \mathfrak{k}_n, 0 = su(2^{n-1}) \otimes I \) is canonically isomorphic to \( su(2^{n-1}) \), so it generates \( \exp(\mathfrak{k}_n, 0 \oplus \text{span}\{I^{n-1}Z\}) \simeq SU(2^{n-1}) \otimes SU(2) \).

Thus, we have accomplished the the complete \( n \)th recurrence step that yields decompositions

\[
G = K^{(1)}F^{(1)}K^{(2)}HK^{(3)}F^{(2)}K^{(4)},
\]

with \( F^{(j)} \in \exp(\mathfrak{f}_n) \), \( H \in \exp(\mathfrak{h}_n) \) and \( K^{(j)} \in SU(2^{n-1}) \otimes SU(2) \).

Note, finally, that we are particularly interested in the ‘Cartan’ factors, i.e. those generated by the Cartan subalgebras \( \mathfrak{h}_n \) of \( (su(2^n), \mathfrak{k}_n) \) and \( \mathfrak{f}_n \) of \( (\hat{\mathfrak{k}}_n, \mathfrak{k}_n, 0) \), that emerge in each step. It is thus convenient to know explicitly a set of basis elements for each of these subalgebras. This can be achieved by the following recurrence formula, starting from \( \mathfrak{h}_2 = \text{span}\{XX, YY, ZZ\}, \)

\[
\begin{align*}
\mathfrak{h}_n &= \text{span}\{a_n\}, \quad n = 2, \ldots, N \\
\mathfrak{f}_n &= \text{span}\{b_n\}, \quad n = 2, \ldots, N \\
\mathfrak{a}(2) &= \{XX, YY, ZZ\}, \quad \mathfrak{b}(2) = \{0\} \\
\mathfrak{a}(n) &= \bigcup_{j=2}^{n} \mathfrak{a}(j) \otimes I^{n-j} \\
\mathfrak{a}(n+1) &= \{I^n, \mathfrak{a}(n)\} \otimes X \\
\mathfrak{b}(n+1) &= \{\mathfrak{a}(n)\} \otimes Z
\end{align*}
\]

The Example below illustrates all the above constructions for the first non-trivial case \( su(8) \):
Example 7 $n = 3 : \mathfrak{su}(8)$

\[
\begin{array}{ccc}
\mathfrak{su}(4) \otimes X & \mathfrak{su}(4) \otimes Y & \mathfrak{su}(4) \otimes Z \\
\mathfrak{su}(8) & \mathfrak{su}(8) & \mathfrak{su}(8)
\end{array}
\]

\[
\mathfrak{b}_3 = \text{span}\{IIX, XXX, YYX, ZZX\}
\]

\[
\mathfrak{f}_3 = \text{span}\{XXZ, YYZ, ZZZ\}
\]

2.3 The Baker-Campbell-Hausdorff formula

The matrix Lie algebra $\mathfrak{g}$ is noncommutative and thus, for general elements $a, b \in \mathfrak{g}$, the product of exponentials $e^a e^b$ does not coincide with the exponential of their sum, $e^{a+b}$. In fact the expression for $\log(e^a e^b)$ has an infinite series of correction terms and is known as the *BCH formula*, after Baker-Campbell-Hausdorff.

Although the original formula was rather complicated and computationally unpractical, a remarkable simplification made by Dynkin [D, B] expresses all the terms as successive commutators of $a$ and $b$

\[
\log(e^a e^b) = \sum_{i,j=1}^{\infty} T_{i,j} (a, b).
\]

Here $T_{i,j} (a, b)$ denotes the homogeneous term of degree $i$ in $a$ and degree $j$ in $b$; its expression is

\[
T_{i,j} (a, b) = \frac{1}{i+j} \sum_{(i_1, j_1, \ldots, i_k, j_k)} (-1)^{k-1} \frac{1}{i_1! j_1! \ldots i_k! j_k!} [a^{i_1} b^{j_1} \ldots a^{i_k} b^{j_k}],
\]

where we abbreviate $[a^{i_1} b^{j_1} \ldots a^{i_k} b^{j_k}] = [a, \ldots [a, [a, [a, \ldots [a, b, \ldots, b, \ldots, b] \ldots]]]_{i_1, j_1, \ldots, i_k, j_k}$

and the sum ranges over all possible $2k$-uples of non-negative integers $(i_1, j_1, \ldots, i_k, j_k)$ such that

\[
\sum_{c=1}^{k} i_c = i, \quad \sum_{c=1}^{k} j_c = j \quad \text{and} \quad i_c + j_c > 0.
\]
The first few terms are
\[
\log(e^a e^b) = a + b + \frac{1}{12} [a, b] + \frac{1}{24} [a, [a, b]] + \frac{1}{12} [b, [b, a]] + \frac{1}{24} [a, [b, a]] + \frac{1}{120} (...) \tag{6}
\]
and the higher order coefficients after \(\frac{1}{120}\) decrease quickly (see e.g. [R]). This will motivate us later on to perform convenient truncations on this convergent series.

