A Sequence of Quantum Gates

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Abstract We study a sequence of quantum gates in finite-dimensional Hilbert spaces given by the normalized eigenvectors of the unitary operators. The corresponding sequence of the Hamilton operators is also given. From the Hamilton operators we construct another hierarchy of quantum gates via the Cayley transform.

1 Introduction

In the finite dimensional Hilbert space \( \mathbb{C}^n \) quantum gates are given by \( n \times n \) unitary matrices \([1, 2, 3, 4, 5]\). For example for \( n = 2 \) we have the phase gate, NOT-gate and Hadamard gate

\[
U_P = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}, \quad U_{NOT} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad U_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.
\]

For the Mach-Zehnder interferometer these quantum gates play the central role \([5]\). The Pauli spin matrices \( \sigma_x, \sigma_y, \sigma_z \) with \( \sigma_x = U_{NOT} \) are also quantum gates. In higher dimensions we have the CNOT gate, Toffoli gate, Fredkin gate

\[
U_{CNOT} = I_2 \oplus \sigma_x, \quad U_T = I_6 \oplus \sigma_x, \quad U_F = (1) \oplus \sigma_x \oplus I_5
\]

where \( \oplus \) denotes the direct sum. Teleportation in the Hilbert space \( \mathbb{C}^8 \) is provided by the unitary matrix \([5]\)

\[
U = U_8 U_7 U_6 U_5 U_4 U_3 U_2 U_1
\]

where

\[
U_1 = I_2 \otimes U_H \otimes I_2, \quad U_2 = I_2 \otimes U_{CNOT},
\]
The $n \times n$ unitary matrices form the compact Lie group $U(n)$. If $\det(U) = 1$ we have the Lie subgroup $SU(n)$. The eigenvalues of a unitary matrix are of the form $e^{i\phi_j} (j = 1, 2, \ldots, n)$, where $\phi_j \in [0, 2\pi)$, i.e. they are elements of the commutative Lie group $U(1)$.

Beside the Hilbert space $\mathbb{C}^n$ we also utilize the Hilbert space of $n \times n$ matrices over $\mathbb{C}$ with the scalar product

$$\langle A, B \rangle := \text{tr}(AB^*) .$$

This implies a norm $\|A\|^2 = \text{tr}(AA^*)$ and a distance measure (Hilbert Schmidt distance)

$$\|A - B\| = \text{tr}((A - B)(A - B)^*) = \text{tr}(AA^*) - \text{tr}(AB^*) - \text{tr}(BA^*) + \text{tr}(BB^*) .$$

In particular if we have two $n \times n$ unitary matrices, say $U$ and $V$ then

$$\|U - V\| = 2n - \text{tr}(UV^*) - \text{tr}(VU^*)$$

since $\text{tr}(UU^*) = n$, $\text{tr}(VV^*) = n$. Consider the two $n \times n$ unitary matrices $U$ and $e^{i\phi}U$. Then

$$\|U - e^{i\phi}U\| = 2n - 2n \cos \phi$$

where $\phi \in [0, 2\pi)$. The norm takes a minimum for $\phi = 0$. We consider two unitary matrices $U$ and $V$ equivalent if and only if $V = e^{i\phi}U$ for $\phi \in [0, 2\pi)$. This leads to equivalence classes. Thus for example $\sigma_y$ and $i\sigma_y$ belong to the same equivalence class. We define the distance measure

$$d(U, V) := \min_{\phi \in [0, 2\pi)} \frac{1}{\sqrt{2n}} \|e^{i\phi}U - V\| .$$

We ask the following question. Given a unitary matrix $U_0$ (not of the form $e^{i\phi}I_n$, where $I_n$ is the identity matrix). We calculate the eigenvalues and corresponding normalized eigenvectors of $U_0$. Using the normalized eigenvectors as columns we form a new unitary matrix $U_1$. This process is repeated and thus provides a sequence of unitary matrices. Now every unitary matrix $U$ can be written as $U = \exp(K)$, where $K$ is a skew-hermitian matrix. $K$ can be identified with a Hamilton operator (hermitian matrix $H$) via $K = -iH$. Thus we find the corresponding sequence of Hamilton operators $H_0, H_1, \ldots$.
From these hermitian matrices we can also form a new hierarchy of unitary matrices via the Cayley transform. The Cayley transform for an \( n \times n \) hermitian matrix \( H \) is given by

\[
V = (H - iI_n)(H + iI_n)^{-1}
\]

where \( V \) is a unitary matrix. Note that +1 cannot be an eigenvalue of the unitary matrix \( V \).

