Sixth-order robust gates for quantum control

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Composite pulse sequences designed for nuclear magnetic resonance experiments are currently being applied in many quantum information processing technologies. We present an analysis of a family of composite pulse sequences used to address systematic pulse-length errors in the execution of quantum gates. It has been demonstrated by Cummins *et al.* [Phys. Rev. A **67**, 042308 (2003)] that for this family of composite pulse sequences, the fidelity of the resulting unitary operation compared with the ideal unitary operation is $1-C\epsilon^6$, where ϵ is the fractional error in the length of the pulse. We derive an exact expression for the sixth-order coefficient C and from this deduce conditions under which this sixth-order dependence is observed. We also present pulse sequences which achieve the same fidelity.

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Systematic errors are always present in any experimental setup. They are best dealt with by stripping down the experiment and finding them one by one. Even after doing this, there is still the possibility of not eliminating them all. Quantum computers operate universally with single-qubit rotations and a controlled-NOT gate between two qubits [1]. Recently, Cummins *et al.* [2] have addressed the issue of systematic errors in single-qubit gates due to pulse-length and off-resonance effects. Off-resonance errors result in a rotation around an axis tilted with respect to the desired rotation axis. Pulse-length errors result in a rotation through an angle which falls short of, or goes beyond, the desired angle of rotation, due to an error in the timing of the pulse. Composite pulse techniques have received much attention as a means to correct systematic errors [2,3,5,6], with [7] a significant recent development. First developed in the NMR setting, these techniques can be very useful in reducing the effects of systematic errors in a wide range of quantum computer proposals. They have been identified as such in numerous quantum information processing technologies such as trapped-ion technologies [8–10], in rare-earth-doped crystal technology [11,12], in superconducting technologies [13,14], and in solid-state quantum information processing technologies [15,16]. The BB1 composite pulse sequence, first developed by Wimperis [3], deals with pulse-length errors in a remarkably efficient manner. It is shown in [2] that the composite pulse sequence has a fidelity of $1-C\epsilon^6$ when compared to the exact qubit rotation. In this article we examine the origin of this sixth-order dependence on the error in the fidelity of the gate and deduce some constraints on the possible composite pulse sequences one may use. We also suggest some other pulse sequences whose fidelities display this sixth-order dependence.

A general single-qubit rotation around an axis in the XY plane of the Bloch sphere can be written as

$$R(\theta,\alpha) = \exp\left(-i\frac{\theta}{2}(X\cos\alpha + Y\sin\alpha)\right), \qquad (1)$$

where θ is the angle through which the qubit is rotated and α is the angle of the axis in the XY plane of the Bloch sphere, $\alpha=0$ being the X axis. We now consider the effects of a systematic error, such as a pulse-length-type error. Using a superscript to denote pulse sequences suffering this type of error, where all rotation angles are altered by the fractional error ϵ, the above one single-qubit rotation becomes

$$R^{\epsilon}(\theta,\alpha) = \exp\left(-i\frac{\theta(1+\epsilon)}{2}(X\cos\alpha + Y\sin\alpha)\right), \qquad (2)$$

where ϵ is the fractional error. In order to compare the error-prone unitary transformation $[V=R^{\epsilon}(\theta,\alpha)]$ with the error-free unitary transformation $[U=R(\theta,\alpha)]$, the following fidelity definition is used:

$$\mathcal{F} = \frac{|\mathrm{Tr}(VU^{\dagger})|}{\mathrm{Tr}(UU^{\dagger})}. \qquad (3)$$

The composite pulse sequence as presented by Wimperis takes the form

$$W^{\epsilon}(\phi_1,\phi_2) = R^{\epsilon}(\pi,\phi_1)R^{\epsilon}(2\pi,\phi_2)R^{\epsilon}(\pi,\phi_1), \qquad (4)$$

so that when $\epsilon=0$, W is simply the identity. When this pulse sequence is carried out before or after the desired single-qubit rotation, the fidelity of the resulting composite pulse sequence is $1-C\epsilon^6$. In fact, $W^{\epsilon}(\phi_1,\phi_2)$ may be placed at any point during a rotation around a given axis—i.e.,

$$R^{\epsilon}(a\theta,\alpha) \leftrightarrow W^{\epsilon}(\phi_1,\phi_2) \leftrightarrow R^{\epsilon}((1-a)\theta,\alpha),$$

with $a\in[0,1]$, and the same fidelity is observed.

