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Use of composite rotations to correct systematic errors in NMR quantum computation

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Abstract. We implement an ensemble quantum counting algorithm on three NMR spectrometers with ^{1}H resonance frequencies of 500, 600 and 750 MHz. At higher frequencies, the results deviate markedly from naive theoretical predictions. These systematic errors can be attributed almost entirely to off-resonance effects, which can be substantially corrected for using fully compensating composite rotation pulse sequences originally developed by Tycko. We also derive an analytic expression for generating such sequences with arbitrary rotation angles.

1. Introduction

Quantum computers are information processing devices which operate by—and exploit—the laws of quantum mechanics, potentially allowing them to tackle otherwise intractable problems [1]. Although there has been a great deal of interest in the theory of quantum computation, actually building a general purpose quantum computer has proved extremely difficult. Since the multiparticle coherent states on which quantum computers rely are extremely vulnerable to the effects of errors, considerable effort has been expended on alleviating the effects of random errors introduced by decoherence. The outcome of this research includes elegant methods of error correction [2, 3] and fault-tolerant computation [4]. Comparatively little effort, however, has been directed at the issue of systematic errors arising from reproducible imperfections in the apparatus used to implement quantum computations.

It makes sense to address systematic errors, as many of them can be eliminated relatively easily. In the Bloch picture, where unitary operations are visualized as rotations of the Bloch vector on the unit sphere, systematic errors are expressed as rotational imperfections. The sensitivity of the final state to these imperfections can be much reduced by replacing single

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rotations with composed rotations. Intuitively, replacing one erroneous operation by several erroneous operations ought to increase the overall error, but this is not necessarily true in the case of rotations as they are nonlinear, and this opens up the possibility of errors cancelling one another.

It is worth stressing the distinction between improved experimental technique, quantum error correcting codes, and the use of composite rotations. Improved experimental technique minimizes conditions which lead to data errors. Error-correcting codes diagnose errors (however obliquely) and use this knowledge of the errors to explicitly reverse them. Composite pulses prevent errors in the first place by reducing the impact on the system of the conditions which cause systematic data errors, without actually eliminating these conditions. Composite pulses cannot, however, correct random errors, as they rely on the reproducible nature of systematic errors to correct them.

2. Systematic errors in NMR quantum computers

In the last few years, nuclear magnetic resonance (NMR) techniques [5–9] have been used to implement small quantum computers [10, 11]. Several simple quantum algorithms have been implemented using NMR, such as Deutsch's algorithm [12–16] and Grover's algorithm [17–19]. The comparative ease with which such experiments have been performed reflects, in part, the fact that more conventional NMR experiments, used throughout the molecular sciences, themselves rely on the generation and manipulation of multi-spin coherent states [6, 7], and so techniques for handling them are highly developed.

Despite this pre-existing experimental sophistication, NMR quantum computers are nonetheless subject to systematic errors. Implementing complex quantum algorithms requires a large network of logic gates, which within an NMR implementation entails even longer cascades of pulses. In these cases small systematic errors in the pulses (which can be largely ignored in many conventional NMR experiments) accumulate and become significant. Interactions between individual spins and between spins and the environment are mediated by RF pulses: applications of an RF field with phase ϕ (in the rotating frame) [5, 6] for some duration τ. In the ideal case, the pulse will drive the Bloch vector through an angle θ about an axis orthogonal to the z-axis and at an angle ϕ to the x-axis. The rotation angle, θ, depends on the rotation rate induced by the RF field, usually written ω_1, and the duration of the pulse, τ. In practice, the RF field is not ideal, and this leads to two important classes of systematic errors, referred to as pulse length errors and off-resonance effects [6].

