

Arbitrary precision composite pulses for NMR quantum computing

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Abstract

We discuss the implementation of arbitrary precision composite pulses developed using the methods of Brown et al. [K.R. Brown, A.W. Harrow, I.L. Chuang, Arbitrarily accurate composite pulse sequences, *Phys. Rev. A* 70 (2004) 052318]. We give explicit results for pulse sequences designed to tackle both the simple case of pulse length errors and the more complex case of off-resonance errors. The results are developed in the context of NMR quantum computation, but could be applied more widely.

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1. Introduction

Composite pulses [1] have long played an important role in many NMR experiments, allowing the effects of systematic errors to be reduced. More recently they have been applied in quantum computing [2], including both magnetic resonance experiments and other implementations [3–6]. Composite pulses developed for quantum computing differ from more conventional NMR approaches in two key ways. Firstly they must perform the desired rotation whatever the starting state of the system, so that they act as *general rotors*; in NMR such pulses are sometimes called type A composite pulses [1], and have the advantage that they can be inserted into any part of a pulse sequence without the need for careful analysis. Secondly, they are usually designed to give extremely accurate rotations in the presence of small errors, rather than to give reasonable rotations in the presence of large errors. Despite these differences, however, composite pulses designed for quantum computation can be

used in conventional NMR experiments, and studying them can give some insight into more conventional approaches.

Type A composite pulses are most commonly used to tackle pulse length errors, which occur when the strength of the driving field differs from its nominal value, for example as a result of inhomogeneity, and off-resonance errors, which occur when the frequency of the driving field is not quite in resonance with the transition of interest. For pulse length errors the BB1 sequence [7], originally developed by Wimperis, has proved highly successful. Designing good type A pulses for off-resonance errors has proved more difficult, with the CORPSE sequence [3,4], based on an early numeric result by Tycko [8], being perhaps the most satisfactory.

More recently Brown et al. have described a general method [9,10] for generating *arbitrary precision* composite pulses, which they claim can be applied to tackle errors of arbitrary kinds. They do not, however, give explicit solutions for more than a small number of cases. We will show that it is simple to apply their methods to generate pulses resistant to pulse length errors, but it is more difficult to tackle off-resonance effects.

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2. Pulse length errors

We consider rotations about axes in the xy plane, for which an ideal rotation is described by the propagator

$$U(\theta, \phi) = \exp[-i\theta(\sigma_x \cos \phi + \sigma_y \sin \phi)/2] \quad (1)$$

where θ , the rotation angle, depends on the strength of the resonant driving field and the time for which it is applied, and ϕ , the phase, depends on the phase of the field with respect to some appropriate reference. Following Brown et al. [9] we describe our rotations in terms of the Pauli matrices, which are trivially related to the corresponding single spin product operator terms [11]. The description above is really only appropriate when $\theta \geq 0$, but also works for negative angles as

$$U(-\theta, \phi) = U(\theta, \phi + \pi) = U^{-1}(\theta, \phi). \quad (2)$$

In the presence of errors, however, this extension may not be appropriate and it is necessary to proceed with some caution.

Pulse length errors occur when the strength of the field is higher or lower than its nominal value, so that all rotation angles are systematically wrong by some constant fraction ϵ . It is convenient to write

$$V(\theta, \phi) = U(\theta[1 + \epsilon], \phi) \quad (3)$$

in such cases, and a series expansion in the error ϵ gives

$$V(\theta, \phi) = U(\theta, \phi) + \mathcal{O}(\epsilon) \quad (4)$$

so that the propagator has first order errors in ϵ . Note that in this paper we write all our composite pulses as sequences of propagators, so that the order of pulses runs from right to left. We classify pulse sequences according to n , the order of error in the propagator, but will occasionally refer to the corresponding propagator fidelity

$$\mathcal{F} = \frac{1}{2} \text{Tr}(VU^{-1}) = 1 - \mathcal{O}(\epsilon^2) \quad (5)$$

in which errors appear to order $2n$. For pulse length errors

$$V(\theta, \phi + \pi) = V^{-1}(\theta, \phi) \quad (6)$$

which will prove very useful throughout this section.