### 3 Numerical algorithm for the KHK decomposition

In this Section we will develop a technique that allows the explicit numerical calculation of the components of a general group element \(G \in \mathbf{G}\) under Cartan decomposition. The idea is to consider the Cartan decomposition (3) in the light of the BCH expansion (6). Let \(g \in \mathfrak{g}, m \in \mathfrak{m}\) and \(k \in \mathfrak{k}_0\) be the generators of \(G, M\) and \(K_0\), respectively. Then (3) reads
\[
G = e^g = e^k e^m. \tag{7}
\]
Since the matrix \(G\) is given, (3) shows that \(k\) can be obtained from \(m\) (and vice-versa) by
\[
k = k(m) = \log(Ge^{-m}). \tag{8}
\]
Hence, the decomposition problem is reduced to finding \(m\).

#### 3.1 Determining \(m\)

First, taking logarithms in (3), we obtain
\[
g = \log(e^k e^m). \tag{9}
\]
We then apply (6) to expand \(g\) in terms of successive brackets of \(k\) and \(m\). In the light of Remark 2 we can easily deduce that each of the brackets belongs in either \(\mathfrak{k}\) or \(\mathfrak{m}\). Hence, the expansion is split into two orthogonal components,
\[
g = k + m + \frac{1}{2} [k, m] + \frac{1}{12} [k, [k, m]] + \frac{1}{12} [m, [m, k]] + \frac{1}{24} [k, [m, k]] + \ldots = g_\mathfrak{k} + g_\mathfrak{m},
\]
where
\[
g_\mathfrak{k} = k + \frac{1}{12} [m, [m, k]] + \frac{1}{24} [k, [m, k]] + \ldots \in \mathfrak{k}, \tag{10}
\]
\[
g_\mathfrak{m} = m + \frac{1}{2} [k, m] + \frac{1}{12} [k, [k, m]] + \ldots \in \mathfrak{m}. \tag{11}
\]
Note that computing $g_k$ and $g_m$ from $g$ is a straightforward task since the Khaneja-Glaser basis (4) makes explicit the partition $g = \mathbf{k} \oplus \mathbf{m}$.

At this stage we can use (3) to eliminate $k = k(m)$ in either of the equations (10,11). Choosing (11) whose first few terms are simpler we obtain

$$g_m = g_m(m) = m + \frac{1}{2} [k(m), m] + \frac{1}{12} [k(m), [k(m), m]] + ..., \quad (12)$$

which is an infinite series with rapidly decreasing coefficients. As $g_m(m)$ is a converging series we can truncate it so that the resulting equation will provide an approximation of $m$ with an error that decreases by including higher commutator terms. If we call $\bar{P}_p(m)$ the truncation that includes all terms with up to $p$ commutators, i.e.

$$g_m(m) = \bar{P}_p(m) + \text{further terms}, \quad (13)$$

we can in principle solve the equation

$$P_p(m) \equiv \bar{P}_p(m) - g_m = 0 \quad (14)$$

with respect to the single matrix variable $m$. However, the expression of $k(m)$ given by (3) is rather complicated. So we propose using again the BCH expansion to obtain

$$k(m) = \log(e^g e^{-m}) = g - m - \frac{1}{2} [g, m] - \frac{1}{12} [g, [g, m]] + \frac{1}{12} [m, [m, g]] + ..., \quad (15)$$

As before, we can truncate (15) to a term that includes all $q$-th order brackets. This yields a polynomial $Q_q(m)$ that approximates $k(m)$ as well as we desire at the cost of taking extra high-order commutators

$$k(m) = Q_q(m) + \text{further terms}. \quad (16)$$

After both truncations, equation (14) is approximated by

$$0 = P_p(m) \simeq -g_m + m + \frac{1}{2} [Q_q(m), m] + \frac{1}{12} [Q_q(m), [Q_q(m), m]] + ..., \quad$$

where $P_p(m)$ is now a polynomial in one matrix variable with matrix coefficients. Our problem of finding $m$ has thus been reduced to finding the zeros of a polynomial. This can be easily performed with a numerical algorithm [D-P-M]. The accuracy of the result can be increased by including more terms in the truncated series $P_p$ and $Q_q$, i.e. increasing $p$ and $q$. Specifically, we prove in Appendix A that, in this way, the errors in determining $m$ by the truncation procedure are well under control.