Pulse length errors arise either when the length of the pulse is set incorrectly, or, more commonly, when the RF field strength deviates from its nominal value, so that the rotation angle achieved deviates from its theoretical value. This effect is most commonly observed within NMR as a result of spatial inhomogeneity in the applied RF field; in this case it is impossible for all the spins within a macroscopic sample to experience the same rotation angle. Off-resonance effects arise from the use of a single RF source to excite transitions in two or more spins which have different resonance frequencies. This is done for a variety of practical reasons. For example, in conventional NMR experiments which seek to analyse molecular systems, there will be a large number of different transition frequencies, whose exact values are unknown at the start of the experiment. Thus the only practical approach is to use a single RF source, with sufficient power that it can excite transitions across a wide range of frequencies. In quantum computation experiments the transition frequencies are known beforehand, but for several reasons the use of a

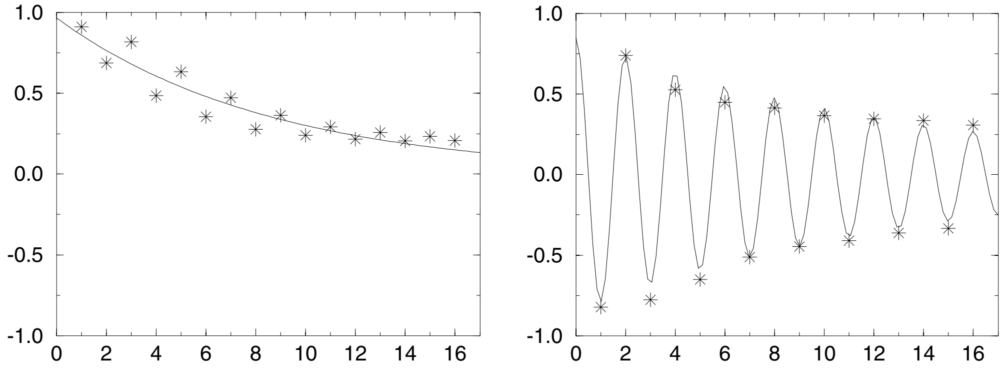


Figure 1. Experimental results from a 500 MHz NMR quantum computer implementing quantum counting over a one-qubit search space; results are shown for two of the four possible functions f: (a) f_{00} (no matches); (b) f_{11} (both match). The observed signal intensity is plotted as a function of r, the number of times the controlled-G operator is applied. Intensities are normalized relative to the case of $r = 0$. The solid lines are exponentially damped cosinusoids with the appropriate theoretical frequencies, and are plotted to guide the eye.

single RF source for each type of atomic nucleus remains the most practical approach (different sources *are* used for different nuclei, such as ^{1}H and ^{13}C).

Composite pulses [6,9,20] are widely used in NMR to minimize the sensitivity of the system to pulse-length and off-resonance errors by replacing direct rotations with composite rotations which are less sensitive 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 or introduce phase errors. These conventional sequences were initially derived by considering the trajectories of Bloch vectors during a pulse [9], and this approach is only useful if the starting point of the Bloch vector is known. Quantum computation requires fully compensating (type A) composite pulse sequences [20]. Fortuitously, a number of such sequences have been developed by Tycko [21]. While these pulse sequences do not offer quite the same degree of compensation as is found with some more conventional sequences, the compensation which does occur is effective whatever the initial position of the Bloch vector. As such behaviour is rarely (if ever) required within conventional NMR experiments, these sequences have previously found no experimental use [22]. They are, however, ideally suited to quantum computation.

3. Example: NMR quantum counting

Systematic errors are an issue with many types of quantum algorithms, but we will focus on a counting algorithm which can involve particularly long pulse trains. Counting the number of items matching a search criterion is a well-known computer science problem, and an efficient quantum counting algorithm based on a variation of Grover's quantum search has been implemented using NMR techniques [23].