Several composite pulse methods for correcting such pulse length errors exist, most notably BBI [7]. This replaces a single pulse with a sequence of pulses such that

$$V(\pi, \phi_a)V(2\pi, \phi_b)V(\pi, \phi_a)V(\theta, 0) = U(\theta, 0) + \mathcal{O}(\epsilon^3) \quad (7)$$

where $\phi_b = 3\phi_a$ and $\phi_a = \arccos(-\theta/4\pi)$, to give a propagator with third order errors in ϵ . This pulse sequence was discovered using geometric arguments, and turns out to be remarkably effective in practice [4,12].

Brown et al. replaced previous methods of finding composite pulses, based on intuitions or special forms, by a systematic procedure [9]. We begin by describing in detail how this procedure can be used to generate a series of composite pulses to correct pulse length errors. As before we only consider target rotations with phase angles of zero, as more

general rotations in the xy plane are trivially derivable from these by offsetting the phase of all pulses appropriately. These pulses can also be used to design sequences for robust evolution under J -couplings [13].

2.1. Isolating the error

The first step is to isolate the error part of a pulse sequence by calculating

$$A_1 = V(\theta, 0)U^{-1}(\theta, 0) = 1 - \frac{i\theta}{2}\epsilon\sigma_x + \mathcal{O}(\epsilon^2) \quad (8)$$

where A_1 indicates a first order error in a sequence correct to zero order. Since

$$A_1^{-1}V = UV^{-1}V = U \quad (9)$$

if we can generate A_1^{-1} *exactly* then we can convert an erroneous rotation into a correct one. More realistically, if we can generate A_1^{-1} *correct to first order* then we can use this to cancel out the first order error in the original pulse. To do this it is useful to note that

$$A_1 = U(\epsilon\theta, 0) + \mathcal{O}(\epsilon^2) \quad (10)$$

so that A_1^{-1} is approximately equal to an x -rotation with angle $-\theta\epsilon$.

2.2. Generating a pure error term

To correct the first order error it is necessary to generate a matching rotation whose angle is *directly proportional* to the error fraction ϵ . A pure error term of this kind is most easily generated by noting that

$$V(2\pi, 0) = -1 + i\pi\epsilon\sigma_x + \mathcal{O}(\epsilon^2) \quad (11)$$

has the correct general form (the global phase of -1 can be ignored as usual). However while the error has the right form it has the wrong magnitude. This can be fixed by using two rotations with different phases [9], as

$$\begin{aligned} X_1(\phi) &= V(2\pi, \phi)V(2\pi, -\phi) \\ &= 1 - i2\pi \cos(\phi)\epsilon\sigma_x + \mathcal{O}(\epsilon^2) \end{aligned} \quad (12)$$

and so the size of the error can be scaled. In particular, solving

$$-2\pi \cos(\phi_1) = \theta/2 \quad (13)$$

to get

$$\phi_1 = \pm \arccos(-\theta/4\pi) \quad (14)$$

allows the first order error to be corrected (note that the sign of the error term must be reversed as we are seeking to approximate A_1^{-1} rather than A_1). This gives

$$X_1(\phi_1)V(\theta, 0) = U(\theta, 0) + \mathcal{O}(\epsilon^2) \quad (15)$$

as a pulse sequence which is correct to second order. Interestingly the key phase angle ϕ_1 has the same size as ϕ_a in the BBI sequence. The sign of ϕ_1 (and ϕ_a) seems arbitrary,

but for definiteness we choose the positive value. This point will be examined in more detail later.

The size and scaling of the errors permits a value of ϕ_1 to be found for any choice of θ , but if larger error terms are needed they can be achieved by simply repeating the sequence of 2π rotations, thus doubling the error. In passing we note that although the approximate form given in Eq. (12) is independent of the sign of ϕ , and thus of the order of the two 2π pulses, the exact form of X_1 does in fact depend on the sign of ϕ , and it is therefore necessary to use a consistent order. This will become important below.

