Exact Solutions of Holonomic Quantum Computation

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Abstract

Holonomic quantum computation is analyzed from geometrical viewpoint. We develop an optimization scheme in which an arbitrary unitary gate is implemented with a small circle in a complex projective space. Exact solutions for the Hadamard, CNOT and 2-qubit discrete Fourier transformation gates are explicitly constructed.

Key words: quantum computer, unitary gate, holonomy, isoholonomic problem, small circle, control theory

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Recently quantum computer attracts great interests from many disciplines. It is strongly desired to find a scheme to implement unitary gates in a physical system. For this purpose it is natural to consider utilizing a quantum system described by a Hamiltonian $H(\lambda)$ that depends on external parameters $\{\lambda\}$. In holonomic quantum computation (HQC) proposed by Zanardi and Rasetti \cite{1,2}, in contrast, the holonomy \cite{3} associated with adiabatic change of the parameters along a loop in a control parameter manifold is employed to implement a unitary gate. Experimental schemes to manipulate the non-Abelian holonomy have been proposed \cite{4} and their uses to realize a unitary gate are also proposed \cite{5,6,7}. For efficient achievement of holonomic computation, it is necessary to find a loop as short as possible in the control manifold. A numerical scheme to search the shortest loop is being developed in \cite{8,9} to implement

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an arbitrary gate. In this Letter we consider an ideal quantum system that has full isospectral parameters as control parameters. In the following we make exact analysis of the shortest loops that generate well-known unitary gates as holonomies. We would like to emphasize that to find an exact solution has remained unsolved [10] even for such an idealized system.

Here we take the relevant terminology from [11,12,13] to define our model. Our formulation can be compared with [14]. Suppose the Hilbert space of a quantum system is an $N$-dimensional complex space $\mathbb{C}^N$. By isospectral parameters, we mean a family of unitary transformations $g(\lambda) \in U(N)$ since the transformed Hamiltonians $H(\lambda) = g(\lambda)H_0g(\lambda)^\dagger$ has spectra independent of $\lambda$. We assume that the ground state of the reference Hamiltonian $H_0$ is $k$-fold degenerate, taking a diagonal form

$$H_0 = \text{diag}(\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_N)$$  \hfill (1)

with $\varepsilon_1 = \varepsilon_2 = \cdots = \varepsilon_k < \varepsilon_{k+j}$ ($j = 1, \ldots, N - k$). The ground state energy may be put to zero, without loss of generality, to get rid of the dynamical phase factor. We concentrate our attention on the ground states of the Hamiltonians $\{H(\lambda)\}$. Associated with the lowest energy for each $H(\lambda)$, there are $k$ orthonormal state vectors $\{|v_1(\lambda)\rangle, \ldots, |v_k(\lambda)\rangle\}$. The set of $k$ orthonormal state vectors is called a $k$-frame and the set of all the $k$-frames,

$$S_{N,k}(\mathbb{C}) = \{V \in M(N, k; \mathbb{C}) | V^\dagger V = I_k\}, \hfill (2)$$

is called the Stiefel manifold. Here $M(n, m; \mathbb{C})$ is the set of $n \times m$ complex matrices and $I_k$ is the $k \times k$ unit matrix. The $k$-frame $V = (|v_1(\lambda)\rangle, \ldots, |v_k(\lambda)\rangle)$ spans a $k$-dimensional subspace in $\mathbb{C}^N$. The set of $k$-dimensional subspaces is the Grassmann manifold

$$G_{N,k}(\mathbb{C}) = \{P \in M(N, N; \mathbb{C}) | P^2 = P, P^\dagger = P, \text{tr}P = k\}. \hfill (3)$$

The Grassmann manifold is regarded as the control manifold in the context of HQC. A projection map $\pi : S_{N,k}(\mathbb{C}) \rightarrow G_{N,k}(\mathbb{C})$ is defined as

$$\pi : V \mapsto \pi(V) = VV^\dagger. \hfill (4)$$

The group $U(k)$ acts on $S_{N,k}(\mathbb{C})$ from the right via matrix product as

$$S_{N,k}(\mathbb{C}) \times U(k) \rightarrow S_{N,k}(\mathbb{C}), \quad (V, h) \mapsto Vh. \hfill (5)$$