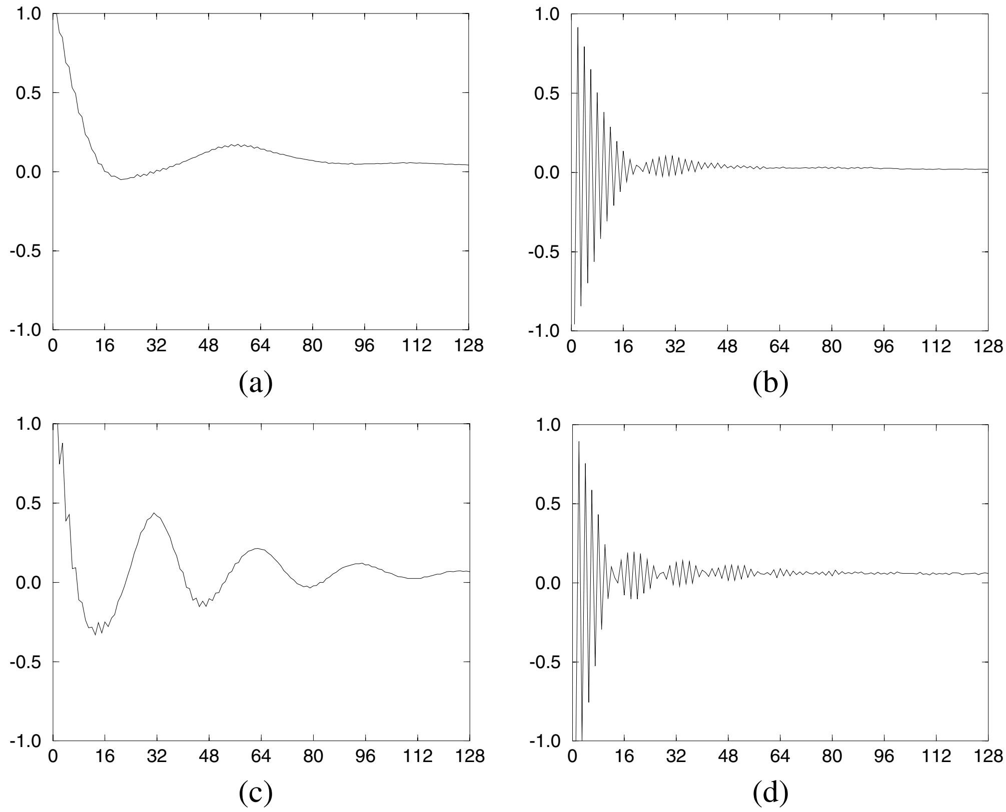


Figure 2. Experimental results from a 600 MHz ((a) and (b)) and 750 MHz ((c) and (d)) NMR quantum computer for f_{00} ((a) and (c)) and f_{11} ((b) and (d)). The observed signal intensity is plotted as a function of r, the number of times the controlled-G operator is applied. Intensities are normalized relative to the case of $r = 0$.

Consider a match function $f(x)$ which maps n-bit binary strings to a single output bit. In general there will be $N = 2^n$ possible input values, of which k will yield a match, $f(x) = 1$. The object of the quantum counting algorithm is to estimate k by estimating an eigenvalue of the Grover iterate $G = HU_0H^{-1}U_{\overline{f}}$, where H represents an n-bit Hadamard transform, U_0 maps $|0\rangle$ to $-|0\rangle$, and $U_{\overline{f}}$ maps $|x\rangle$ to $(-1)^{f(x)+1}|x\rangle$. The algorithm involves applying G repeatedly and observing the variation in signal intensity. The signal intensity is modulated in r, the number of applications of G, with frequency proportional to k, the number of matches. A more detailed explanation of this algorithm is given in reference [23].

Figure 1 shows experimental results for a search over a one-qubit search space, using a two-qubit quantum computer based on the two ^{1}H nuclei of cytosine in solution in D_2O [15]. The NMR spectrometer used a ^{1}H operating frequency of 500 MHz. On a one-qubit search space, there are three possible results corresponding to four possible functions f: no inputs match (in which case $f = f_{00}$), the first input matches ($f = f_{01}$), the second input matches ($f = f_{10}$), or both inputs match ($f = f_{11}$). For simplicity, only the cases f_{00} and f_{11} are shown.