**Example 8** Take the “first order” truncations $p = 1$, $q = 1$:

$$P_1(m) = -g_m + m + \frac{1}{2} [k(m), m],$$

$$Q_1(m) = g - m - \frac{1}{2} [g, m].$$
Then, approximating \( k(m) \simeq Q_1(m) \), we obtain

\[
P_1(m) \simeq -g_m + m + \frac{1}{2} \left[ g - m - \frac{1}{2} [g, m], m \right]
= -g_m + m + \frac{1}{2} [g, m] - \frac{1}{4} [m, [m, g]].
\]

### 3.2 The \( M = K_1 H K_1^\dagger \) decomposition

Once \( m \) is known, it remains to find the subgroup element \( K_1^\dagger \in K \) whose adjoint action rotates \( M \) onto \( H = e^h, h \in \mathfrak{h} \).

**Lemma 9** The following properties are associated to \( H = \exp(\mathfrak{h}) \):

1. \( H \) is a torus (compact connected Abelian Lie subgroup) of \( G \);
2. any vector \( v \in \mathfrak{h} \) whose 1-parameter subgroup \( \{\exp(tv)\} \) is dense in \( H \) is centralized in \( m \) just by \( \mathfrak{h} \):

\[
\{u \in m \mid [u, v] = 0\} = \mathfrak{h}
\]  

**Proof.** see e.g. [W, §8.6].

As shown in Appendix B, the first necessary ingredient to perform the decomposition \( M = K_1 H K_1^\dagger \) is some vector \( v \in \mathfrak{h} \) that generates a dense 1-parameter subgroup \( \exp(tv) \subset \mathfrak{h} \). This may seem abstract, but since we have an explicit basis \( (5) \) for \( \mathfrak{h} \), it suffices to take any irrational combination of the Cartan generators.

**Example 10** In \( \mathfrak{su}(8) \), take e.g.

\[
v = II X + \pi.XXX + \pi^2.YYX + \pi^3.ZZX.
\]

The reluctant reader may verify that, indeed, the centralizer of such \( v \) in \( m \) is just \( \mathfrak{h} \).

Now, we may define \( f_{v,m} \) as in the Appendix B to be given by

\[
f_{v,m}(K) = \langle v, \Ad_K(m) \rangle = \sum_{a,b,c,d} C_{ac}^d C_{bd}^c v^a (K_1^\dagger m K)^b
\]  

and recover \( K_1 \) numerically as a minimum of \( f_{v,m} \).

We conclude that \( m \) can be rotated into \( h = \Ad_{K_1}(m) \). Thus we have completed the decomposition

\[
\therefore G = K_0 K_1 e^h K_1^\dagger
\]
4 Step-by-step summary

What we have described so far consists of the main building blocks necessary to perform the Khaneja-Glaser decomposition. Here, we will summarize all the steps one needs to take when given an arbitrary unitary $G \in SU(2^n)$.

1. Calculate its (matrix) logarithm $g = \log(G) \in g = su(2^n)$.
2. Compute the Khaneja-Glaser basis following the recurrence in diagram (4); take $g_m$, the component of $g$ on the subspace $m_n$.
3. Truncate (12) including $p$-th commutators to get $\tilde{P}_p(m)$; let $P_p(m) = \tilde{P}_p(m) - g_m$.
4. Truncate (15) including $q$-th commutator to get $Q_q(m)$, as in (16).
5. Replace $Q_q(m)$ for $k(m)$ in the expression of $P_p(m)$ obtained in 3, so that $P_p(m)$ becomes a polynomial in $m$.
6. Solve the zeros of $P_p(m)$ to get a solution $m$ to (14).
7. Use $m$ from item 6 above to calculate $K_0 = Ge^{-m}$ as in (3).
8. Compute $h_n$ following (5); order its elements $\{u_j\}$ e.g. alphabetically and define $v = \sum \pi^{-1}u_j$ to satisfy the density hypothesis of Lemma 9.
9. Use $m$ and $v$ to define $f_{v,m}(K) = \sum_{a,b,c,d} C_{ad}^c C_{bc}^d v^a (K^\dagger mK)^b$ as in (18); minimize $f$ on $K = \exp(t_n)$ to find $K_1$.
10. Calculate $h = K_1^\dagger mK_1$, and thus $H = \exp(h)$.
11. Assembling the results from items 7, 9, and 10, obtain $G = K_0 K_1 H K_1^\dagger$.
12. Repeat the above steps for $G = K_0 \hat{K}_1$ and then for $G = \hat{K}_1$, replacing $t_n \rightarrow t_{n,0}$, $m_n \rightarrow t_{n,1}$ and $h_n \rightarrow f_n$.
13. Items 11 and 12 yield the decomposition $G = K^{(1)} F^{(1)} K^{(2)} H K^{(3)} F^{(2)} K^{(4)}$, with $F^{(j)} \in \exp(j_n), H \in \exp(h_n)$ and $K^{(j)} \in SU(2^{n-1}) \otimes SU(2)$.
14. Decrease $n \rightarrow n - 1$ and iterate this process to further decompose each factor $K^{(j)} \in SU(2^{n-1}) \otimes SU(2)$ until they all reduce to a product of Cartan factors $F^{(j)}_n$ and $H^{(j)}_n$ and local unitaries in $SU(2)^{\otimes N}$.

