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Quantum Gates and Hamilton Operators

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Quantum gates are described by unitary operators. We discuss the construction of Hamilton operators from the unitary operators. Different techniques are applied.

KEY WORDS: quantum gates; hamilton operators; unitary operators.

Quantum gates are described by unitary operators (Hardy and Steeb, 2001; Nielsen and Chuang, 2000; Steeb and Hardy, 2004). Here, we consider a finite dimensional Hilbert space and thus the unitary operators are described by $n \times n$ unitary matrices. A unitary matrix U is defined by $U^* = U^{-1}$. The eigenvalues of U lie on the unit circle in the complex plane; that is they may be expressed as $\exp(i\phi_k)$, $\phi_k \in [0, 2\pi)$ and $k = 1, 2, \ldots, n$. Now any unitary matrix U can be written as $U = \exp(iK)$, where K is a Hermitian matrix ($K^* = K$). In this paper, we describe several methods to construct the Hermitian matrix K from a given unitary matrix U which represents a quantum gate. Then we will relate the Hermitian matrix K to a Hamilton operator H given by $U = \exp(-iHt/\hbar)$ with $H = \hbar\omega A$, where A is a Hermitian matrix. Thus $K = -A\omega t$ and with the frequency $\omega = 1/t$ we obtain $K = -A$. We consider 1-qubit and 2-qubit gates.

The methods, we apply for the construction of the Hermitian matrix K are the sine-cosine decomposition, the Schur decomposition (calculating the eigenvalues and eigenvectors of U and then rotating the matrix into diagonal form), the Putzer method and calculating the log of a square matrix.

The most common 1-qubit gates are the NOT-gate given by

$$U_{\mathrm{NOT}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{1}$$

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the Hadamard gate given by

$$U_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{2}$$

and the phase gate

$$U_P = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}. \tag{3}$$

Other gates could be the Pauli spin matrices σ_y, σ_z which are unitary and Hermitian. The phase gate contains the σ_z-gate with $\phi = \pi$.

A useful identity for our computation is that for any $n \times n$ matrix A we have

$$\det\ \exp(A) \equiv \exp(\mathrm{tr}\ A). \tag{4}$$

Thus if $A = iK$ and $U = \exp(iK)$ we obtain

$$\det \exp(iK) \equiv \exp(i \mathrm{tr} K). \tag{5}$$

or $\det U = \exp(i\ \mathrm{tr}\ K)$. Thus if $\det U = -1$, we obtain $\mathrm{tr} K = \pi$. Another useful identity is: Let A be an $n \times n$ matrix over $\mathbf{C}$. Assume that $A^2 = cI_n$, where $c \in \mathbf{R}$. Then

$$\exp(A) = I_n \cosh(\sqrt{c}) + \frac{A}{\sqrt{c}} \sinh(\sqrt{c}). \tag{6}$$

If we apply the result to the 2×2 matrix ($z \neq 0$)

$$A = \begin{pmatrix} 0 & z \\ -\bar{z} & 0 \end{pmatrix}$$

(i.e., A is skew-Hermitian $\overline{A}^T = -A$) we obtain

$$e^B = I_2 \cos(|z|) + \frac{A}{|z|} \sin(|z|).$$

We first apply the cosine-sine decomposition. Any unitary $2^n \times 2^n$ matrix U can be decomposed as

$$U = \begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix} \begin{pmatrix} C & S \\ -S & C \end{pmatrix} \begin{pmatrix} U_3 & 0 \\ 0 & U_4 \end{pmatrix} \tag{7}$$

where U_1, U_2, U_3, U_4 are $2^{n-1} \times 2^{n-1}$ unitary matrices and C and S are the $2^{n-1} \times 2^{n-1}$ diagonal matrices

$$C = \mathrm{diag}(\cos\alpha_1, \cos\alpha_2, \ldots, \cos\alpha_{2^{n-1}}), \quad S = \mathrm{diag}(\sin\alpha_1, \sin\alpha_2, \ldots, \sin\alpha_{2^{n-1}}) \tag{8}$$

where $\alpha_{xj} \in \mathbf{R}$. Consider first the NOT-gate given by (1). We find a 2×2 Hermitian matrix K such that $U_{\text{NOT}} = \exp(iK)$. We have ($\alpha \in \mathbf{R}$.)

