Tackling Systematic Errors in Quantum Logic Gates with Composite Rotations

Holly K. Cummins, Gavin Llewellyn, and Jonathan A. Jones
Centre for Quantum Computation, Clarendon Laboratory,
University of Oxford, Parks Road, OX1 3PU, United Kingdom
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We describe the use of composite rotations to combat systematic errors in single qubit quantum logic gates and discuss three families of composite rotations which can be used to correct off-resonance and pulse length errors. Although developed and described within the context of NMR quantum computing these sequences should be applicable to any implementation of quantum computation.

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I. INTRODUCTION

Quantum computers [1] are information processing devices that use quantum mechanical effects to implement algorithms which are not accessible to classical computers, and thus to tackle otherwise intractable problems [2]. Quantum computers are extremely vulnerable to the effects of errors, and considerable effort has been expended on alleviating the effects of random errors arising from decoherence processes [3, 4, 5]. It is, however, also important to consider the effects of systematic errors, which arise from reproducible imperfections in the apparatus used to implement quantum computations.

The effects of systematic errors are clearly visible in nuclear magnetic resonance (NMR) experiments [6] which have been used to implement small quantum computers [7, 8, 9, 10, 11, 12]. Implementing complex quantum algorithms require some sort of spin–spin interaction, which in NMR is provided by the scalar spin–spin coupling (J coupling) interaction. While this does not have quite the form needed for standard two qubit gates, it can be easily sculpted into the desired form by combining free evolution under the background Hamiltonian (which includes spin–spin coupling terms) with the application of single qubit gates [13].

NMR quantum computers are implemented [11] using the two spin states of spin-1/2 atomic nuclei in a magnetic field as the qubits. Transitions between these states, and thus single qubit gates, are achieved by the application of radio frequency (RF) pulses. Two qubit gates require some sort of spin–spin interaction, which in NMR is provided by the scalar spin–spin coupling (J coupling) interaction. While this does not have quite the form needed for standard two qubit gates, it can be easily sculpted into the desired form by combining free evolution under the background Hamiltonian (which includes spin–spin coupling terms) with the application of single qubit gates [14].

As single qubit gates involve the application of external fields they are vulnerable to systematic errors in these fields. In the ideal case, the application of a RF field in resonance with the corresponding transition with relative phase \( \phi \) (in the rotating frame [15]) will drive the Bloch vector through some angle about an axis orthogonal to the \( z \)-axis and at an angle \( \beta \) to the \( x \)-axis. The rotation angle, \( \theta \), depends on the rotation rate induced by the RF field, usually written \( \nu \), and the duration of the pulse, \( \tau \). In practice the RF field is not ideal, and this leads to two important types of systematic errors, pulse length errors and off-resonance effects [15].

Pulse length errors occur when the duration of the RF pulse is set incorrectly, or (equivalently) when the RF field strength deviates from its nominal value, so that the rotation angle achieved deviates from its theoretical value. Within NMR this effect is most commonly observed as a result of spatial inhomogeneity in the applied RF field, so that it is impossible for all the spins within a macroscopic sample to experience the same rotation angle. Off-resonance effects arise when the RF field is not quite in resonance with the relevant transition, so that the rotation occurs around some tilted axis.

Composite pulses [6, 14, 15] are widely used in NMR...
to minimize the sensitivity of the system to these errors by replacing simple rotations with composite rotations which are less susceptible to such effects. However, conventional composite pulse sequences are rarely appropriate for quantum computation because they usually incorporate assumptions about the initial state of the spins. Such starting states are not known for pulses in the middle of complex quantum computations, and it is therefore necessary to use fully-compensating (type A) composite pulse sequences [13], which work for any initial state. Composite pulses of this kind, which do not offer quite the same degree of compensation as is found with more conventional sequences, are of little use in conventional NMR, and have received relatively little study. They are, however, ideally suited to quantum computation.

III. OFF-RESONANCE ERRORS

The problem of tackling off-resonance errors was initially studied by Tycko [14]; his results were then extended by Cummins and Jones [15, 16]. Here we describe two families of composite pulses which can be used to compensate for off-resonance errors, and show how they can be derived using quaternions.