2 Sequence of Unitary Matrices

Let \( \{ e_{1,n}, \ldots, e_{n,n} \} \) denote the standard basis in \( \mathbb{C}^n \). Let \( < \) denote an ordering on \( \mathbb{C}^n \) and let \( F_n : U(n) \to U(n) \) be a function with the properties that \( F_n(U)e_{j,n} \) is an eigenvector of \( U \) for \( j = 1, 2, \ldots, n \) and the columns of \( F_n(U) \) are in order with respect to \( < \), i.e.

\[
F_n(U)e_{1,n} < F_n(U)e_{2,n} < \cdots < F_n(U)e_{j,n}.
\]

Consider a sequence \( U_0 \) (given), \( U_1, U_2, \ldots \) of unitary matrices acting on \( \mathbb{C}^n \) defined by

\[
U_{k+1} := F_n(U_k).
\]

We have the spectral decompositions

\[
U_k := F_n(U_k) \text{ diag } (e^{i\theta_{k,1}}, e^{i\theta_{k,2}}, \ldots, e^{i\theta_{k,n}}) F_n(U_k)^* \]

where \( e^{i\theta_{k,j}} \) is the \( j \)-th eigenvalue of \( U_k \) with corresponding eigenvector \( F_n(U_k)e_{j,n} \).

It follows that the corresponding Hamilton operators are

\[
H_k := F_n(U_k) \text{ diag } (-\theta_{k,1}, -\theta_{k,2}, \ldots, -\theta_{k,n}) F_n(U_k)^*
\]

and the Cayley transforms are given by

\[
V_k := -F_n(U_k) \text{ diag } \left( \frac{i + \theta_{k,1}}{i - \theta_{k,1}}, \frac{i + \theta_{k,2}}{i - \theta_{k,2}}, \ldots, \frac{i + \theta_{k,n}}{i - \theta_{k,n}} \right) F_n(U_k)^*.
\]

Suppose that the sequence converges in the sense of the Hilbert Schmidt distance. Then

\[
\lim_{k \to \infty} U_{k+1}^* U_k = \lim_{k \to \infty} \text{ diag } (e^{i\theta_{k,1}}, e^{i\theta_{k,2}}, \ldots, e^{i\theta_{k,n}}) F_n(U_k)^* = I_n
\]

from which follows

\[
\lim_{k \to \infty} U_k = \lim_{k \to \infty} F_n(U_k) = \lim_{k \to \infty} \text{ diag } (e^{i\theta_{k,1}}, e^{i\theta_{k,2}}, \ldots, e^{i\theta_{k,n}}) .
\]
Thus for convergence we must have
\[ e^{i\alpha_1}e_{1,n} \lhd e^{i\alpha_2}e_{2,n} \lhd \cdots \lhd e^{i\alpha_n}e_{n,n} \]
for all \( \alpha_1, \alpha_2, \ldots, \alpha_n \in \mathbb{R} \).

We note that even though the eigenvalues need never explicitly appear in the definition of \( F_n \), they still play a role in the convergence of the sequence.

3 Examples

To define the sequence we need
1. the ordering \( \lhd \),
2. the function \( F_n \),
3. and the initial unitary matrix \( U_0 \).

We consider a few different \( U_0 \). For each of the sequences we will use the same ordering and the same definition of \( F_n \) (dependent on \( n \)).

Example \( \lhd \).

The ordering \( \lhd \) we consider is
\[ x \prec y \Leftrightarrow \left( |e^*_{u(x,y)}x| > |e^*_{u(x,y)}y| \right) \lor \left( |e^*_{u(x,y)}x| = |e^*_{u(x,y)}y| \wedge \arg(e^*_{u(x,y)}x) < \arg(e^*_{u(x,y)}y) \right) \]
where
\[ u(x,y) := \min \{ v \in \{1, \ldots, n\} : e^*_v x \neq e^*_v y \}. \]

Example \( F_n \).