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} u_1 & 0 \\ 0 & u_2 \end{pmatrix} \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} u_3 & 0 \\ 0 & u_4 \end{pmatrix}$$

where $u_1, u_2, u_3, u_4 \in \mathbf{C}$ with $|u_1| = |u_2| = |u_3| = |u_4| = 1$. Matrix multiplication yields

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} u_1 u_3 \cos\alpha & u_1 u_4 \sin\alpha \\ -u_2 u_3 \sin\alpha & u_2 u_4 \cos\alpha \end{pmatrix}.$$

Since $u_1, u_2, u_3, u_4 \neq 0$ we obtain $\cos\alpha = 0$. We select the solution $\alpha = \pi/2$. Thus $\sin(\pi/2) = 1$ and $u_1 u_4 = 1, -u_1 u_3 = 1$. We select the solution $u_1 = u_4 = 1$, $u_2 = u_3 = i$. Thus we obtain the decomposition

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} i & 0 \\ 0 & 1 \end{pmatrix} = e^{iK}.$$

We set $V = \text{diag}(-i, 1)$. Consequently V is unitary. It follows that

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = V^* e^{i(K - \pi I_2/2)} V = e^{iV^*(K - \pi I_2/2)V}.$$

For $\alpha = \pi/2$ we obtain

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} \cos(\pi/2) & \sin(\pi/2) \\ -\sin(\pi/2) & \cos(\pi/2) \end{pmatrix} = \exp\left(\alpha \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\right)\Big|_{\alpha=\pi/2}.$$

Comparing the exponents yields

$$\begin{pmatrix} 0 & \pi/2 \\ -\pi/2 & 0 \end{pmatrix} = iV^*(K - \pi I_2/2)V.$$

Since K is a Hermitian matrix we can write

$$K = \begin{pmatrix} a & b \\ \bar{b} & d \end{pmatrix}, \quad a, d \in \mathbf{R}.$$

Thus we obtain $a = d = \pi/2$, $b = -\pi/2$. Finally

$$K = \begin{pmatrix} \pi/2 & -\pi/2 \\ -\pi/2 & \pi/2 \end{pmatrix} = \frac{\pi}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Next we consider the cosine-sine decomposition of the Hadamard gate given by (2). We have ($\alpha \in \mathbf{R}$)

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} u_1 & 0 \\ 0 & u_2 \end{pmatrix}\begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}\begin{pmatrix} u_3 & 0 \\ 0 & u_4 \end{pmatrix}$$

where $u_1, u_2, u_3, u_4 \in \mathbf{C}$ with $|u_1| = |u_2| = |u_3| = |u_4| = 1$. Matrix multiplication yields

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} u_1 u_3 \cos\alpha & u_1 u_4 \sin\alpha \\ -u_2 u_3 \sin\alpha & u_2 u_4 \cos\ \alpha \end{pmatrix}.$$

Thus we obtain four equations with a solution $\alpha = \pi/4$ and $u_1 = u_3 = u_4 = 1$, $u_2 = -1$. Therefore we have the decomposition

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \exp\left(\alpha \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\right)\Big|_{\alpha=\pi/4}.$$

Note that the two matrices on the right-hand side do not commute. Thus we have a Hamilton operator for each unitary matrix. We can transform the NOT-gate to the σ_z-gate using the Hadamard gate

$$U_H U_{\mathrm{NOT}} U_H^{-1} = \sigma_z.$$

In the Schur decomposition every $n \times n$ matrix A is similar to a matrix in upper triangular form, and a unitary matrix may be chosen to produce the transformation. If the matrix A is Hermitian then the matrix is in diagonal form after the unitary transformation. Let K be the Hermitian matrix

$$K = \begin{pmatrix} a & b \\ \bar{b} & a \end{pmatrix}, \qquad a \in \mathbf{R}, \quad b \in \mathbf{C}$$

with $b \neq 0$. We calculate e^{iK} using the normalized eigenvectors of K to construct a unitary matrix V such that $V^* K V$ is a diagonal matrix. Then we specify a, b such that we find the U_{NOT} gate. The eigenvalues of K are given by ($|b| = \sqrt{b\bar{b}}$)

$$\lambda_1 = a + |b|, \qquad \lambda_2 = a - |b|$$

with the corresponding normalized eigenvectors

$$\mathbf{x}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ |b|/b \end{pmatrix}, \qquad \mathbf{x}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -|b|/b \end{pmatrix}.$$