In order to show where this comes from, we need to examine the definition of the fidelity. First we let

$$A = X\cos\phi_1 + Y\sin\phi_1,$$

$$B = X\cos\phi_2 + Y\sin\phi_2,$$

$$C = X\cos\alpha + Y\sin\alpha$$

be three axes in the XY plane of the Bloch sphere. C is the axis around which we wish to perform the rotation and A and B are the two axes in $W^{\epsilon}(\phi_1,\phi_2)$. The fidelity is

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$$\mathcal{F} = \frac{1}{2}\left|\mathrm{Tr}(e^{-i[\theta(1+\epsilon)/2]C}W^{\epsilon}(\phi_1,\phi_2)e^{i(\theta/2)C})\right|$$
$$= \frac{1}{2}\left|\mathrm{Tr}(e^{-i(\theta/2)C}e^{-i(\epsilon\theta/2)C}W^{\epsilon}(\phi_1,\phi_2)e^{i(\theta/2)C})\right|$$
$$= \frac{1}{2}\left|\mathrm{Tr}(e^{-i(\epsilon\theta/4)C}W^{\epsilon}(\phi_1,\phi_2)e^{-i(\epsilon\theta/4)C})\right|.$$

The last step is due to the trace property of invariance under cyclic permutations. $W^{\epsilon}(\phi_1,\phi_2)$ can be simplified to

$$W^{\epsilon}(\phi_1,\phi_2) = e^{-i[\pi(1+\epsilon)/2]A}e^{[-i(1+\epsilon)\pi B]}e^{-i[\pi(1+\epsilon)/2]A}$$
$$= e^{-i(\epsilon\pi/2)A}(-iA)e^{-i\epsilon\pi B}(-\mathbb{I})(-iA)e^{-i(\epsilon\pi/2)A}$$
$$= e^{-i(\epsilon\pi/2)A}e^{-i\epsilon\pi ABA}e^{-i(\epsilon\pi/2)A},$$

since $A^2=\mathbb{I}=B^2$. $ABA=X\cos(2\phi_1-\phi_2)+Y\sin(2\phi_1-\phi_2)$ is another axis in the XY plane of the Bloch sphere. The fidelity now takes on a more symmetric look when written as

$$\mathcal{F} = \frac{1}{2}\left|\mathrm{Tr}(e^{-i(\epsilon\theta/4)C}e^{-i(\epsilon\pi/2)A}e^{-i\epsilon\pi ABA}e^{-i(\epsilon\pi/2)A}e^{-i(\epsilon\theta/4)C})\right|.$$

This form for the fidelity turns out to be the reason the BB1 sequence performs so well. The symmetric Baker-Campbell-Hausdorff formula is stated and derived in [4] as

$$e^{tR/2}e^{tS}e^{tR/2} = e^{F_{sbch}(t;R,S)}, \tag{5}$$

with,

$$F_{sbch}(t;R,S) = t(R+S) - \frac{1}{24}t^3[R+2S,[R,S]] + \mathcal{O}(t^5).$$

If we define $Q=-i\theta C$, $R=-i\pi A$, and $S=-i\pi ABA$ to simplify the notation, we can reduce the expression in the trace above by twice applying the symmetric BCH formula, yielding