The observed signal loss with r could arise from a number of sources. Clearly one possibility is the effects of decoherence, but the observed decay rate is too rapid to be so simply explained, and patterns in the signal loss (this is especially clear for f_{00}, where data points lie alternately above

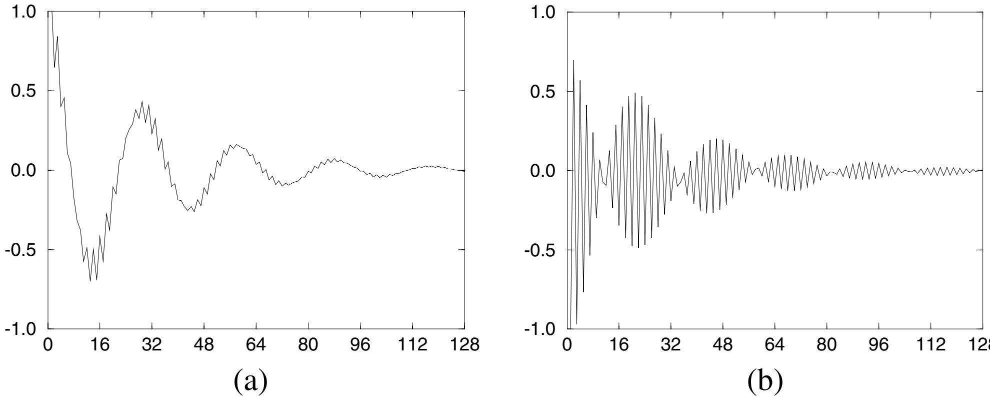


Figure 3. Theoretical prediction for 750 MHz spectra once off-resonance effects are included. An (arbitrary) exponential damping has been applied.

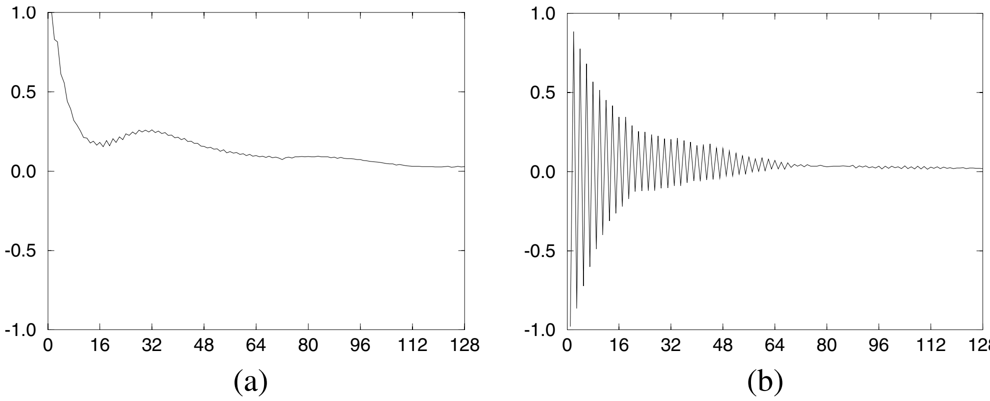
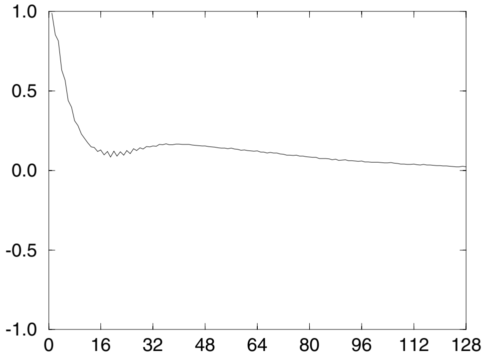