2.3. Treating the second order error

The process described above can then be repeated to isolate the second order error

$$A_2 = X_1(\phi_1)V(\theta, 0)U^{-1}(\theta, 0) \quad (16)$$

with the result

$$A_2 = 1 - \frac{i\theta\sqrt{16\pi^2 - \theta^2}}{8}\epsilon^2\sigma_z + O(\epsilon^3). \quad (17)$$

To correct this will require an error term dependent on ϵ^2 , rather than on ϵ , and directed along the z axis rather than the x axis. This can be achieved by using the properties of *group commutators*. As these properties play a key role in the proof of the Solovay–Kitaev theorem [14] Brown et al. refer to the results as SK pulse sequences, but beyond the role of group commutators there is no need to understand the Solovay–Kitaev theorem to see how their methods work. The key result

$$\begin{aligned} \exp(-iA\epsilon^l)\exp(-iB\epsilon^m)\exp(iA\epsilon^l)\exp(iB\epsilon^m) \\ = \exp([A, B]\epsilon^{l+m}) + O(\epsilon^{l+m+1}) \end{aligned} \quad (18)$$

shows that two different first order pure error terms can be combined to make a single second order pure error term as long as their directions are chosen properly *and* inverses are available for each error term. This restriction will not be important for pulse length errors but will be more problematic for off-resonance errors.

As the commutator $[\sigma_x, \sigma_y] = -2i\sigma_z$ the desired second order error term along z can be generated from x and y terms. The x term can be generated as before, Eq. (12), and the equivalent y term Y_1 can be generated in the same way by shifting the phase of both pulses by $\pi/2$. (Brown et al. in fact described an alternative method [9] for implementing Y_1 , but this alternative is more complex.) Inverse terms can be generated by reversing the order of the two 2π pulses and shifting their phases by π . Note that it is necessary to reverse the sequence of pulses even though Eq. (12) appears to be independent of this, as the two alternatives differ to second order in ϵ ; it is *not* sufficient to generate an inverse which only accurate to first order. Hence

$$\begin{aligned} Z_2(\phi) &= X_1(\phi)Y_1(\phi)X_1^{-1}(\phi)Y_1^{-1}(\phi) \\ &= 1 - i8\pi^2 \cos^2(\phi)\epsilon^2\sigma_z + O(\epsilon^3) \end{aligned} \quad (19)$$

allows a second order z error of some desired size to be generated. If an error of the opposite sign is needed then the X_1 and Y_1 sequences can be interchanged to give

$$\begin{aligned} Z'_2(\phi) &= Y_1(\phi)X_1(\phi)Y_1^{-1}(\phi)X_1^{-1}(\phi) \\ &= 1 + i8\pi^2 \cos^2(\phi)\epsilon^2\sigma_z + O(\epsilon^3). \end{aligned} \quad (20)$$

As before we can solve

$$8\pi^2 \cos^2(\phi_2) = \theta\sqrt{16\pi^2 - \theta^2}/8. \quad (21)$$

to remove the second order error, giving

$$\phi_2 = \pm \arccos \left[\pm \frac{\sqrt{16\pi^2\theta^2 - \theta^4}}{8\pi} \right] \quad (22)$$

where the signs may be chosen independently, and we choose initially to take both positive signs. Thus

$$Z'_2(\phi_2)X_1(\phi_1)V(\theta, 0) = U(\theta, 0) + O(\epsilon^3) \quad (23)$$

is our desired pulse sequence, correct to third order. The explicit expansion

$$\begin{aligned} &V(2\pi, \pi/2 + \phi_2)V(2\pi, \pi/2 - \phi_2)V(2\pi, \phi_2)V(2\pi, -\phi_2) \\ &V(2\pi, 3\pi/2 - \phi_2)V(2\pi, 3\pi/2 + \phi_2)V(2\pi, \pi - \phi_2)V(2\pi, \pi + \phi_2) \\ &V(2\pi, \phi_1)V(2\pi, -\phi_1)V(\theta, 0) \end{aligned} \quad (24)$$

shows that this contains a total of ten correction pulses in addition to the main pulse.