$$\mathcal{F} = \frac{1}{2}\left|\mathrm{Tr}(e^{-i(\epsilon\theta/4)C}e^{-i(\epsilon\pi/2)A}e^{-i\epsilon\pi ABA}e^{-i(\epsilon\pi/2)A}e^{-i(\epsilon\theta/4)C})\right|$$
$$= \frac{1}{2}\left|\mathrm{Tr}(e^{(\epsilon/4)Q}e^{(\epsilon/2)R}e^{\epsilon S}e^{(\epsilon/2)R}e^{(\epsilon/4)Q})\right|$$
$$= \frac{1}{2}\left|\mathrm{Tr}(e^{(\epsilon/4)Q}e^{(\epsilon/2)((2/\epsilon)F_{sbch}(\epsilon;R,S))}e^{(\epsilon/4)Q})\right|$$
$$= \frac{1}{2}\left|\mathrm{Tr}(e^{F_{sbch}((\epsilon/2);Q,(2/\epsilon)F_{sbch}(\epsilon;R,S))})\right|.$$

Letting $P(\epsilon)=F_{sbch}(\epsilon/2;Q,(2/\epsilon)F_{sbch}(\epsilon;R,S))$, we find that

$$P(\epsilon) = \epsilon\left(\frac{1}{2}Q+R+S\right) + \epsilon^3\left(-\frac{1}{24}[R+2S,[R,S]] - \frac{1}{192}[Q,[Q,2(R+S)]] - \frac{1}{24}[R+S,[Q,R+S]]\right) + \mathcal{O}(\epsilon^5).$$

Given that all the operators in $P(\epsilon)$ are proportional to the Pauli operators, $\mathrm{Tr}[P(\epsilon)]=0$, and, therefore,

$$\mathrm{Tr}(e^{P(\epsilon)}) = \mathrm{Tr}(\mathbb{I}) + \mathrm{Tr}\left\{\frac{1}{2}[P(\epsilon)]^2\right\} \Rightarrow \mathcal{F} = 1 + \frac{1}{4}\mathrm{Tr}\{[P(\epsilon)]^2\} + \cdots.$$

For the next step we let the first derivative of the total pulse sequence with respect to the error ϵ equal the zero matrix at $\epsilon=0$ to find a relation between the rotation axis C and the axes A and B.

The total pulse sequence is given by

$$BB(\epsilon) = e^{[(1+\epsilon)/2]Q}e^{[(1+\epsilon)/2]R}e^{(1+\epsilon)S}e^{[(1+\epsilon)/2]R},$$

so that

$$\left.\frac{dBB(\epsilon)}{d\epsilon}\right|_{\epsilon=0} = 0$$

$\Rightarrow \frac{1}{2}Q+(R+S)=0.$

This allows us to simplify the expression for $P(\epsilon)$,

$$P(\epsilon) = \epsilon^3\left(-\frac{1}{24}[R+2S,[R,S]] + \frac{1}{192}[Q,[Q,Q]] - \frac{1}{96}[Q,[Q,Q]]\right) + \mathcal{O}(\epsilon^5)$$
$$= -\frac{1}{24}[R+2S,[R,S]]\epsilon^3 + \mathcal{O}(\epsilon^5).$$

Next we expand the commutator $[R+2S,[R,S]]$ to get

$$([R+2S,[R,S]])^2 = -\pi^6([A+2ABA,[A,ABA]])^2$$
$$= -\pi^6(40\mathbb{I} + 8(AB+BA) - 20(ABAB + BABA) - 8(ABABAB + BABABA))$$
$$= -\pi^6[40 + 16\cos(\phi_2-\phi_1) - 40\cos 2(\phi_2 - \phi_1) - 16\cos 3(\phi_2-\phi_1)]\mathbb{I},$$

since $AB=\exp[i(\phi_2-\phi_1)Z]$.