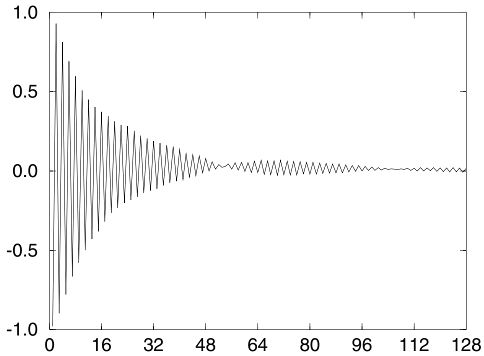
Figure 4. Experimental results from the 750 MHz quantum computer when 90°_y pulses are replaced by $385^\circ_y 320^\circ_{-y} 25^\circ_y$ pulse sequences.

and below a smooth curve) suggest a more complex explanation. Repeating the experiments on spectrometers with higher operating frequencies markedly degrades the results, as shown in figure 2, which shows data from computations implemented on 600 and 750 MHz spectrometers. Once more, only the f_{00} and f_{11} cases are shown. These results clearly demonstrate that the use of expensive high field magnets does not always give better results. An unwanted beat frequency and high frequency chatter have been introduced, and the signal decays more rapidly. These effects are more severe at 750 MHz than at 600 MHz.

The observed field dependence strongly suggests that these errors arise from off-resonance effects. These arise because only a single RF transmitter is used to excite both ^{1}H nuclei, and it cannot be on-resonance with both sets of transitions. Instead the transmitter frequency is chosen to lie halfway between the two resonance frequencies, resulting in equal and opposite off-resonance terms. Two factors are responsible for the poor results at higher frequencies. Firstly, the frequency offsets, $\pm\delta\nu$, are proportional to the resonance frequency, and thus are larger at high frequencies. Secondly, the RF field strength is typically weaker at higher frequencies. These combine to make the off-resonance effects much more serious. This diagnosis can be confirmed by including off-resonance effects in simulations of the NMR experiment. After this correction is made, the theoretical results, shown in figure 3, agree strikingly well with the experimental



(a)



(b)

Figure 5. Experimental results on the 750 MHz spectrometer when 90°_y pulses are replaced by $385^\circ_y 320^\circ_{-y} 25^\circ_y$ pulse sequences and 180°_x pulses are replaced by $90^\circ_x 225^\circ_{-x} 315^\circ_x$ pulse sequences.

results. Even the high-frequency 'noise' on the peaks is reproduced.

Since our simulations confirm that the major errors in NMR quantum counting arise from off-resonance effects in the 90°_y pulses, we chose to use Tycko's $385^\circ_y\ 320^\circ_{-y}\ 25^\circ_y$ composite 90°_y sequence [21], which offers good compensation for off-resonance errors while remaining fairly insensitive to pulse-length errors. Substituting this sequence for the 90°_y pulses produced a significant improvement in the experimental results at 750 MHz, as shown in figure 4. The low-frequency beating almost disappears, and the high-frequency noise is much reduced. The remaining damping is due to the effects of decoherence and pulse length errors.

When using composite pulses, there is a trade-off between the cancellation of errors and the extra manipulation of the system necessary to induce this cancellation. While there exist sequences which in theory compensate for an extraordinary range of errors, these sequences involve prohibitively long cascades of pulses. In practice, three-pulse sequences seem to provide a good balance between insensitivity and simplicity. The hazards of over-manipulation can be seen when the counting experiment is repeated using composite 180° pulses as well as 90° ones, shown in figure 5. The composite 180°_x pulse used was $90^\circ_x\ 225^\circ_{-x}\ 315^\circ_x$ [24]. Although simulations predict that the results should be slightly better when both 180° and 90° compensated pulses are used, the results for f_{11} are in fact slightly worse. The errors introduced by the extra manipulation outweigh the small gain achieved by the use of more sophisticated pulse sequences.