2.4. Rotating and redividing the error

The sequence described above is not in fact the sequence originally described by Brown et al. Their approach [9] is instead based on generating an X_2 error correction term using appropriate Y_1 and Z_1 sequences and then rotating this onto the z axis. In the absence of systematic errors, such rotations are easily performed. For example the identity

$$U(\pi/2, 3\pi/2)U(\theta, 0)U(\pi/2, \pi/2) = \exp(-i\theta\sigma_z/2) \quad (25)$$

allows a z rotation to be generated from x and y rotations, a composite Z -pulse [16]. In the presence of systematic errors it is necessary to proceed with more caution, as the errors in different pulses will combine in a complex manner. However, in the presence of pulse length errors it is possible to use imperfect pulses to rotate pure error terms, as

$$V(\pi/2, 3\pi/2)X_nV(\pi/2, \pi/2) = Z_n + O(\epsilon^{n+1}) \quad (26)$$

for any error order n , and similarly for other error terms. This approach requires the ability to generate accurate inverse operators, and while this is easy for pulse length errors it can be tricky in other cases.

For pulse length errors we can implement the second order correction sequence using

$$Z'_2(\phi_2) \approx V(\pi/2, 3\pi/2)X'_2(\phi_2)V(\pi/2, \pi/2) \quad (27)$$

$$X'_2(\phi_2) = Z_1(\phi_1)Y_1(\phi_1)Z_1^{-1}(\phi_1)Y_1^{-1}(\phi_1) \quad (28)$$

$$Z_1(\phi_2) \approx V(\pi/2, 3\pi/2)X_1(\phi_2)V(\pi/2, \pi/2). \quad (29)$$

This alternative sequence gives identical performance at second order (complete correction of errors) but differs in its third order behaviour, as we shall see later.

We can also consider many other possibilities: firstly we can instead generate Z'_2 from any of Y'_2 , X_2 , or X'_2 ; secondly we can use alternative rotations to generate Z_1 ; thirdly we can use the negative sign for ϕ_1 in the first order correction sequence (in which case the second order error changes sign). Beyond these possibilities, built around rotating the error, we can also choose how to divide up the relative contributions to the second order error term arising from the two first order terms. For example we can write

$$\begin{aligned} Z_2(\alpha, \beta) &= X_1(\alpha)Y_1(\beta)X_1^{-1}(\alpha)Y_1^{-1}(\beta) \\ &= 1 - i8\pi^2 \cos(\alpha) \cos(\beta)\epsilon^2\sigma_z + O(\epsilon^3) \end{aligned} \quad (30)$$

and control the size of the second order error term by varying α and β . More simply still, we can use the fact that $V(2\pi, 0)$ gives an *unscaled* pure error term along x to use the form

$$\begin{aligned} V(2\pi, 0)Y_1(\beta)V(2\pi, \pi)Y_1^{-1}(\beta) \\ = 1 - i4\pi^2 \cos \beta \epsilon^2 \sigma_x + O(\epsilon^3) \end{aligned} \quad (31)$$

which only has six pulses, rather than the usual eight, and obtain the correct error term by choosing

$$\beta = \pm \arccos \left[-\frac{\theta\sqrt{16\pi^2 - \theta^2}}{32\pi^2} \right]. \quad (32)$$

2.5. Choosing between sequences

Given this plethora of subtly different sequences it is reasonable to ask which is the best. In some sense *all* second order pulse sequences are equally good, as they all suppress errors to the same order, but it is possible to choose between them either by considering higher order errors, or by considering sensitivity to *other* types of error [4].

Here, we adopt the first approach, choosing to minimize the size of the third order error term, and initially specializing to the case of 180° pulses, so that $\theta = \pi$. The smallest error term we have so far been able to find occurs when using Eqs. (27)–(29) to create the second order term, and taking positive signs throughout Eqs. (14) and (22). There is no obvious reason *why* this choice is best, but it does give a third order error more than 15 times smaller than some other alternatives.