Therefore, we can write the fidelity as

$$\mathcal{F} = 1 + \frac{1}{2304}\epsilon^6\mathrm{Tr}\{([R+2S,[R,S]])^2\} + \mathcal{O}(\epsilon^8)$$
$$= 1 - \frac{\epsilon^6\pi^6}{144}[5 + 2\cos(\phi_2-\phi_1) - 5\cos 2(\phi_2-\phi_1) - 2\cos 3(\phi_2-\phi_1)] + \mathcal{O}(\epsilon^8)$$

Finally, by writing A, B, and C in terms of the Pauli operators, X and Y, the condition $\frac{1}{2}Q+R+S=0$ implies

$$\cos\phi_1 + \cos(2\phi_1-\phi_2) = -\frac{\theta}{2\pi}\cos\alpha, \tag{6}$$

$$\sin\phi_1 + \sin(2\phi_1-\phi_2) = -\frac{\theta}{2\pi}\sin\alpha, \tag{7}$$

and these two equations lead to the following rule for choosing ϕ_1 and ϕ_2 given θ and α:

$$\phi_1 = \alpha - \frac{1}{2}\arccos\left(\frac{\theta^2}{8\pi^2} - 1\right), \tag{8}$$

$$\phi_2 = 3\phi_1 - 2\alpha. \tag{9}$$

To give a concrete example, we choose $\alpha=0$, $\theta=\pi$ corresponding to a 180° rotation about the X axis of the Bloch sphere. This gives us

$$\phi_1 = \arccos\left(-\frac{1}{4}\right),$$

$$\phi_2 = 3\phi_1,$$

and a fidelity

$$\mathcal{F} = 1 - \frac{5}{1024}\pi^6\epsilon^6 + \mathcal{O}(\epsilon^8),$$

which agrees with the findings in [5].

It can be readily seen that if n copies of $W^\epsilon(\phi_1,\phi_2)$ are carried out one after the other, then the condition that $dBB/d\epsilon|_{\epsilon=0}=0$,

$$\Rightarrow \frac{1}{2}Q + n(R+S) = 0,$$

and also $P(\epsilon)=\epsilon\left[\frac{1}{2}Q+n(R+S)\right]+\mathcal{O}(\epsilon^3)$. This defines the general Wn pulses, introduced in [2] as

$$\phi_1 = \alpha - \frac{1}{2}\arccos\left(\frac{\theta^2}{8n^2\pi^2} - 1\right),$$

$$\phi_2 = 3\phi_1 - 2\alpha,$$

and shows that they all perform with a fidelity $1-\mathcal{O}(\epsilon^6)$. We note that it is only necessary to show the sequence works for one angle—say, $\alpha=0$—with other axes accounted for by phase shifting each pulse by some angle α.

Other sixth-order pulse sequences. We now look at whether there are other types of pulse sequences similar to those above which can achieve the same fidelity. The most general three-pulse sequence is

$$W^\epsilon(\phi_1,\phi_2,\phi_3) = R^\epsilon(\zeta,\phi_1)R^\epsilon(\eta,\phi_2)R^\epsilon(\gamma,\phi_3).$$

As before we define axes A, B, and C in the XY plane of the Bloch sphere by the angles ϕ_1, ϕ_2, and α, respectively. The first condition to satisfy is that the pulse sequence must be symmetric so that it can be reduced using the symmetric BCH formula, thus keeping the fidelity for the total pulse sequence sixth order in ϵ. This means we need $\zeta=\gamma$ and $\phi_1=\phi_3$. Also to satisfy the condition that $W^\epsilon(\phi_1,\phi_2)=\mathbb{I}$, we require

$$2\gamma + \eta = 4m\pi, \quad m = 1,2,\ldots\ . \tag{10}$$

We are then left with sequences of the form

$$W^\epsilon(\phi_1,\phi_2) = R^\epsilon(\gamma,\phi_1)R^\epsilon(2(2m\pi-\gamma),\phi_2)R^\epsilon(\gamma,\phi_1).$$

Finally, we let the first derivative of the total pulse sequence with respect to ϵ equal zero at $\epsilon=0$ and obtain the constraint