Note that this action satisfies $\pi(Vh) = \pi(V)$. Thus the set $(S_{N,k}(\mathbb{C}), G_{N,k}(\mathbb{C}), \pi, U(k))$ forms a principal fiber bundle with the structure group $U(k)$. The group $U(N)$ also acts on the manifolds from the left as
We now state the main problem: Given a unitary matrix $U ∈ U(k)$ find the shortest closed loop $P(t) = \pi(V(t))$ in the Grassmann manifold that yields the matrix $U$ as its associated holonomy. This problem is called the isoholonomic problem and various representations of the problem have been given by Montgomery [10]. Let us consider a familiar example, a two-dimensional sphere, to illustrate our idea to find the solution. Suppose we parallel transport a tangent vector on the unit sphere along a loop starting from and ending at the North Pole, where the parallel transport is defined with respect to the Levi-Civita connection [11]. In general, the vector is get rotated from the initial direction when it comes back to the initial point. What is the shortest loop which implements the given rotation angle $\omega$? The holonomy angle in this case is equal to the area surrounded by the loop and the problem is reduced to the so-called isoperimetric problem. The solution is well-known to be a small circle which surrounds an area of $\omega$. We use this analogy to find a small circle solution to the isoholonomic problem in HQC.

Here we describe a generalized small circle in the Grassmann manifold. Take

$$V_0 = \begin{pmatrix} I_k \\ 0 \end{pmatrix} ∈ S_{N,k}(\mathbb{C})$$

as a reference point and put $P_0 = \pi(V_0) = V_0V_0^\dagger ∈ G_{N,k}(\mathbb{C})$ as the initial point of a curve in the control manifold. Taking an antihermitian matrix $X ∈ u(N)$, we define a curve $V(t) = e^{tX}V_0$ ($0 ≤ t ≤ 1$) in $S_{N,k}(\mathbb{C})$ and define a curve $P(t) = \pi(V(t)) = e^{tX}P_0e^{-tX}$ in $G_{N,k}(\mathbb{C})$ by projecting $V(t)$ into $G_{N,k}(\mathbb{C})$. We call the curve $P(t)$ a small circle if it satisfies $P(1) = P(0)$. The connection evaluated along the curve $V(t)$ is $V(t)^*A = V(t)^{\dagger}dV(t) = V_0^\dagger XV_0 dt$, from which we obtain the holonomy associated with the loop $P(t)$ as

$$U = e^{-\int V^*A} = e^{-V_0^\dagger XV_0} ∈ U(k).$$

(10)
Note that the integrand in the exponent has no $t$-dependence and $\int_0^1 dt$ simply yields a factor unity.

Suppose that we are to implement a unitary gate $U_{gate}$ by HQC. Our task is to find a control matrix $X \in u(N)$ such that the holonomy (10) reproduces $U_{gate}$. In general, computing the holonomy $U$ for a given $X$ is easy but the inverse problem is considerably difficult; we need to find $X$ for a given $U$ while keeping the closed loop condition $P(1) = P(0)$ satisfied. Here we report some of the exact solutions of this inverse problem for several important gates.

Define the logarithmic matrix $\Omega \in u(k)$ of the gate such that $U_{gate} = e^{-\Omega}$. If the eigenvalues of $U_{gate}$ are $(e^{-i\omega_1}, e^{-i\omega_2}, \ldots, e^{-i\omega_k})$, $\Omega$ has eigenvalues $(i\omega_1, i\omega_2, \ldots, i\omega_k)$ in the range $-\pi < \omega_j \leq \pi$ and the same eigenvectors as $U_{gate}$. Then the problem (10) reduces to find $X \in u(N)$ such that

$$V_0^\dagger XV_0 = \Omega.$$ \hfill (11)

The general solution to this problem takes the form

$$X = \left( \begin{array}{cc} \Omega & W \\ -W^\dagger & Z \end{array} \right),$$ \hfill (12)

with matrices $Z \in u(N-k)$ and $W \in M(k; N-k; \mathbb{C})$. Montgomery [10] has shown that any optimal solution necessarily satisfies $Z = 0$. The remaining problem is to find the matrix $W$ that satisfies the loop condition $P(1) = P(0)$. This condition demands that $e^X$ be of the form

$$e^X = \left( \begin{array}{cc} * & 0 \\ 0 & ** \end{array} \right),$$ \hfill (13)

where $*$ and $**$ are nonvanishing matrices. The solution $W = 0$ is not acceptable since it gives a constant curve $P(t) \equiv P_0$, leaving the Hamiltonian unchanged. To seek a nontrivial solution we introduce a penalty function $p(X)$, which measures the norm of the off-diagonal-block elements of $e^X$, by

$$p(X) = \sum_{i=1}^{k} \sum_{j=k+1}^{N} |\langle i | e^X | j \rangle|^2,$$ \hfill (14)

where $\{|i\rangle\}$ being the set of orthonormal basis vectors of $\mathbb{C}^N$. Then the closed loop condition (13) is rephrased as an equivalent condition $p(X) = 0$. It is apparent that $p(X) \geq 0$ by definition and this nonnegativity is suitable for numerical
search of the zeroes of \( p(X) \). Through numerical studies we have arrived at a method to construct systematically exact solutions of the equation \( p(X) = 0 \).