Interestingly, the second best choice we have found is the BB1 sequence, which for the case $\theta = \pi$ has an error only about 10% larger than the best sequence. Furthermore for BB1 the size of the third order error term scales approximately linearly with θ , while the behavior of the “best” sequence, described above, is more complex. Thus for most

flip angles (specifically, $\theta < 168^\circ$) BB1 is the best second order sequence known. For the case of 180° pulses it has a fidelity

$$\mathcal{F} = 1 - \frac{5\pi^6}{1024}\epsilon^6 + O(\epsilon^8). \quad (33)$$

2.6. Third order errors

We can of course correct the third order error term in much the same way as the first and second order errors. As pointed out by Brown et al. there is no need to use a fully systematic approach of correcting error orders in sequence; instead we can begin with BB1 and correct the third order error term.

The third order error term for BB1 (and indeed for all the other sequences considered above) lies in the xy plane, with the size and position depending on the value of θ . Here, we do not give complete results, but simply sketch a partial solution. There are many possibilities for generating a third order error, but one simple example is

$$\begin{aligned} X_3(\phi) &= Y_1(\phi)Z_2(\phi)Y_1^{-1}(\phi)Z_2^{-1}(\phi) \\ &= 1 - i32\pi^3 \cos^3(\phi)\epsilon^3\sigma_x + O(\epsilon^4) \end{aligned} \quad (34)$$

where $Z_2(\phi)$ is generated from $X_1(\phi)$ and $Y_1(\phi)$ as before, Eq. (19), and $Z_2^{-1} = Z'_2$, so that this sequence only requires x and y rotations. The error term can then be rotated into the correct position, either by composite z rotations or, more simply, by shifting the phases of all the pulses in the X_3 term.

As before we need to choose a value of ϕ_3 to cancel the third order error, but as the calculations become very complicated we here consider only the special case of 180° pulses, $\theta = \pi$. Even in this case the analytic result is complicated, and so we simply give the numerical value, $\phi_3 \approx 73.1^\circ$; the required phase shift can also be calculated as approximately -1.6° .

3. Off-resonance errors

The treatment of off-resonance errors is superficially similar but much more difficult in practice. The fundamental problem is that, unlike the case of pulse length errors, it is not possible to generate perfect inverses of arbitrary rotations in the presence of off-resonance errors.

Off-resonance errors occur when the frequency of the driving field is not quite in resonance with the transition of interest, so that all rotations occur around a tilted axis. They can be parameterized in terms of the off-resonance fraction f , equal to the ratio of the frequency error and the driving frequency. The basic rotation is then

$$\begin{aligned} V(\theta, \phi) &= \exp[-i\theta(\sigma_x \cos \phi + \sigma_y \sin \phi + f\sigma_z)/2] \\ &= U(\theta, \phi) + O(f) \end{aligned} \quad (35)$$

which has first order errors in f . Unlike the case of pulse length errors this definition should *only* be used for positive

values of θ . The CORPSE family of sequences [3,4] for correcting off-resonance errors uses the three pulse sequence

$$\begin{aligned} C(\theta, \phi) &= V(\theta_c, \phi)V(\theta_b, \phi + \pi)V(\theta_a, \phi) \\ &= U(\theta, \phi) + \mathcal{O}(f^2) \end{aligned} \quad (36)$$

where

$$\theta_a = n_a 2\pi + \theta/2 - \arcsin[\sin(\theta/2)/2] \quad (37)$$

$$\theta_b = n_b 2\pi - 2 \arcsin[\sin(\theta/2)/2] \quad (38)$$

$$\theta_c = n_c 2\pi + \theta/2 - \arcsin[\sin(\theta/2)/2] \quad (39)$$

and the size of the second order error term depends on the values chosen for the integers n_a , n_b and n_c . The smallest errors are seen for the original CORPSE sequence, which has $n_a = n_b = 1$ and $n_c = 0$; for the case of 180° pulses the fidelity is

$$\mathcal{F} = 1 - \frac{12 + \pi^2 - 4\sqrt{3}}{32} f^4 + \mathcal{O}(f^6). \quad (40)$$

Short-CORPSE, defined by $n_a = n_c = 0$ and $n_b = 1$ is the shortest possible sequence but has a much larger error term [4].