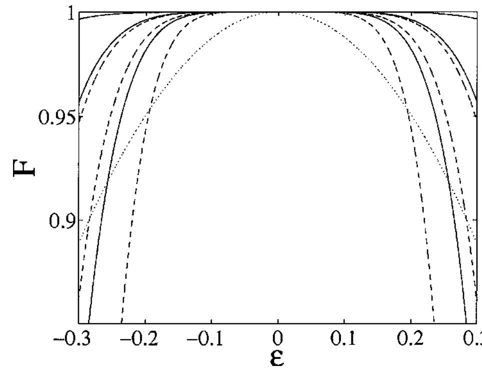

FIG. 1. Fidelity of composite pulse sequences for (a) the three-pulse sequences (solid) and (b) the five-pulse sequences (dashed), with coefficients for the sixth-order term of the fidelity given in Table I. The fidelity of the single error-prone pulse is also shown (dotted line).

$$0 = \frac{\theta}{2}C + \gamma A + (2m\pi - \gamma)e^{-i(\gamma/2)A}Be^{i(\gamma/2)A}$$
$$\Rightarrow \sin\gamma\sin(\phi_2-\phi_1)$$
$$= 0,$$

giving $\gamma=p\pi$, $\eta=2q\pi$ with $p+q=2m$ and $p,q=1,2,\ldots$. The most general three-pulse sequences are $R^\epsilon(p\pi,\phi_1)$ $R^\epsilon(2q\pi,\phi_2)$ $R^\epsilon(p\pi,\phi_1)$ with ϕ_1, ϕ_2 determined from

$$\frac{\theta}{2\pi}C + pA + qA^pBA^p = 0.$$

For even p,

$$p\sin\phi_1 + q\sin\phi_2 = \frac{-\theta}{2\pi}\sin(\alpha),$$

$$p\cos\phi_1 + q\cos\phi_2 = \frac{-\theta}{2\pi}\cos(\alpha),$$

meaning that either $\phi_1=\alpha-\arcsin[(q/p)\sin(\phi_2-\alpha)]$ or $\phi_2=\alpha+\arcsin[(p/q)\sin(\alpha-\phi_1)]$. Hence $p/q\leqslant 1$ since $-1\leqslant(p/q)\sin(\alpha-\phi_1)\leqslant 1\ \forall\alpha$. Similarly, $q/p\leqslant 1$—i.e., $q=p$ and $\phi_1+\phi_2=2\alpha$. The same is true for odd p except $3\phi_1-\phi_2=2\alpha$.

We are left with the general three-pulse sequences

$$W_m^\epsilon(\phi_1,\phi_2) = R^\epsilon(m\pi,\phi_1)R^\epsilon(2m\pi,\phi_2)R^\epsilon(m\pi,\phi_1).$$

The Wn family is obtained from repeating the $W_1^\epsilon(\phi_1,\phi_2)$ sequence n times. When $m=2$, the "passband" Wimperis sequence [3,6] is recovered. Moreover, these are the only three-pulse sequences which achieve this sixth-order fidelity. The first three of these composite sequences are plotted in Fig. 1. In other three-pulse sequences, the first-order term in the fidelity always disappears due to the fact that by collapsing the entire pulse sequence using the BCH formula to

$$BB(\epsilon) = e^{-i\theta(1+\epsilon)/2}W^\epsilon(\phi_1,\phi_2) = e^{P_1(\epsilon)},$$

the fidelity is $\mathcal{F}=1+\frac{1}{4}\mathrm{Tr}\{[P_1(\epsilon)]^2\}+\cdots$ and the leading term in $P_1(\epsilon)$ is $\mathcal{O}(\epsilon)$.