Thus the unitary matrices V, V^* which diagonalize K are

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ |b|/b & -|b|/b \end{pmatrix}, \quad V^* = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & b/|b| \\ 1 & -b/|b| \end{pmatrix}$$

with

$$D := V^* K V = \begin{pmatrix} a + |b| & 0 \\ 0 & a - |b| \end{pmatrix}.$$

From $U = e^{iK}$ it follows that $V^* U V = V^* e^{iK} V = e^{iV^* K V} = e^{iD}$. Thus,

$$e^{iD} = \begin{pmatrix} e^{i(a+|b|)} & 0 \\ 0 & e^{i(a-|b|)} \end{pmatrix}$$

and since $V^* = V^{-1}$ the unitary matrix U is given by $U = V e^{iD} V^*$. We obtain

$$U = e^{ia} \begin{pmatrix} \cos(|b|) & ib/|b| \sin(|b|) \\ i|b|/b \sin(|b|) & \cos(|b|) \end{pmatrix}.$$

If $a = \pi/2$ and $b = -\pi/2$ we find U_{NOT}.

Calculating $\exp(A)$ we can also use the Cayley–Hamilton theorem, and the Putzer method. We apply this method to find K for the Hadamard gate U_H. Using the Cayley-Hamilton theorem, we can write

$$f(A) = a_{n-1} A^{n-1} + a_{n-2} A^{n-2} + \cdots + a_2 A^2 + a_1 A + a_0 I_n \tag{9}$$

where the complex numbers $a_0, a_1, \ldots, a_{n-1}$ are determined as follows: Let

$$r(\lambda) := a_{n-1} \lambda^{n-1} + a_{n-2} \lambda^{n-2} + \cdots + a_2 \lambda^2 + a_1 \lambda + a_0$$

which is the right-hand side of (9) with A^j replaced by $\lambda^j (j = 0, 1, \ldots, n-1)$. For each distinct eigenvalue λ_j of the matrix A, we consider the equation

$$f(\lambda_j) = r(\lambda_j). \tag{10}$$

If λ_j is an eigenvalue of multiplicity k, for $k > 1$, then we consider also the following equations

$$f'(\lambda)|_{\lambda=\lambda_j} = r'(\lambda)|_{\lambda=\lambda_j}, \quad \ldots \quad , f^{(k-1)}(\lambda)|_{\lambda=\lambda_j} = r^{(k-1)}(\lambda)|_{\lambda=\lambda_j}.$$

We apply the method given above to calculate $\exp(iK)$, where the Hermitian 2×2 matrix K is given by

$$K = \begin{pmatrix} a & b \\ \overline{b} & c \end{pmatrix}, \quad a, c \in \mathbf{R}, \quad b \in \mathbf{C}.$$

Then we find the condition on a, b and c such that $e^{iK} = U_H$. The eigenvalues of iK are given by

$$\lambda_{1,2} = \frac{i(a+c)}{2} \pm \frac{1}{2}\sqrt{2ac - a^2 - c^2 - 4b\bar{b}}.$$

We set in the following

$$\Delta := \lambda_1 - \lambda_2 = \sqrt{2ac - a^2 - c^2 - 4b\bar{b}}.$$

To apply the method given above we have

$$r(\lambda) = \alpha_1\lambda + \alpha_0 = f(\lambda) = e^{\lambda}.$$

Thus we obtain the two equations

$$e^{\lambda_1} = \alpha_1\lambda_1 + \alpha_0, \qquad e^{\lambda_2} = \alpha_1\lambda_2 + \alpha_0.$$

It follows that

$$\alpha_1 = \frac{e^{\lambda_1} - e^{\lambda_2}}{\lambda_1 - \lambda_2}, \qquad \alpha_0 = \frac{e^{\lambda_2}\lambda_1 - e^{\lambda_1}\lambda_2}{\lambda_1 - \lambda_2}.$$

Thus we have the condition

$$e^{iK} = \alpha_1 iK + \alpha_0 I_2 = \begin{pmatrix} i\alpha_1 a + \alpha_0 & i\alpha_1 b \\ i\alpha_1\bar{b} & i\alpha_1 c + \alpha_0 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