The CORPSE family will play a key role in the following sections, not simply because it provides a pulse sequence with no first order errors, but mostly because it provides a route to sufficiently accurate inverse propagators. In the presence of off-resonance errors $V(\theta, \phi + \pi)$ is *not* an accurate inverse for $V(\theta, \phi)$ as

$$V(\theta, \pi)V(\theta, 0) = 1 + \mathcal{O}(f). \quad (41)$$

The corresponding CORPSE pulses perform much better,

$$C(\theta, \pi)C(\theta, 0) = 1 + \mathcal{O}(f^3), \quad (42)$$

and provide sufficiently accurate inverses to allow error terms to be rotated as for pulse length errors. As before the size of the third order error term depends on the exact choice of sequence, but is now smallest for short-CORPSE.

3.1. Correcting first order errors

We now explore the systematic correction of error orders using the methods previously described. The first order error can be isolated as before,

$$\begin{aligned} A_1 &= V(\theta, 0)U^{-1}(\theta, 0) \\ &= 1 - i \sin(\theta)/2f \sigma_z + i \sin^2(\theta/2)f \sigma_y + \mathcal{O}(f^2) \end{aligned} \quad (43)$$

and in general lies in the yz plane. Tunable pure error terms can be created either by using the form given by Brown et al. [9],

$$\begin{aligned} B_1(\phi) &= V(\phi, 0)V(2\phi, \pi)V(\phi, 0) \\ &= 1 - i2 \sin(\phi)f \sigma_z + \mathcal{O}(f^2), \end{aligned} \quad (44)$$

or the alternative form

$$\begin{aligned} Y'_1(\phi) &= V(\pi, \phi)V(\pi, \pi + \phi)V(\pi, -\phi)V(\pi, \pi - \phi) \\ &= 1 + i4 \cos(\phi)f \sigma_y + \mathcal{O}(f^2). \end{aligned} \quad (45)$$

Designing a sequence for the case $\theta = \pi$ is easy as the error lies solely along the y axis in this case, and so

$$Y'_1(\phi_1)V(\pi, 0) = U(\pi, 0) + \mathcal{O}(f^2) \quad (46)$$

with the choice $\phi_1 = \arccos(-1/4) \approx 104.5^\circ$. Interestingly, the key phase angle in this sequence turns out to be the same as that used in a BB1 pulse with $\theta = \pi$. The size of the second order error term is significantly larger than for CORPSE (and somewhat larger than for short-CORPSE), with a fidelity

$$\mathcal{F} = 1 - \frac{60 + \pi^2}{32} f^4 + \mathcal{O}(f^5). \quad (47)$$

but this sequence does have the relative simplicity of being constructed solely from 180° rotations, albeit with complicated phases.

Designing a sequence for other values of θ is, however, much trickier. In the general case the error does not lie along a principal axis, and so it might seem that we should rotate one of the two pure error terms. This cannot be done directly using simple rotations, as accurate inverse propagators are required to rotate error terms. It could be achieved using CORPSE pulses, but this is not sensible as CORPSE is already correct to first order.

An alternative approach is to note that pure error sequences can simply be combined, and so build up a tilted error by combining the z and y error sequences,

$$\begin{aligned} B_1(\phi_1^z)Y'_1(\phi_1^y) &= 1 - i2 \sin(\phi_1^z)f \sigma_z + i4 \cos(\phi_1^y)f \sigma_y \\ &\quad + \mathcal{O}(f^2) \end{aligned} \quad (48)$$

with any cross terms between the two parts if the pulse sequence being swallowed up into the $\mathcal{O}(f^2)$ term. Choosing $\phi_1^y = \arccos[-\sin^2(\theta/2)/4]$ and $\phi_1^z = -\arcsin[\sin(\theta)/4]$ allows first order off-resonance errors to be suppressed in the general case. However, the size of the second order error term remains significantly larger than for CORPSE, and this general sequence does not have the simplicity seen for the special case of 180° pulses. Thus CORPSE remains the best currently known type A sequence correct to first order in the presence of off-resonance errors.