NB.: As far as accuracy in step 6 is concerned, tasks 3 to 5 should be performed in the light of Appendix A. Namely, truncations at higher order should be tried until numerical errors are satisfactory, which will happen after a finite number of attempts.
5 Conclusions

As the advances in quantum technologies move beyond the control of one or two spins, or qubits, it is important to minimize the overall cost of processing quantum information. The Khaneja-Glaser decomposition of $SU(2^N)$ offers an upper bound for this optimization procedure given by $4^{N-1}$ multi-local $SU(2)^\otimes N$ rotations together with $4^{N-1} - 1$ purely entangling operations. The latter can be reduced, if desired, into bipartite interactions, or two-qubit gates. Moreover, in [N], Nielsen gives lower bounds for such optimization. Here we exploit the Khaneja-Glaser approach to build a constructive method for decomposing a general unitary in terms of its local unitary components. Abstract as it may seem, the decomposition problem can be cast in such a way that can be easily solved by a numerical algorithm that can be found at http://cam.qubit.org/users/jiannis/lie_solve[1].tar.gz.

Finally, one should notice that the solutions we obtained are not necessarily unique. In general, neither the zeros of the matrix polynomials, $P_p(m)$, nor the minima of the functions, $f$, are unique. In particular, viewing the minimization procedure from the equivalent point of view of the diagonalization of the matrix $m$, where $K_1$ is constructed out of the eigenvectors of $m$, there are many equivalent solutions depending on the particular ordering of the eigenvectors. Moreover, one should also take into account that the exponential function has a natural $2\pi$ periodicity and the adjoint action is $\mathbb{Z}_2$-symmetric [K-C, H-V-C]. While our approach is not concerned with the actual parametrizations of the group elements, this is an important issue which should be addressed in the future.

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A Appendix: Accuracy of BCH truncations

Here, a generalised version of Rouché’s theorem [L] is employed to show that the truncations performed in Subsection 3.1 yield a rigorous approximation for the zeros of (12).

Theorem 11 Let $\varphi, \psi : \mathbb{C}^r \to \mathbb{C}^r$ be holomorphic functions and $D \subset \mathbb{C}^r$ be an open domain such that neither $\varphi$ nor $\psi$ have zeros on $\partial D$; if

$$|\varphi(m) - \psi(m)| < |\varphi(m)| + |\psi(m)|, \quad \forall m \in \partial D,$$

then $\varphi$ and $\psi$ have the same number of zeros in $D$.

NB.: We adopt, e.g., the norm $|\varphi| = \max_{i,j} |\varphi_{ij}|$, but the argument holds for any $L^p$-norm.

Let $r = 2^{2n}$ be the number of entries of a matrix $m \in \mathfrak{su}(2^n)$, seen as a complex vector. Consider then a BCH-type series $\varphi(m)$ and its truncated version $\psi(m) = \mathcal{P}_p(m)$ containing all its terms of up to $p$ successive brackets, calling $R_p(m)$ the truncation remainder

$$\varphi(m) = \mathcal{P}_p(m) + R_p(m).$$

Suppose $\hat{m} \in \mathfrak{su}(2^n)$ is a zero of $\mathcal{P}_p(m)$; then $\varphi(m)$ will also have a zero inside the polydisc $D = \Delta_\delta(\hat{m}) \subset \mathbb{C}^r$ of radius $\delta > 0$ about $\hat{m}$ if the following (stronger) instance of (19) holds

$$|R_p(m)| < |\mathcal{P}_p(m)|, \quad \forall m \in \partial \Delta_\delta(\hat{m}).$$

In other words, $\hat{m}$ approximates at least one zero of $\varphi(m)$ with error inferior to an arbitrarily chosen $\delta$.