We obtain the four equations

$$i\alpha_1 a + \alpha_0 = \frac{1}{\sqrt{2}}, \quad i\alpha_1 c + \alpha_0 = -\frac{1}{\sqrt{2}}, \quad i\alpha_1 b = \frac{1}{\sqrt{2}}, \quad i\alpha_1\bar{b} = \frac{1}{\sqrt{2}}.$$

From the last two equations we find that $\bar{b} = b$, i.e., b is real. From the first two equations we find $\alpha_0 = -i\alpha_1(a+c)/2$ and therefore, using the last two equations, $c = a - 2b$. Thus

$$\begin{pmatrix} i\alpha_1 a + \alpha_0 & i\alpha_1 b \\ i\alpha_1\bar{b} & i\alpha_1 c + \alpha_0 \end{pmatrix} = \begin{pmatrix} i\alpha_1 b & i\alpha_1 b \\ i\alpha_1 b & -i\alpha_1 b \end{pmatrix}.$$

From the eigenvalues of e^{iK} we find $e^{\lambda_1} - e^{\lambda_2} = 2$ and

$$\Delta = \sqrt{2ac - a^2 - c^2 - 4b^2} = 2\sqrt{2}ib.$$

Furthermore,

$$\lambda_1 = i(a-b) + \sqrt{2}ib, \qquad \lambda_2 = i(a-b) - \sqrt{2}ib.$$

Thus, we arrive at the equation

$$e^{i(a-b)+\sqrt{2}ib} - e^{i(a-b)-\sqrt{2}ib} = 2.$$

It follows that

$$ie^{i(a-b)}\sin(\sqrt{2}b) = 1$$

and, therefore,

$$i\cos(a-b)\sin(\sqrt{2}b) - \sin(a-b)\sin(\sqrt{2}b) = 1$$

with a solution

$$b = \frac{\pi}{2\sqrt{2}}, \quad a = \frac{\pi}{2}\left(3 + \frac{1}{\sqrt{2}}\right), \quad c = a - 2b = \frac{\pi}{2}\left(3 - \frac{1}{\sqrt{2}}\right)$$

Then the matrix K is given by

$$K = \frac{\pi}{2}\begin{pmatrix} 3 + 1/\sqrt{2} & 1\sqrt{2} \\ 1\sqrt{2} & 3 - 1/\sqrt{2} \end{pmatrix} = \frac{3\pi}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{\pi}{2} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

We note that the second matrix on the right-hand side is the Hadamard gate again.

Another method to find the Hermitian matrix K is to consider the principal logarithm (Steeb *et al.*. 2005) of a matrix $A \in \mathbf{C}^{n\times n}$ with no eigenvalues on $\mathbf{R}^-$ (the closed negative real axis). This logarithm is denoted by $\log A$ and is the unique matrix B such that $\exp(B) = A$ and the eigenvalues of B have imaginary parts lying strictly between $-\pi$ and π. For $A \in \mathbf{C}^{n\times n}$ with no eigenvalues on $\mathbf{R}^-$ we have the following integral representation

$$\log(s(A - I_n) + I_n) = \int_0^s (A - I_n)(t(A - I_n) + I_n)^{-1} dt. \qquad (11)$$

Thus with $s = 1$, we obtain

$$\log A = \int_0^1 (A - I_n)(t(A - I_n) + I_n)^{-1} dt \qquad (12)$$

where I_n is the $n \times n$ identity matrix. Note that, this method cannot be applied to U_{NOT} and U_H since they admit the eigenvalue -1. As an example, consider the unitary operator

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

We calculate $\log U$ to find i_K given by $U = \exp(i_K)$. We set $B = i_K$ in the following. The eigenvalues of U are given by

$$\lambda_1 = \frac{1}{\sqrt{2}}(1 + i), \quad \lambda_2 = \frac{1}{\sqrt{2}}(1 - i).$$

Thus the condition to apply the Eq. (12) is satisfied. We consider first the general case $U = (u_{jk})$ and then simplify to $u_{11} = u_{22} = 1/\sqrt{2}$ and $u_{21} = -u_{12} = 1/\sqrt{2}$.