3.2. Correcting higher order errors

The systematic approach can, more sensibly, be used to correct higher order errors. As the equations for arbitrary values of θ become extremely complicated we will again limit ourselves to the special case $\theta = \pi$. We extend our definitions

$$\begin{aligned} X_1(\phi) &= V(\pi, \pi/2 - \phi)V(\pi, 3\pi/2 - \phi)V(\pi, \pi/2 + \phi)V(\pi, 3\pi/2 + \phi) \\ &= 1 - i4 \cos(\phi)f \sigma_x + \mathcal{O}(f^2) \end{aligned} \quad (49)$$

$$\begin{aligned} Y_1(\phi) &= V(\pi, \pi - \phi)V(\pi, -\phi)V(\pi, \pi + \phi)V(\pi, \phi) \\ &= 1 - i4 \cos(\phi)f \sigma_y + \mathcal{O}(f^2) \end{aligned} \quad (50)$$

$$\begin{aligned} X'_1(\phi) &= V(\pi, 3\pi/2 + \phi)V(\pi, \pi/2 + \phi)V(\pi, 3\pi/2 - \phi)V(\pi, \pi/2 - \phi) \\ &= 1 + i4 \cos(\phi)f \sigma_x + \mathcal{O}(f^2) \end{aligned} \quad (51)$$

and note that $X'_1(\phi) \approx X_1^{-1}(\phi)$. The approximation is good enough that these terms can be used to build higher order propagators; in particular

$$Z_2(\phi) = X_1(\phi)Y_1(\phi)X'_1(\phi)Y'_1(\phi) = 1 - i32 \cos^2(\phi)f^2\sigma_z \quad (52)$$

and

$$Z'_2(\phi) = Y_1(\phi)X_1(\phi)Y'_1(\phi)X'_1(\phi) = 1 + i32 \cos^2(\phi)f^2\sigma_z. \quad (53)$$

The second order error can be isolated as usual

$$\begin{aligned} A_2 &= Y'_1(\phi_1)V(\pi, 0)U^{-1}(\pi, 0) \\ &= 1 - i\sqrt{15}/2f^2\sigma_z - i\pi/4f^2\sigma_x + O(f^3) \end{aligned} \quad (54)$$

and lies in the xz plane with magnitude $\sqrt{60 + \pi^2}/4$.

One approach to correcting this is by using CORPSE pulses to rotate an appropriate Z_2 error around the y axis to get the final sequence

$$\begin{aligned} C(\psi_2, \pi/2)Z'_2(\phi_2)C(\psi_2, 3\pi/2)Y'_1(\phi_1)V(\pi, 0) \\ = U(\pi, 0) + O(f^3) \end{aligned} \quad (55)$$

with

$$\phi_2 = \arccos\left(\frac{\sqrt[4]{60 + \pi^2}}{8\sqrt{2}}\right) \approx 75.2^\circ \quad (56)$$

and

$$\psi_2 = \arctan\left(\frac{\pi}{2\sqrt{15}}\right) \approx 22.1^\circ. \quad (57)$$

This approach can, of course, be generalized to other angles and higher orders, but the resulting algebra is very complex. For simplicity it is possible to check results using ideal rotations in place of CORPSE based rotations: this will give the right result for error terms which are completely suppressed, but the wrong values for higher order errors.