Here we describe the method briefly. We restrict ourselves to the cases such that \( N = k + 1 \) for simplicity. In this case the Grassmann manifold \( G_{N,k}(\mathbb{C}) \) reduces to the complex projective space \( \mathbb{C}P^{N-1} = G_{N,N-1}(\mathbb{C}) \). A given unitary gate \( U_{\text{gate}} = e^{-\Omega} \) has a set of eigenvectors and eigenvalues \( \{(u_j, e^{-i\omega_j}) \mid u_j \in \mathbb{C}^k, \omega_j \in \mathbb{R}, -\pi < \omega_j \leq \pi, \Omega u_j = i\omega_j u_j, \langle u_j, u_l \rangle = \delta_{jl}\} \). Then choose a pair of eigenvector and eigenvalue, \( (u_\mu, \omega_\mu) \), and substitute

\[
W_{(\mu,n)} = a_{(\mu,n)} u_\mu, \quad a_{(\mu,n)} = \frac{1}{2} \sqrt{(2\pi n + \omega_\mu)(2\pi n - \omega_\mu)}
\]  

into \( W \) of \( X \) in (12) for \( n = \pm 1, \pm 2, \ldots \). Then we obtain the solution \( X_{(\mu,n)} \) that satisfies \( p(X_{(\mu,n)}) = 0 \). Therefore, the integer \( n \) generates a family of solutions and there are inequivalent families of solutions as many as different eigenvalues of \( U_{\text{gate}} \). The proof of the above method is lengthy and will be published elsewhere. In the rest of this Letter we show results exemplifying this method.

We first consider the Hadamard gate

\[
U_H = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 1 \\
1 & -1
\end{pmatrix},
\]

which has two eigenvalues and corresponding eigenvectors

\[
e^{-i\omega_1} = 1, \quad u_1 = \begin{pmatrix}
\cos \frac{\pi}{8} \\
\sin \frac{\pi}{8}
\end{pmatrix}, \quad e^{-i\omega_2} = -1, \quad u_2 = \begin{pmatrix}
-\sin \frac{\pi}{8} \\
\cos \frac{\pi}{8}
\end{pmatrix}.
\]

Hence there are two families of exact solutions of the equation \( p(X) = 0 \). We construct the first family by substituting the eigenvector and eigenvalue \( (u_1, \omega_1) \) into (15). Then the control matrix \( X \) of the first family is

\[
X_{H}^{(1)} = i\pi \begin{pmatrix}
\sin^2 \frac{\pi}{8} & -\sin \frac{\pi}{8} \cos \frac{\pi}{8} & ne^{i\theta} \cos \frac{\pi}{8} \\
-\sin \frac{\pi}{8} \cos \frac{\pi}{8} & \cos^2 \frac{\pi}{8} & ne^{i\theta} \sin \frac{\pi}{8} \\
ne^{-i\theta} \cos \frac{\pi}{8} & ne^{-i\theta} \sin \frac{\pi}{8} & 0
\end{pmatrix},
\]

where \( \theta \) is an arbitrary real number, which parametrizes unitarily equivalent solutions. The integer \( n \) counts the winding number of the loop \( P(t) =
\( e^{tX} P_0 e^{-tX} \) as seen below. The eigenvalues and eigenvectors of \( X^{(1)} \) are easily found to be

\[
x_1 = i\pi, \quad |x_1\rangle = \begin{pmatrix} -\sin \frac{\pi}{8} \\ \cos \frac{\pi}{8} \\ 0 \end{pmatrix}
\]

\[
x_2 = in\pi, \quad |x_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta} \cos \frac{\pi}{8} \\ e^{i\theta} \sin \frac{\pi}{8} \\ 1 \end{pmatrix}
\]

\[
x_3 = -in\pi, \quad |x_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta} \cos \frac{\pi}{8} \\ e^{i\theta} \sin \frac{\pi}{8} \\ -1 \end{pmatrix}
\]

(19)

Using the spectral decomposition of \( X^{(1)} \) we can calculate its exponentiation \( e^{tX} \), from which we obtain the penalty function as

\[
p(tX^{(1)}) = \sin^2(n\pi t).
\]

(20)

This clearly shows that the loop \( P(t) \) passes through the initial point \( P_0 \) \(|n| - 1 \) times in the interval \( 0 < t < 1 \). Accordingly, the number \( n \) describes how many times the loop winds as \( t \) changes from 0 to 1. It is clear that \( n = \pm 1 \) is nontrivial and optimal in this family of solutions.