For each of the sequences we will use the same definition of \( F_n \) (dependent on \( n \)).

We choose \( F_n(U) \) as follows. Let \( \{x_1, x_2, \ldots, x_n\} \) be an orthonormal set of eigenvectors of \( U \). The eigenvectors are determined as follows. Let \( \Pi_\lambda \) denote the projection operator onto an eigenspace of \( U \) for the eigenvalue \( \lambda \). Then the Gram-Schmidt orthonormalization process applied to \( \{ \Pi_\lambda e_{1,n}, \Pi_\lambda e_{2,n}, \ldots, \Pi_\lambda e_{n,n} \} \), in that order (and discarding zero vectors), yields an orthonormal basis \( \{x_j, x_{j+1}, \ldots\} \) for that eigenspace. Define
\[ y_k := \frac{|e^*_{l(x_k),n}x_k|}{e^*_{l(x_k),n}x_k}, \quad l(x) := \min \{ v \in \{1, \ldots, n\} : e^*_v x_k \neq 0 \}. \]

Now let \( \sigma : \{1, 2, \ldots, n\} \to \{1, 2, \ldots, n\} \) be the permutation such that
\[ y_{\sigma(1)} \lhd y_{\sigma(2)} \lhd \cdots \lhd y_{\sigma(n)}. \]
Then we define

$$F_n(U) := \sum_{j=1}^{n} y_{\sigma(j)} e_{j,n}^*.$$  

**Example 1.1.**

As a first example we consider the $U_0 = U_{\text{NOT}} = \sigma_x$ gate. This is a special case of example 1.2 below. The corresponding Hamilton operator $H_0$ is

$$H_0 = -\frac{\pi}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

and the unitary operator given by the Cayley transform of $H_0$ is

$$V_0 = -\frac{1}{1 + i\pi} \begin{pmatrix} 1 & i\pi \\ i\pi & 1 \end{pmatrix}$$

with the eigenvalues $+i$ and $-i$. The eigenvalues of $U_0$ are $+1$ and $-1$ and the corresponding normalized eigenvectors are

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$  

This leads us to the Hadamard gate

$$U_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$  

The eigenvalues of $U_1$ are $+1$ and $-1$ with the corresponding normalized eigenvectors

$$\frac{1}{\sqrt{8}} \begin{pmatrix} \sqrt{4 + 2\sqrt{2}} \\ \sqrt{4 - 2\sqrt{2}} \end{pmatrix}, \quad \frac{1}{\sqrt{8}} \begin{pmatrix} \sqrt{4 - 2\sqrt{2}} \\ -\sqrt{4 + 2\sqrt{2}} \end{pmatrix}.$$  

The corresponding Hamilton operator is

$$H_1 = -\frac{\pi}{8} \begin{pmatrix} 4 - 2\sqrt{2} & -\sqrt{8} \\ -\sqrt{8} & 4 + 2\sqrt{2} \end{pmatrix}$$

with the Cayley transform of $H_1$

$$V_1 = \frac{1}{2(\pi + i)} \begin{pmatrix} -\sqrt{2}\pi - 2i & -\sqrt{2}\pi \\ -\sqrt{2}\pi & 2\pi - 2i \end{pmatrix}.$$  

At the next step we find

$$U_2 = \frac{1}{\sqrt{8}} \begin{pmatrix} \sqrt{4 + 2\sqrt{2}} & \sqrt{4 - 2\sqrt{2}} \\ \sqrt{4 - 2\sqrt{2}} & -\sqrt{4 + 2\sqrt{2}} \end{pmatrix}.$$
and \((\alpha := 2 + \sqrt{2}, \beta := 2 - \sqrt{2})\)

\[
H_2 = \frac{-\pi \beta}{8 + 4\sqrt{\alpha}} \left( \frac{1}{(2 + \sqrt{\alpha})/\sqrt{\beta}} \left( \frac{2 + \sqrt{\alpha}}{4\sqrt{\alpha} + \sqrt{2} + 6} / \beta \right) \right).
\]

The distances between the unitary matrices are

\[
\|U_0 - U_1\| = \sqrt{4 - 2\sqrt{2}}, \quad \|U_1 - U_2\| = \sqrt{4 - \sqrt{4 + 2\sqrt{2}} - \sqrt{4 - 2\sqrt{2}}}.\]