4. Composite pulses for arbitrary rotation angles

Discussion of composite pulses in the NMR literature has focused almost exclusively on 90° and 180° pulses, for the simple reason that these are the rotation angles most commonly used in conventional pulse sequences. While these composite pulses can be very useful for quantum computation, as demonstrated above, it would be preferable to have composite pulses for other rotation angles as well. For example, a 45° pulse could be used in the implementation of a true Hadamard gate [25], which might be applied many times in a single network.

We use the method of coherent averaging [7] to generate an analytic expression for composite pulses similar to Tycko's 90° pulse, but with arbitrary rotation angles. The basic idea of the

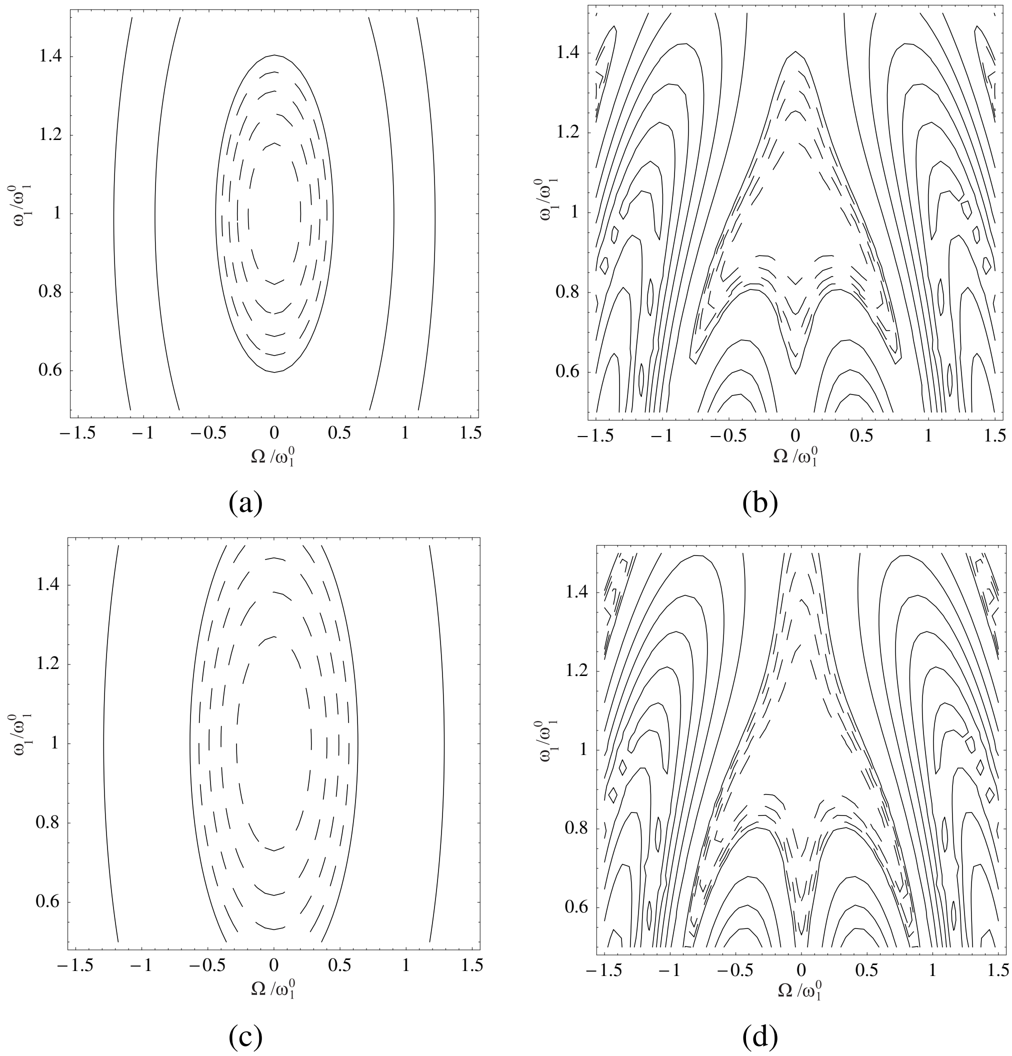


Figure 6. Numerical evaluation of the fidelity of some composite pulses. The x-axis represents radio-frequency inhomogeneity and the y-axis represents off-resonance effects. The sequences are (a) an uncompensated 90°_x pulse, (b) Tycko's 90°_x pulse, $385^\circ_x 320^\circ_{-x} 25^\circ_x$, (c) an uncompensated 60°_x pulse, and (d) a new 60°_x composite pulse, $375^\circ_x 331^\circ_{-x} 15^\circ_x$. Solid contour lines are spaced at 15% intervals, and dashed contour lines are spaced at 1% intervals, beginning at 95%.

method is to split the Hamiltonian of the system into intended and error components

$$H(t) = H_0(t) + V \tag{1}$$

where the 'ideal' Hamiltonian (written in the rotating frame and using product operator notation [26]) is

$$H_0(t) = \omega_1 \left(I_x \cos\phi + I_y \sin\phi \right) \tag{2}$$

and the error term arising from off-resonance effects is

$$V = \delta\omega I_z \tag{3}$$

where $\delta\omega$ is the resonance offset angular frequency. We then seek to minimize the propagator of the error component by expanding it as a power series [21]. (This is essentially equivalent to time-dependent perturbation theory.) Knowing V, we can rewrite the propagator as a product