The second family of solutions is constructed by substituting the second eigenvector and eigenvalue \((u_2, \omega_2)\) of \( U_H \) into (15) as

\[
X^{(2)} = i\pi \begin{pmatrix} \sin^2 \frac{\pi}{8} & -\sin \frac{\pi}{8} \cos \frac{\pi}{8} & -a_n e^{i\theta} \sin \frac{\pi}{8} \\ -\sin \frac{\pi}{8} \cos \frac{\pi}{8} & \cos^2 \frac{\pi}{8} & a_n e^{i\theta} \cos \frac{\pi}{8} \\ -a_n e^{-i\theta} \sin \frac{\pi}{8} & a_n e^{-i\theta} \cos \frac{\pi}{8} & 0 \end{pmatrix},
\]

(21)

where \( a_n = \sqrt{4n^2 - 1/2} \). The eigenvalues and corresponding eigenvectors of \( X^{(2)} \) are
\( x_1 = 0, \quad |x_1⟩ = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos \frac{\pi}{8} \\ \sin \frac{\pi}{8} \\ 0 \end{pmatrix} \)

\[
\begin{align*}
x_2 &= i\pi \left(n + \frac{1}{2}\right), \quad |x_2⟩ = \begin{pmatrix} -b_n e^{i\theta} \sin \frac{\pi}{8} \\ b_n e^{i\theta} \cos \frac{\pi}{8} \\ c_n \end{pmatrix} \\
x_3 &= i\pi \left(-n + \frac{1}{2}\right), \quad |x_3⟩ = \begin{pmatrix} -c_n e^{i\theta} \sin \frac{\pi}{8} \\ c_n e^{i\theta} \cos \frac{\pi}{8} \\ -b_n \end{pmatrix},
\end{align*}
\] (22)

where \( b_n = \sqrt{(2n + 1)/4n} \) and \( c_n = \sqrt{(2n - 1)/4n} \). This time the penalty function is evaluated as

\[
p(tX^{(2)}_H) = \left(1 - \frac{1}{4n^2}\right) \sin^2(n\pi t). \quad (23)
\]

The integer \( n \) is again interpreted as the winding number of the loop and the choice \( n = \pm 1 \) provides the optimal solution in this family.

We have shown that there are two families of exact solutions to the holonomic implementation of the Hadamard gate. To determine the shortest loop we need to calculate length of each loop employing the Fubini-Study metric of the Grassmann manifold. Consequently, the velocity of the point \( P(t) \) and therefore the length of the loop are proportional to the norm \( \|W\| \) of the matrix \( W \). These norms are evaluated to be

\[
\|W^{(1)}_H\| = \pi|n|, \quad \|W^{(2)}_H\| = \frac{\pi}{2} \sqrt{4n^2 - 1}. \quad (24)
\]

Therefore, we conclude that the simple loop solution \( n = \pm 1 \) in the second family is in fact optimal in the whole class of solutions.

Next we turn to the CNOT gate

\[
U_{\text{CNOT}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \quad (25)
\]
For this case there are two families of solutions. The first one is given by

\[
X^{(1)}_{\text{CNOT}} = i\pi \begin{pmatrix}
0 & 0 & 0 & 0 & nd_1 e^{i\theta_1} \\
0 & 0 & 0 & 0 & nd_2 e^{i\theta_2} \\
0 & 0 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} nd_3 e^{i\theta_3} \\
0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{\sqrt{2}} nd_3 e^{-i\theta_3} \\
d_1 e^{-i\theta_1} & nd_2 e^{-i\theta_2} & \frac{1}{\sqrt{2}} nd_3 e^{-i\theta_3} & \frac{1}{\sqrt{2}} nd_3 e^{i\theta_3} & 0
\end{pmatrix}
\]  
(26)

with real numbers \(\{d_1, d_2, d_3\}\) with a constraint \(d_1^2 + d_2^2 + d_3^2 = 1\). The parameters \(\{\theta_1, \theta_2, \theta_3\}\) are arbitrary real numbers. The integer \(n\) again counts the winding number of the loop. The second one is

\[
X^{(2)}_{\text{CNOT}} = i\pi \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{\sqrt{2}} a_n e^{i\theta} \\
0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{\sqrt{2}} a_n e^{i\theta} \\
0 & 0 & -\frac{1}{\sqrt{2}} a_n e^{-i\theta} & \frac{1}{\sqrt{2}} a_n e^{-i\theta} & 0
\end{pmatrix}
\]  
(27)

with \(a_n = \sqrt{4n^2 - 1/2}\). By similar comparison of the norms \(\|W_{\text{CNOT}}\|\) as in (24), we conclude that the choice \(n = \pm 1\) in the second family yields the optimal loop.