From example 1.2 we find

\[
\lim_{k \to \infty} U_k = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

**Example 1.2.**

Consider the unitary matrix

\[
U_0 = \begin{pmatrix} a & b \\ b & -a \end{pmatrix}
\]

where \(a, b \in \mathbb{R}, b \neq 0\) and \(a^2 + b^2 = 1\). If \(a > 0\) then we find

\[
U_1 = \begin{pmatrix} a' & b' \\ \text{sgn}(b)b' & -\text{sgn}(b)a' \end{pmatrix}, \quad a' := \sqrt{\frac{1 + a}{2}}, \quad b' := \sqrt{\frac{1 - a}{2}},
\]

and for \(a < 0\) we have

\[
U_1 = \begin{pmatrix} a' & b' \\ -\text{sgn}(b)b' & \text{sgn}(b)a' \end{pmatrix}, \quad a' := \sqrt{\frac{1 - a}{2}}, \quad b' := \sqrt{\frac{1 + a}{2}},
\]

while for \(a = 0\) we find that \(U_1\) is the Hadamard gate

\[
U_1 = \begin{pmatrix} a' & b' \\ b' & -a' \end{pmatrix}, \quad a' := \frac{1}{\sqrt{2}}, \quad b' := \frac{1}{\sqrt{2}}.
\]

In each case, by construction, we have \(a' > 0\) and \(b' \neq 0\). We also note that for \(a \geq 0\) we have \(a' > |a|\) and \(b' < |b|\). Since \(a', b' \in (0, 1]\) we find that sequences beginning with

\[
U_0 = \begin{pmatrix} a & b \\ b & -a \end{pmatrix}
\]

where \(a \geq 0\), converge to \(\sigma_z\).
Example 2.

As our second example we consider the Pauli matrix
\[
U_0 = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}
\]
with
\[
H_0 = -\frac{\pi}{2} \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}, \quad V_0 = -\frac{1}{1 + i\pi} \begin{pmatrix} 1 & \pi \\ -\pi & 1 \end{pmatrix}.
\]
The eigenvalues of \(U_0\) are 1 and \(-1\) and we obtain the unitary matrix
\[
U_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}.
\]
The eigenvectors of \(U_1\) are
\[
\frac{1}{\sqrt{12 + 4\sqrt{3}}} \begin{pmatrix} 2 \\ -(1 - i)(\sqrt{3} + 1) \end{pmatrix}, \quad \frac{1}{\sqrt{12 - 4\sqrt{3}}} \begin{pmatrix} 2 \\ (1 - i)(\sqrt{3} - 1) \end{pmatrix}.
\]
Thus
\[
U_2 = \frac{1}{4\sqrt{6}} \begin{pmatrix} 2\sqrt{12 - 4\sqrt{3}} & 2\sqrt{12 + 4\sqrt{3}} \\ (1 - i)\sqrt{24 + 8\sqrt{3}} & (1 - i)\sqrt{24 - 8\sqrt{3}} \end{pmatrix}.
\]

Example 3.

As last example we consider the \(3 \times 3\) matrix
\[
U_0 = \begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \end{pmatrix}.
\]
Then
\[
H_0 = -\frac{\pi}{8} \begin{pmatrix} 4 - 2\sqrt{2} & 0 & -\sqrt{8} \\ 0 & 0 & 0 \\ -\sqrt{8} & 0 & 4 + 2\sqrt{2} \end{pmatrix},
\]
\[
V_0 = \frac{1}{2(\pi + i)} \begin{pmatrix} -\sqrt{2}\pi - 2i & 0 & -\sqrt{2}\pi \\ 0 & -2(\pi + i) & 0 \\ -\sqrt{2}\pi & 0 & \sqrt{2}\pi - 2i \end{pmatrix}.
\]
The eigenvalues of \(U_0\) are +1 and \(-1\) with the corresponding normalized eigenvectors
\[
\frac{1}{\sqrt{8}} \begin{pmatrix} \sqrt{4 + 2\sqrt{2}} \\ 0 \\ \sqrt{4 - 2\sqrt{2}} \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \frac{1}{\sqrt{8}} \begin{pmatrix} \sqrt{4 - 2\sqrt{2}} \\ 0 \\ -\sqrt{4 + 2\sqrt{2}} \end{pmatrix}.
\]
For the first step in the sequence we find
\[ U_1 = \frac{1}{\sqrt{8}} \begin{pmatrix} \sqrt{4 + 2\sqrt{2}} & \sqrt{4 - 2\sqrt{2}} & 0 \\ 0 & 0 & \sqrt{8} \\ \sqrt{4 - 2\sqrt{2}} & -\sqrt{4 + 2\sqrt{2}} & 0 \end{pmatrix}. \]