$$\begin{aligned} U(t) &= U_0(t)U_V(t) & (4) \\ &= T\exp\left(-\mathrm{i}\int_0^\tau \mathrm{d}t\, H_0(t)\right) T\exp\left(-\mathrm{i}\int_0^\tau \mathrm{d}t\, \tilde{V}(t)\right) & (5) \end{aligned}$$

where T is the Dyson time-ordering operator and

$$\tilde{V}(t) = U_0(t)^{-1} V U_0(t). \tag{6}$$

Since U_V varies rather slowly with time, it can be expanded as a power series in $\tilde{V}$:

$$U_V(\tau) = \exp\left(-\mathrm{i}\tau\left(V^{(0)} + V^{(1)} + \ldots\right)\right) \tag{7}$$

using the Magnus expansion [7,27]

$$V^{(0)} = \frac{1}{\tau}\int_0^\tau \mathrm{d}t\, \tilde{V}(t) \tag{8}$$

$$V^{(1)} = \frac{-\mathrm{i}}{2\tau}\int_0^\tau \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \left[\tilde{V}(t_1), \tilde{V}(t_2)\right] \tag{9}$$

and so on. Complete expressions for the higher-order terms are given in [28,29]. Our objective is to find a pulse sequence which satisfies the requirement that it perform an ideal rotation under ideal conditions†

$$T\prod_{i=1}^{m} U_i(\tau_i) = U_0(\tau) \tag{10}$$

while minimizing $V^{(0)}$. (Here $U_0(\tau)$ is the propagator of an ideal uncomposed pulse and the $U_i(\tau_i)$ are the constituent propagators of the ideal composite pulse.) We do not consider higher-order terms as we wish to restrict the length of our composite sequence to three pulses. Ordinarily, a numerical search for a solution must be conducted for each set of target values, θ and ϕ, but an analytic solution exists if the axes of rotation are taken to be $\phi_1 = \phi$, $\phi_2 = \phi + \pi$, and $\phi_3 = \phi$. While this is nominally a loss of generality, the solutions we find are perfectly compensated to first order, and so no more general solution would be better to first order. The solutions also exhibit reasonable tolerance of RF field inhomogeneity.