Our final example is the 2-qubit discrete Fourier transform (DFT2) gate

\[
U_{\text{DFT2}} = \frac{1}{2} \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & i & -1 & -i \\
1 & -1 & 1 & -1 \\
1 & -i & -1 & i
\end{pmatrix}
\]  
(28)

There are three families of the solutions for this gate. The first family takes
the form

\[
X_{\text{DFT}2}^{(1)} = i\pi \begin{pmatrix}
\frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & nw_1 \\
\frac{1}{4} & -\frac{1}{2} & -\frac{1}{4} & 0 & nw_2 \\
\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & nw_3 \\
\frac{1}{4} & 0 & -\frac{1}{4} & -\frac{1}{2} & nw_4 \\
nw_1^* & n w_2^* & n w_3^* & n w_4^* & 0
\end{pmatrix}
\]

(29)

with the parameters

\[
w_1 = \frac{1}{2} f_1 e^{i\theta_1} + \frac{1}{\sqrt{2}} f_2 e^{i\theta_2}, \quad w_2 = w_4 = \frac{1}{2} f_1 e^{i\theta_1},
\]

\[
w_3 = -\frac{1}{2} f_1 e^{i\theta_1} + \frac{1}{\sqrt{2}} f_2 e^{i\theta_2}
\]

(30)

with a constraint \( f_1^2 + f_2^2 = 1 \). The second family is

\[
X_{\text{DFT}2}^{(2)} = i\pi \begin{pmatrix}
\frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & 0 \\
\frac{1}{4} & -\frac{1}{2} & -\frac{1}{4} & 0 & -\frac{1}{\sqrt{2}} g_n e^{i\theta} \\
\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & 0 \\
\frac{1}{4} & 0 & -\frac{1}{4} & -\frac{1}{2} & \frac{1}{\sqrt{2}} g_n e^{i\theta} \\
0 & -\frac{1}{2} g_n e^{-i\theta} & 0 & \frac{1}{2} g_n e^{-i\theta} & 0
\end{pmatrix}
\]

(31)

with \( g_n = \sqrt{16n^2 - 1} \). The third family is

\[
X_{\text{DFT}2}^{(3)} = i\pi \begin{pmatrix}
\frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & -\frac{1}{2} a_n e^{i\theta} \\
\frac{1}{4} & -\frac{1}{2} & -\frac{1}{4} & 0 & \frac{1}{2} a_n e^{i\theta} \\
\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{2} a_n e^{i\theta} \\
\frac{1}{4} & 0 & -\frac{1}{4} & -\frac{1}{2} & \frac{1}{2} a_n e^{i\theta} \\
-\frac{1}{2} a_n e^{-i\theta} & \frac{1}{2} a_n e^{-i\theta} & \frac{1}{2} a_n e^{-i\theta} & \frac{1}{2} a_n e^{-i\theta} & 0
\end{pmatrix}
\]

(32)

with \( a_n = \sqrt{4n^2 - 1} \). The norm of the matrix \( W \) with \( n = \pm 1 \) for each family is now evaluated as

\[
\|W_{\text{DFT}2}^{(1)}\| = \pi, \quad \|W_{\text{DFT}2}^{(2)}\| = \pi \sqrt{\frac{15}{16}}, \quad \|W_{\text{DFT}2}^{(3)}\| = \pi \sqrt{\frac{3}{4}}.
\]

(33)
Thus the simple loop \((n = \pm 1)\) in the third family gives the optimal control.

In this Letter we considered an ideal system which has full isospectral parameters as control parameters. We found exact implementation of Hadamard, CNOT and DFT2 gates with a small circle in the complex projective space \(\mathbb{C}P^{N-1} = \mathbb{G}_{N,N-1}\). Implementation of larger-qubit gates is under progress and will be published elsewhere.

A realistic system has a restricted control manifold \(M\) and a control map \(f : M \rightarrow \mathbb{G}_{N,k}(\mathbb{C})\). For physical realization of HQC it is required to find an optimal loop for the holonomy in the pullback bundle \(f^*(S_{N,k}(\mathbb{C}))\) as discussed in [2,4,5,6,7]. The exact solutions we have obtained here are pulled back by \(f^*\) to be loops in \(M\). Detailed analysis of physical realization is beyond the scope of this Letter and will be published elsewhere.

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