So there are no pulse sequences constructed from three pulses which achieve this sixth-order dependence for the fidelity for the resulting rotation other than the above family of pulse sequences. There is, however, the option of creating a five-pulse sequence by introducing a third axis. The general form for such a sequence is

$$R^{\epsilon}(\zeta,\phi_1)R^{\epsilon}(\eta,\phi_2)R^{\epsilon}(\gamma,\phi_3)R^{\epsilon}(\mu,\phi_4)R^{\epsilon}(\nu,\phi_5).$$

We define the axes A, B, C, and D in the XY plane of the Bloch sphere by the angles ϕ_1, ϕ_2, ϕ_3, and α, respectively. D is now the axis around which we wish to rotate by θ. Again, we will require $\zeta=\nu$, $\eta=\mu$ and $\phi_1=\phi_5$, $\phi_2=\phi_4$ in order to keep symmetry in the sequence and hence the sixth-order fidelity dependence. In order that the pulse sequence be the identity when $\epsilon=0$, we need to satisfy $2\zeta+2\eta+\gamma=4m\pi$, $m=1,2,\ldots$. The first derivative of the total pulse sequence is zero at $\epsilon=0$ when $\zeta=p\pi$, $\eta=q\pi$ for positive integers p and q. We arrive at general five-pulse sequences of the form

$$W^{\epsilon}_{pqr}=R^{\epsilon}(p\pi,\phi_1)R^{\epsilon}(q\pi,\phi_2)R^{\epsilon}(2r\pi,\phi_3)\times R^{\epsilon}(q\pi,\phi_2)R^{\epsilon}(p\pi,\phi_1),$$

where $p+q+r=2m$ and ϕ_1, ϕ_2, and ϕ_3 are determined from

$$\frac{\theta}{2\pi}D + pA + qA^pBA^p + rA^pB^qCB^qA^p = 0. \qquad (11)$$

One solution to find five-pulse sequences is at $p=q=r$, analogously to the three-pulse sequence case. In this case $p=2m/3$ and, as it must remain an integer, m must be a multiple of 3 with now $p=2,4,6\ldots$. Equation (11) is satisfied for $p=2$ when $\phi_1=0$, $\phi_2=\arccos[(\theta-4\pi)/8\pi]$ and $\phi_3=-\phi_2$ for a rotation around the X axis. However, while the fidelity displays a sixth-order dependence on the fractional error, the coefficient of the leading term, shown in Table I is so much larger that the sequence is only better than the error-prone pulse for small values of ϵ (~ 0.2). The situation does not improve for higher values of p and so these sequences are of no real practical use.

TABLE I. The coefficients C in the fidelity expansion $F=1-C\epsilon^6$ for six composite pulse sequences which compensate for an error-prone π pulse around the X axis.

Three-pulse	C	Five-pulse	C
W^{ϵ}_1(BB1)	4.7	W^{ϵ}_{121}	72.3
W^{ϵ}_2(PB1)	59.1	W^{ϵ}_{112}	190.6
W^{ϵ}_3	283.4	W^{ϵ}_{222}	877.8

Another five-pulse sequence which achieves the same sixth-order dependence for the fidelity is found by setting $p=1$, $q=2$, and $r=1$. Equation (11) is now satisfied when $\phi_1=\arccos[(\theta-4\pi)/4\pi]$, $\phi_2=2\phi_1$, and $\phi_3=3\phi_1$ for a rotation around the X axis ($\alpha=\pi$). As before, other axes may be accounted for by phase shifting each pulse by the appropriate angle. The fidelity of this sequence is much better than the previous five-pulse sequence and is quite close to that of the PB1 sequence as seen in Fig. 1. Other sequences can be constructed by varying p, q, and r.

Conclusion. We have presented an analysis of the composite pulse sequences presented by Jones and co-workers [2,6] to combat systematic pulse-length errors in single-qubit rotations. We have derived an explicit form for the fidelity and shown how it is possible to set up other three-pulse sequences which achieve the same order error dependence for the fidelity. We have shown that there are also five-pulse sequences which do achieve the sixth-order dependence of the fidelity on the error.

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