All we have to show is that condition (20) holds for suitably large $p$; this is a relatively straightforward consequence of the uniform convergence of the BCH series $\varphi(m) = \lim_{p \to \infty} \mathcal{P}_p(m)$, as we will now see. For any (small) $\varepsilon_0 > 0$, there is a $p_0$ such that

$$p > p_0 \Rightarrow |\mathcal{P}_p(m) - \mathcal{P}_{p_0}(m)| < \varepsilon_0, \quad \forall m,$$

hence

$$|\mathcal{P}_p(m)| > |\mathcal{P}_{p_0}(m)| - \varepsilon_0, \quad \forall m.$$

In particular, if $m_0$ is a zero of $\mathcal{P}_{p_0}(m)$, equation (21a) restricted to the boundary $\partial \Delta_\delta(m_0)$ implies that all polynomials $\mathcal{P}_p(m), p > p_0$, also have at least one zero inside $\Delta_\delta(m_0)$, by Rouché’s theorem.

On the other hand, convergence also implies $\lim_{p \to \infty} |R_p(m)| = 0$, hence, for a given $\varepsilon_1 > 0$, there is $p_1$ such that

$$p > p_1 \Rightarrow |R_p(m)| < \varepsilon_1, \quad \forall m.$$
Set $\varepsilon_1 = \min_{m \in \partial \Delta_b(m_0)} |P_p(m)| - \varepsilon_0$; assuming this is positive (if not, take a larger $p_0$ for a smaller $\varepsilon_0$), take some $p > \max\{p_0, p_1\}$ and find $m_1 \in \Delta_b(m_0)$ such that $P_p(m_1) = 0$. Then consider any smaller polydisc $\Delta_{b'}(m_1) \subset \Delta_b(m_0)$, and restrict equations (21b) and (22) to its boundary. We obtain

$$|R_p(m)| < |P_p(m)|, \quad \forall m \in \partial \Delta_{b'}(m_1),$$

thus, by Rouché’s theorem again, $\varphi(m) = P_p(m) + R_p(m)$ has a zero inside $\Delta_{b'}(m_1) \subset \Delta_b(m_0)$.

**B Appendix: Proof of Proposition 4**

In this Appendix we will develop the proof of Proposition 4, following [W, §8.3]. This argument contains most of the crucial elements to understanding the KHK decomposition in detail.

**Proof of Proposition 4.**

1. Given $m \in \mathfrak{m}$, we want to find $K_1^+ \in K$ whose action rotates $m$ onto some element $h$ of the Cartan subalgebra $\mathfrak{h}$. First, take any $v \in \mathfrak{h}$ that generates a dense 1-parameter subgroup $\exp(tv) \subset H = \exp(\mathfrak{h})$, as in Lemma 9 and define the function

$$f_{v,m} = f : K \to \mathbb{R}$$

$$K \mapsto f(K) = \langle v, \text{Ad}_K(m) \rangle$$

where $\langle a, b \rangle = \text{tr}(\text{ad}_a \text{ad}_b)$ is the Killing form on $\mathfrak{g}$. Since $f$ is continuous and $K$ is compact, $f$ admits an absolute minimum $K_1 \in K$. If we consider a local perturbation of $K_1$ by $e^{tk}$, for any $k \in \mathfrak{k}$, we have

$$0 = \left. \frac{d}{dt} \right|_{t=0} f(e^{tk}K_1) = \left. \frac{d}{dt} \right|_{t=0} \langle v, \text{Ad}_{e^{tk}} \text{Ad}_{K_1}(m) \rangle$$

$$= \left. \langle v, \left[ k, \text{Ad}_{K_1}(m) \right] \right|_{h} = \text{tr}(\text{ad}_v \text{ad}_{[k,h]})$$

$$= \text{tr}(\text{ad}_v(\text{ad}_k \text{ad}_h - \text{ad}_h \text{ad}_k)) \overset{(c.p.t.)}{=} \text{tr}(\text{ad}_{[h,v]} \text{ad}_k)$$

$$\Leftrightarrow \langle [h, v], k \rangle = 0, \forall k \in \mathfrak{k}.$$

But the Killing form is non-degenerate on $\mathfrak{k}$, so we must have $[h, v] = 0$ and thus $h \in \mathfrak{h}$, as $v$ is centralized by $\mathfrak{h}$ (2); hence, we have shown that

$$m = \text{Ad}_{K_1^+}(h), \quad h \in \mathfrak{h}.$$  

2. By 1, there exists $K \in K$ such that

$$\text{Ad}_K(v) \in \mathfrak{h}'.$$  

Now take centralizers on both sides.
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