We obtain

$$t(U - I_2) + I_2 = \begin{pmatrix} 1 + t(u_{11} - 1) & tu_{12} \\ tu_{21} & 1 + t(u_{22} - 1) \end{pmatrix}$$

and

$$d(t) := \det(t(U - I_2) + I_2) = 1 + t(-2 + \mathrm{tr}U) + t^2(1 - \mathrm{tr}U + \det U).$$

Let $X \equiv \det U - \mathrm{tr}U + 1$. Then

$$(U - I_2)(t(U - I_2) + I_2)^{-1} = \frac{1}{d(t)} \begin{pmatrix} tX + u_{11} - 1 & u_{12} \\ u_{21} & tX + u_{22} - 1 \end{pmatrix}.$$

With $u_{11} = u_{22} = 1/\sqrt{2}$, $u_{21} = -u_{12} = 1/\sqrt{2}$ we obtain

$$d(t) = 1 + t(-2 + \sqrt{2}) + t^2(2 - \sqrt{2})$$

and $X = 2 - \sqrt{2}$. Thus the matrix takes the form

$$\frac{1}{d(t)} \begin{pmatrix} t(2 - \sqrt{2}) + 1/\sqrt{2} - 1 & -1\sqrt{2} \\ 1\sqrt{2} & t(2 - \sqrt{2}) + 1/\sqrt{2} - 1 \end{pmatrix}.$$

Since

$$\int_0^1 \frac{1}{d(t)} dt = \frac{2}{\sqrt{2}} \left| \arctan\left(\frac{2(2 - \sqrt{2})t + \sqrt{2} - 2}{\sqrt{2}} \right) \right|_0^1 = \sqrt{2}\frac{\pi}{4}$$

and

$$\int_0^1 \frac{t}{d(t)} dt = \frac{1}{\sqrt{2}} \frac{\pi}{4}$$

we obtain

$$K = \begin{pmatrix} 0 & i\pi/4 \\ -\pi/4 & 0 \end{pmatrix}.$$

The unitary matrices are elements of the Lie group $U(n)$. The corresponding Lie algebra are the matrices with the condition $X^* = -X$. An important subgroup of $U(n)$ is the Lie group $SU(n)$ with the condition that $\det U = 1$. Note that the Hadamard gate and the NOT-gate are not elements of the Lie algebra $SU(2)$ since the determinants of these unitary matrices are -1. The corresponding Lie algebra $SU(n)$ of the Lie group $SU(n)$ are the $n \times n$ matrices given by $X^* = -X$ and $\mathrm{tr}X = 0$.

Let $\sigma_1, \sigma_2, \sigma_3$ be the Pauli spin matrices. Then any unitary matrix in $U(2)$ can be represented by

$$U(\alpha, \beta, \gamma, \delta) = e^{i\alpha I_2} e^{-i\beta\sigma_3/2} e^{-i\gamma\sigma_2/2} e^{-i\delta\sigma_3/2}$$

where $0 \le \alpha < 2\pi, 0 \le \beta < 2\pi, 0 \le \gamma \le \pi$ and $0 \le \delta < 2\pi$. Then

$$U(\alpha,\beta,\gamma,\delta) = \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{i\alpha} \end{pmatrix} \begin{pmatrix} e^{-i\beta/2} & 0 \\ 0 & e^{i\beta/2} \end{pmatrix} \begin{pmatrix} \cos(\gamma/2) & -\sin(\gamma/2) \\ \sin(\gamma/2) & \cos(\gamma/2) \end{pmatrix} \begin{pmatrix} e^{-i\delta/2} & 0 \\ 0 & e^{i\delta/2} \end{pmatrix}.$$

Obviously this is the sine-cosine decomposition described above. Each of the four matrices on the right-hand side are unitary and $e^{i\alpha}$ is unitary. Thus U is unitary and $\det(U) = e^{2i\alpha}$. We obtain the special case of the Lie group $SU(2)$ if $\alpha = 0$. The most important two-qubit gates are the controlled-NOT-gate

$$U_{\text{CNOT}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

and the swap-gate

$$U_{\text{SWAP}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Both gates can be written as direct sums, i.e.

$$U_{\text{CNOT}} = I_2 \oplus U_{\text{NOT}}, \quad U_{\text{SWAP}} = \oplus U_{\text{NOT}} \oplus 1.$$

Thus, we can apply the result given above for the construction of the Hermitian matrix K. The same applies for the Fredkin gate and the Toffoli gate which are three qubit gates.

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