The original method used to develop many type A composite pulse sequences [15, 16] was based on dividing the propagator describing the evolution of the quantum system into intended and error components, and then seeking to minimise the error term. While this approach is effective, it is cumbersome, and a much simpler approach can be adopted for single qubit gates, which are simply rotations on the Bloch sphere and so can be modelled by quaternions. The quaternions corresponding to individual pulses can be multiplied together to give a quaternion description of the composite pulse, which can then be compared with the quaternion of the ideal system.

A quaternion is often thought of as a vector with four coefficients, but when describing a rotation it is more useful to regroup these coefficients as a scalar and a three-vector,

\[ q = \{s, v\} \]  

(1)

where

\[ s = \cos(\theta/2) \]  

(2)

depends solely on the rotation angle, \( \theta \), and

\[ v = \sin(\theta/2)\mathbf{a} \]  

(3)

depends on both the rotation angle, \( \theta \), and a unit vector along the rotation axis, \( \mathbf{a} \). Thus the quaternion describing an on-resonance pulse with phase angle \( \phi \) is

\[ q_{\theta,\phi} = \{\cos(\theta/2), \sin(\theta/2)\{\cos(\phi), \sin(\phi), 0\}\} \]  

(4)

An off-resonance pulse is conveniently parameterised by its off-resonance fraction \( f = \delta/\nu_1 \) (where \( \delta \) is the off-resonance frequency, and \( \nu_1 \) the nutation rate), and is described by the quaternion

\[ q_{\theta,\phi} = \{\cos(\theta'/2), \frac{\sin(\theta'/2)}{\sqrt{1+f^2}}\{\cos(\phi), \sin(\phi), f\}\} \]  

(5)

where \( \theta' = \theta \sqrt{1+f^2} \), and \( \theta \) is now the nominal rotation angle, that is the rotation achieved when \( f = 0 \). The quaternion describing a sequence of pulses is obtained by multiplying the quaternions for each pulse according to the rule

\[ q_1 \cdot q_2 = \{s_1 \cdot s_2 - v_1 \cdot v_2, s_1 v_2 + s_2 v_1 + v_1 \wedge v_2\} \]  

(6)

Finally, two quaternions can be compared using the quaternion fidelity [15]

\[ F(q_1, q_2) = |q_1 \cdot q_2| = |s_1 \cdot s_2 + v_1 \cdot v_2| \]  

(7)

(it is necessary to take the absolute value, as the two quaternions \( \{s, v\} \) and \( \{-s, -v\} \) correspond to equivalent rotations, differing in their rotation angle by integer multiples of \( 2\pi \)).

Following our previous work [15] we seek to tackle off-resonance errors in a \( \theta_x \) pulse using a sequence of three pulses applied along the \( x \), \(-x\) and \( x \) axes; pulses with any other phase angle can then be trivially derived by simply adding the desired value to the phase angles of all the pulses in the sequence. Such sequences can be described completely by the nominal rotation angles of the three pulses, \( \theta_1 \), \( \theta_2 \) and \( \theta_3 \). The composite quaternion for this composite pulse is complicated, but the situation can be greatly simplified by expanding it as a Maclaurin series in \( f \) and neglecting all terms above the first power. This gives

\[ s = \cos(2) \left( \frac{\theta_1 - \theta_2 + \theta_3}{2} \right) \]  

(8)

and

\[ v = \left\{ \sin(2) \sin(\theta_1/2), \sin(\theta_2/2), 2 \cos(\theta_3/2) \sin(\theta_1/2) + 2 \sin(\theta_1/2) \sin(\theta_2/2) \right\} \]  

(9)

while the ideal quaternion has the form

\[ \{\cos(\theta/2), \{\sin(\theta/2), 0, 0\}\} \].  

(10)

It now remains to chose the three nominal rotation angles so that these equations agree.

First we note that in order to achieve the correct rotation angle, \( s = \cos(\theta/2) \), we must choose our angles such that \( \theta_1 - \theta_2 + \theta_3 = \theta + 2a\pi \) (where \( a \) is any integer). We
also note that the $y$ component of $\mathbf{v}$ should equal zero, and that this can be achieved by choosing $\theta_1 = \theta_3 + 2b\pi$ (where $b$ is any integer). These two choices give
\[
\mathbf{v} = \left\{ \sin \frac{\theta}{2}, 0, f \left( \sin \frac{\theta}{2} - 2\sin \left( \frac{\theta}{2} - \theta_1 \right) \right) \right\}.
\] (11)