Alternatively, we can construct the tilted error term out of a combination of z and x errors as in the previous section. We begin by noting that $B_1(3\pi/2)$ provides a good inverse for the pure error term $B_1(\pi/2)$, and that this allows us to construct a second order x error using

$$X_2(\phi) = Y_1(\phi)B_1(\pi/2)Y'_1(\phi)B_1(3\pi/2) = 1 - i16 \cos(\phi)f^2\sigma_x. \quad (58)$$

This can be combined with a z error to get the pulse sequence

$$X_2(\phi_2^x)Z'_2(\phi_2^z)Y'_1(\phi_1)V(\pi, 0) = U(\pi, 0) + O(f^3) \quad (59)$$

where $\phi_2^x = \arccos(-\pi/64) \approx 92.8^\circ$ and $\phi_2^z = \arccos(\sqrt[4]{15}/8) \approx 75.8^\circ$. This sequence has the advantage over the CORPSE based approach of requiring only 90° and 180° pulses.

3.3. Time symmetric sequences

In passing we consider the use of time-symmetry in composite pulse sequences [4]. In the presence of off-resonance errors time symmetric composite pulses have fidelities

which are even functions of the off-resonance fraction f [15], and so give the same fidelity for $+f$ and $-f$, although the details of the error may differ. Although such symmetric fidelities have no advantage in principle, the results are certainly easier to interpret.

As an example we consider a time symmetric version of the pulse sequence to correct first order errors arising from off-resonance effects in a 180° pulse, which takes the form

$$Y'_1(\phi'_1)V(\pi, 0)Y_1(\phi'_1) = U(\pi, 0) + O(f^2) \quad (60)$$

where $\phi'_1 = \arccos(-1/8) \approx 97.2^\circ$. The fidelity of this sequence has no fifth order term, unlike that of the previous version, Eq. (46), but as both fidelities are dominated by fourth order errors this is largely a cosmetic improvement.

3.4. Simultaneous errors

So far we have only considered the effects of pulse length errors and off-resonance errors in isolation, while in real physical systems both sorts of error can occur simultaneously. It is generally difficult to find pulse sequences which suppress both sorts of error simultaneously, but it is still important to consider whether insensitivity to one type of error is obtained at the cost of increased sensitivity to other types of errors [4].

As noted previously [4], the response of the time symmetric version of BB1 to off-resonance errors is very similar to that of a simple pulse. This occurs because *in the absence of pulse length errors* the correction sequence

$$V(\pi, \phi_1)V(2\pi, 3\phi_1)V(\pi, \phi_1) = 1 + O(f^2) \quad (61)$$

has no first order terms arising from off-resonance errors, and so does not contribute significantly to the total error. In the same way *in the absence of off-resonance errors* the correction sequence

$$V(\pi, \phi_1)V(\pi, \pi + \phi_1)V(\pi, -\phi_1)V(\pi, \pi - \phi_1) = 1 \quad (62)$$

has no error terms arising from pulse length errors at all. Thus these two sequences can be combined, giving the composite 180° pulse

$$\begin{aligned} V(\pi, \phi_1)V(\pi, \pi + \phi_1)V(\pi, -\phi_1)V(\pi, \pi - \phi_1) \\ V(\pi, \phi_1)V(2\pi, 3\phi_1)V(\pi, \phi_1)V(\pi, 0) \end{aligned} \quad (63)$$

with $\phi_1 = \arccos(-1/4)$. This has a fidelity

$$\mathcal{F} = 1 - \frac{15}{8}f^4 - \frac{5\pi^6}{1024}\epsilon^6 - \frac{169\pi^2}{32}f^2\epsilon^2 + \text{higher terms} \quad (64)$$

so in the absence of off-resonance errors the correction of pulse length errors is identical to a BB1 sequence, and in the absence of pulse length errors the correction of off-resonance errors is even better than the simple pulse, Eq. (46). This pulse can correct well for *either* pulse length errors *or* off-resonance errors; in the presence of *simultaneous* errors the performance is not so good, but is still much better than a simple 180° pulse.

4. Summary

The methods of Brown et al. can indeed be used to derive arbitrary precision composite pulses, but the process can be somewhat complicated. For the case of pulse length errors the situation is simple, as it is possible both to generate a wide range of pure error terms and their inverses, and to rotate these terms using uncorrected pulses. The case of off-resonance errors is much more complicated because the difficulty of generating accurate inverses of incorrect rotations means that the most direct approach cannot be used.

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