4 Kronecker Product, Direct Sum and Star Product

From the 2×2 case we can easily construct these sequences for the 4×4 case given by the direct sum, Kronecker product and star product. The star product of two 2×2 matrices \( A \) and \( B \) is defined by
\[ A \star B := \begin{pmatrix} a_{11} & 0 & 0 & a_{12} \\ 0 & b_{11} & b_{12} & 0 \\ 0 & b_{21} & b_{22} & 0 \\ a_{21} & 0 & 0 & a_{22} \end{pmatrix}. \]

Note that if \( A \) and \( B \) are unitary, then \( A \star B \) is unitary. We also have \( \det(A \star B) = \det(A) \det(B) \) and \( \text{tr}(A \star B) = \text{tr}(A) + \text{tr}(B) \).

In particular if \( F \) distributes over any of these operations i.e.
\[
\begin{align*}
F_{mn}(U_A \otimes U_B) &= F_m(U_A) \otimes F_n(U_B), \\
F_{m+n}(U_A \oplus U_B) &= F_m(U_A) \oplus F_n(U_B), \\
F_{m+n}(U_A \star U_B) &= F_m(U_A) \star F_n(U_B)
\end{align*}
\]

for \( U_A \in U(m) \) and \( U_B \in U(n) \), then the sequence for \( U_0 := U_{0,0} \otimes U_{0,1} \) etc. is completely determined by the sequence for \( U_{00} \) and \( U_{01} \). In other words if \( F_{mn}(U_A \otimes U_B) = F_m(U_A) \otimes F_n(U_B) \) then we construct the sequences for \( U_{0,0} \in U(m) \) and \( U_{0,1} \in U(n) \)
\[
\begin{align*}
U_{0,0}, & \quad U_{1,0} = F_m(U_{0,0}), \quad U_{2,0} = F_m(U_{1,0}), \quad \ldots \\
U_{0,1}, & \quad U_{1,1} = F_n(U_{0,1}), \quad U_{2,1} = F_n(U_{1,1}), \quad \ldots
\end{align*}
\]

and
\[
\begin{align*}
U_0, & \quad U_1 = F_{mn}(U_0) = U_{1,0} \otimes U_{1,1}, \quad U_2 = F_{mn}(U_2) = U_{2,0} \otimes U_{2,1}, \quad \ldots
\end{align*}
\]
5 Conclusion

We defined a sequence of unitary operators on the Hilbert space $\mathbb{C}^n$. The eigenvectors of each unitary operator is used to construct the next. We found some necessary criteria for convergence.

Some open questions remain. The role of the eigenvalues in the convergence of the sequence has not been determined. Due to the implicit role of the eigenvalues we have not examined the sequence of eigenvalues and their convergence properties.

Obviously this construction can also be applied to other invertible matrices. For example the matrix ($\alpha \in \mathbb{R}$)

$$A(\alpha) = \begin{pmatrix} \cosh(\alpha) & \sinh(\alpha) \\ \sinh(\alpha) & \cosh(\alpha) \end{pmatrix}$$

is an element of the non-compact Lie group $SO(1,1)$ (Lorentz transformation). The matrix is also hermitian. Applying the construction described above we find the Hadamard gate $U_H$ which is an element of the compact Lie group $U(2)$ \[7\]. Since $A(\alpha)$ is hermitian we can apply the Cayley transform and find the quantum gate

$$U(\alpha) = \frac{1}{\cosh(\alpha)} \begin{pmatrix} -i & \sinh(\alpha) \\ \sinh(\alpha) & -i \end{pmatrix}$$

with $U(\alpha \to \infty) = \sigma_z = U_{NOT}$.

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