Finally we choose $\theta_1$ such that the $z$ component of $\mathbf{v}$ equals zero; this gives
\[
\theta_1 = \frac{\theta}{2} - \arcsin \left( \frac{\sin(\theta/2)}{2} \right).
\] (12)

Combining this value with our previous relations between the angles gives
\[
\theta_1 = 2n_1\pi + \frac{\theta}{2} - \arcsin \left( \frac{\sin(\theta/2)}{2} \right)
\] (13)
\[
\theta_2 = 2n_2\pi - 2\arcsin \left( \frac{\sin(\theta/2)}{2} \right)
\] (14)
\[
\theta_3 = 2n_3\pi + \frac{\theta}{2} - \arcsin \left( \frac{\sin(\theta/2)}{2} \right)
\] (15)

where $n_1$, $n_2$ and $n_3$ are integers, subject to the physical restriction that the resulting pulse angles must be positive.

These solutions have the same general form as those found previously [17]. Although they appear to differ in detail the expressions are, in fact, identical: taking the values $n_1 = 1$, $n_2 = 1$ and $n_3 = 0$ gives our previous family of solutions, referred to by the acronym CORPSE (Compensation for Off-Resonance with a Pulse SEquence). This family is now seen to be just one member of a larger group of families. To choose between these it is necessary to look at higher order terms, and this is most conveniently achieved using the quaternion fidelity, Equation (14). As a baseline we take the fidelity of a single off-resonance $\theta_\phi$ pulse compared with its (ideal) on-resonance form,
\[
\mathcal{F} \approx 1 + f^2 \left( \cos \frac{\theta}{4} - 1 \right)
\] (16)

where terms in $f^4$ and higher have been neglected. Note that the fidelity only contains even order terms in $f$ as the composite pulse perform symmetrically for positive and negative values of $f$.

As expected all members of our general group of solutions result in much better fidelities; in particular the term in $f^2$ is always completely removed. The behaviour of the term in $f^4$ is much more complicated, but it can be shown that this term depends only on the value of $n = n_1 - n_2 + n_3$, that is the total number of additional $2\pi$ rotations performed by the composite pulse sequence, and has the smallest absolute value when the three integers are chosen so that $n = 0$. As our previous values ($n_1 = 1$, $n_2 = 1$ and $n_3 = 0$) are the smallest numbers that fit this criterion, it seems that the CORPSE family of pulse sequences is indeed the best member of this group.

\[
\begin{array}{cccc}
\theta & \theta_1 & \theta_2 & \theta_3 \\
30^\circ & 367.6 & 345.1 & 7.6 \\
45^\circ & 371.5 & 337.9 & 11.5 \\
90^\circ & 384.3 & 318.6 & 24.3 \\
180^\circ & 420.0 & 300.0 & 60.0 \\
\end{array}
\]

TABLE I: Pulse rotation angles for a CORPSE composite pulse with a target rotation of $\theta_1$: CORPSE pulse phases are $+x, -x, +x$.

![Fidelity of simple (dashed line) and CORPSE composite pulses (solid line) as a function of the off-resonance fraction $f$ for pulses with a target rotation angle of 180°.](image)

The only other family of interest is that with $n_1 = 0$, $n_2 = 1$ and $n_3 = 0$, previously referred to as SHORT-CORPSE [18]; while this performs less well than CORPSE it is somewhat shorter. Numerical values of individual pulse rotation angles for CORPSE sequences with a variety of target angles are given in Table I.

The performance of the CORPSE sequence for a 180° pulse is demonstrated in Figure (1); the CORPSE pulse performs better than a simple pulse as long as $|f| \leq 0.663$. For smaller values of $\theta$ the effective range of $f$ is reduced, but not dramatically so: for a 30° pulse the CORPSE pulse outperforms a simple pulse as long as $|f| \leq 0.297$.

### IV. PULSE LENGTH ERRORS

A similar approach can be used to develop composite pulses to tackle pulse length errors. As before we begin with a sequence of three pulses, but the subsequent development is quite different. In particular we allow the three pulses to have arbitrary phase angles, as well as arbitrary rotation angles, thus giving us six variable parameters, although this number is soon reduced to three.

The quaternion corresponding to each pulse takes the simple form
\[
q_{\theta_\phi} = \{\cos(\theta/2), \sin(\theta/2)\{\cos(\phi), \sin(\phi), 0\}\}.
\] (17)

where $\theta = \theta(1 + g)$ is the actual rotation angle achieved by a pulse with nominal rotation angle $\theta$, and $g$ is the fractional error in the pulse power. The quaternion describing the composite pulse is very complicated, but can be simplified by restricting attention to the time symmetric case, where $\theta_1 = \theta_3$ and $\phi_1 = \phi_3$. This automatically
ensures that the composite quaternion has no \( z \) component, as any time symmetric sequence of rotations about axes in the \( xy \) plane is itself a rotation about an axis in the \( xy \) plane.

Even after this simplification, the composite quaternion remains extremely complicated. To make further progress we note that a composite pulse of this kind has been previously described for the case of a 180° rotation: the sequence

\[
180_{60} \ 180_{300} \ 180_{60}
\]

will perform a 180° rotation with compensation for pulse length errors (see [14], but note the corrected phase angles). It seems likely that other members of this family will have either \( \theta_1 = \pi \) or \( \theta_2 = \pi \); both possibilities were initially explored, but the second choice seemed more productive and forms the basis of our subsequent work.

As before, the composite quaternion can be expanded as a Maclaurin series in \( g \), and it is most useful to concentrate on the first order error term. This can be set equal to zero by choosing

\[
\phi_2 = \phi_1 \pm \arccos(-\pi/2\theta_1) \quad (19)
\]

and, for consistency with equation [18] we will use the minus sign in future. Sequences obeying this equation will be insensitive to pulse length errors; the rotation and phase angle can then be adjusted by choosing suitable values for \( \theta_1 \) and \( \phi_1 \). As before we will derive values for a \( \theta_2 \) pulse; pulses with other phase angles can be obtained by offsetting all the phase angles by the desired amount.

Solving these equations is complex, but the solutions are fairly straightforward:

\[
\theta_1 = \theta_3 = \arcsin\left(\frac{2 \cos(\theta/2)}{\pi}\right) \quad (20)
\]

\[
\theta_2 = \pi \quad (21)
\]

\[
\phi_1 = \phi_3 = \arccos\left(\frac{-\pi \cos \theta_1}{2\theta_1 \sin(\theta/2)}\right) \quad (22)
\]

\[
\phi_2 = \phi_1 - \arccos(-\pi/2\theta_1) \quad (23)
\]

where \( \text{sinc}(x) \) is defined as \( \sin(x)/x \). We refer to this as a Short Composite RRotation For Undoing Length Over and Under Shoot or SCROFULOUS sequence.

Numerical values of individual pulse rotation and phase angles for a variety of target angles are given in Table [1]. The performance of SCROFULOUS and plain 180° pulses are compared in Figure [2].

### V. THE BB1 FAMILY

Another approach to composite pulse design has been described by Wimperis [20]. While sequences such as CORPSE and SCROFULOUS seek a single composite pulse which performs the desired rotation with reduced sensitivity to errors, an alternative approach is to combine a

| \( \theta \) | \( \theta_1 \) | \( \phi_1 \) | \( \theta_2 \) | \( \phi_2 \) |
|---|---|---|---|---|
| 30° | 93.0 78.6 180.0 273.3 |
| 45° | 96.7 73.4 180.0 274.9 |
| 90° | 115.2 62.0 180.0 280.6 |
| 180° | 180.0 60.0 180.0 300.0 |

Table II: Pulse rotation and phase angles for a SCROFULOUS composite pulse with a target rotation of \( \theta_x \); note that \( \theta_3 = \theta_1 \) and \( \phi_3 = \phi_1 \).

FIG. 2: Fidelity of simple (dashed line) and SCROFULOUS composite pulses (solid line) as a function of the fractional pulse length error \( g \) for pulses with a target rotation angle of 180°.

The positive solution is then identical to that previously described [20]. Examining higher order error terms shows that this pulse sequence is even better than it first appears, as these choices also completely remove the second order error terms. As discussed below, this effect appears
TABLE III: Pulse phase angles for a W1 correction sequence with a target rotation of $\theta_x$; pulse rotation angles are $\theta_1 = 180^\circ$ and $\theta_2 = 360^\circ$.

| $\theta$ | $\phi_1$ | $\phi_2$ |
|---------|---------|---------|
| $30^\circ$ | 92.4 | 277.2 |
| $45^\circ$ | 93.6 | 280.8 |
| $90^\circ$ | 97.2 | 291.5 |
| $180^\circ$ | 104.5 | 313.4 |

FIG. 3: Fidelity of simple (dashed line) and BB1 composite pulses (solid line) as a function of the fractional pulse length error $g$ for pulses with a target rotation angle of $180^\circ$.

VI. SIMULTANEOUS ERRORS

So far we have only considered the case of either off-resonance effects or pulse length errors being present. In reality both problems may well occur simultaneously. It is therefore important to consider how such simultaneous errors might be tackled. Ideally we would like to design pulse sequences which can compensate for both problems at the same time; this, however, is a complicated and as yet unresolved problem, and here we simply analyse the sensitivity of each of our pulse sequences to the other kind of error.

We proceed as before, calculating composite pulse and simple pulse quaternions in the presence of errors, and determining the quaternion fidelity. This fidelity can then be expanded as a Maclaurin series in the error, and the lower order terms examined. Note that this procedure still assumes that only one type of error is present at a time; in order to detail with the case where both errors are present simultaneously it would be possible to use a Maclaurin expansion in both errors, but this is unlikely to lead to much insight. Instead we will simply plot the fidelity as function of both errors for some chosen target angles.

We begin by considering the response of the CORPSE pulse sequence to pulse length errors. In the absence of off-resonance effects the behaviour of CORPSE is trivial to calculate, as the three pulses are applied along the $+x$, $-x$ and $+x$ axes, so that the behaviour is identical to

\[
\phi_1 = \pm \arccos \left( -\frac{\theta}{4n\pi} \right). \tag{27}
\]

where $n$ is the total number of sequences used. As before the fidelity is independent of where the Wn sequences are placed, but it does depend on the value of $n$. The second and fourth order error terms are cancelled in all cases, and the size of the sixth order error term now depends on both $\theta$ and $n$. The smallest sixth order term is achieved when $n = 2$, but the term is not completely removed. The gain over $n = 1$ is fairly small, and in practice the simpler composite pulses based on the W1 sequence are likely to be the most effective.

Having varied the position and number of the error correcting pulse sequences the next logical step is to vary their form. In principle any sequence that has no overall effect in the absence of errors could be used. In practice we find that many possible sequences allow the second order error term in the fidelity expression to be removed, but the simultaneous cancellation of second and fourth order errors seems to be a special feature of the Wn family of sequences.

Given the success of this approach to tackling pulse length errors, it seems obvious to apply the method to tackle off-resonance effects. As yet, however, this approach has had no success.
that of a simple pulse. The behaviour of a 180° pulse in the presence of simultaneous errors is shown in Figure 4.

The behaviour of the scrofulous pulse sequence is difficult to calculate for general target rotation angles, due to the dependence of $\theta_1$ on the arcsinc function, and so we concentrate on the case of 180° pulses. For this case the dependence of the fidelity on off-resonance effects is given by $F \approx 1 - 2f^2$, while a simple pulse has a fidelity $F \approx 1 - f^2/2$ (see Equation 16). In general scrofulous is considerably more sensitive to off-resonance effects than plain pulses.

Finally we consider the BB1 family of pulse sequences, taking the time-symmetrised version of BB1, Equation 24, as our standard. In this case we can solve the problem for any target rotation angle, and up to second order the result is identical to that of a plain pulse, Equation 16. Thus, unlike scrofulous, the BB1 sequence achieves its impressive tolerance to pulse length errors at little or no cost in sensitivity to off-resonance effects. This is confirmed for simultaneous errors by Figure 4.

VII. CONCLUSIONS

Composite pulses show great promise for reducing data errors in NMR quantum computers. More generally, any implementation of a quantum computer must be concerned on some level with rotations on the Bloch sphere, and so composite pulse techniques may find very broad application in quantum computing. Composite pulses are not, however, a panacea, and some caution must be exercised in their use.

The corpse pulse sequence appears to be the best approach for tackling small off-resonance errors (for large known off-resonance effects the resonance offset tailored, or rotten, scheme [21] is preferable). For pulse length errors variations on the BB1 scheme of Wimperis [20] give the best results; the scrofulous family of pulses is less effective, but does have the advantage of being considerably shorter.

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FIG. 4: Fidelity of (a) plain, (b) CORPSE, (c) SCROFULOUS and (d) BB1 180° pulses as a function of simultaneous off resonance effects, $f$, and fractional pulse length error, $g$. Contours are plotted at 5% intervals.