With these phases, it follows trivially from equation (10) that

$$\theta_2 = \theta_1 + \theta_3 - \theta. \tag{11}$$

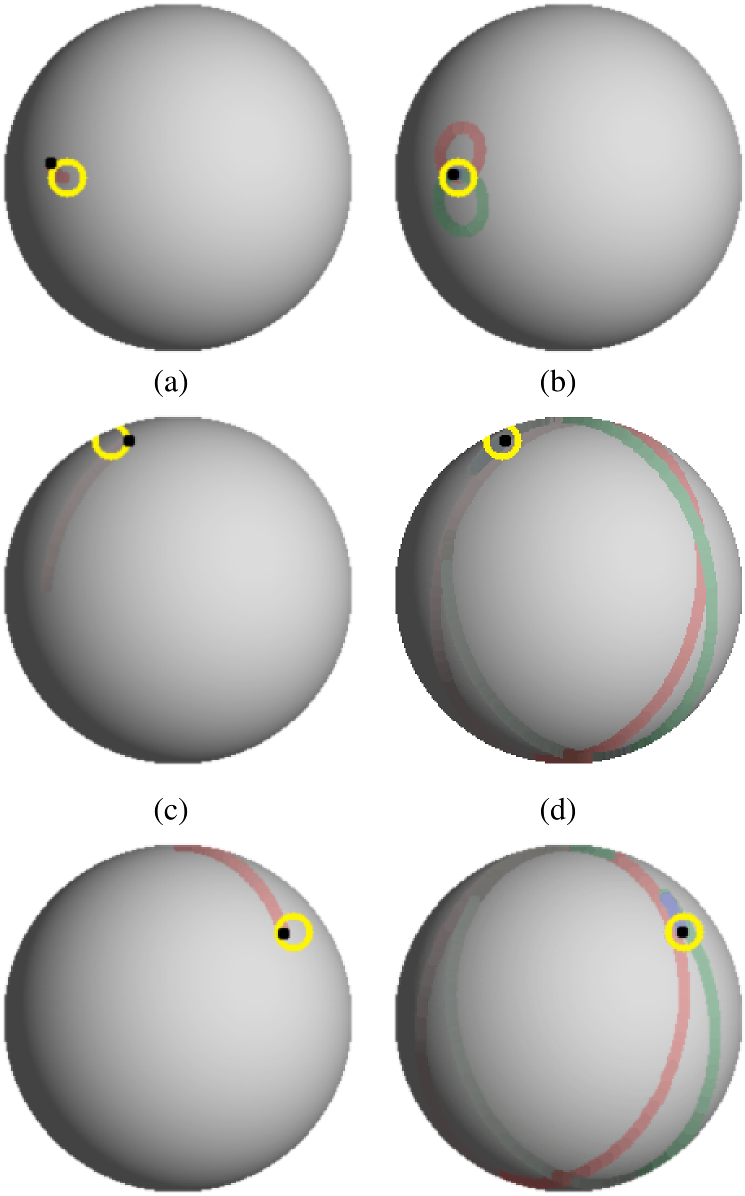
Evaluating $V^{(0)}$ with these values of ϕ and θ_2 and setting $V_y^{(0)}$ and $V_z^{(0)}$ to zero (in this case $V_x^{(0)}$ is identically zero) gives a restriction on θ_3

$$\theta_3 = \pm\theta_1 + 2n\pi \qquad n = 0, \pm 1, \pm 2, \ldots \tag{12}$$

Taking the positive result, $\theta_3 = \theta_1 + 2n\pi$, and back-substituting appears to give two solution families

$$\theta_1 = \pm\arccos\left(\frac{(1-\cos\theta)^2 \pm \sin\theta\sqrt{(1-\cos\theta)(7+\cos\theta)}}{4(1-\cos\theta)}\right) + 2n\pi \tag{13}$$

† This condition is perhaps not necessary, since these ideal conditions will not normally occur. Since the resonance offsets in quantum computation sequences are always known, an intriguing alternative approach would be to develop composite pulses which perform best at some pre-determined resonance offset.



(a) (b) (c) (d) (e) (f)

Figure 7. Magnetization trajectories on the Bloch sphere for a 60° uncompensated pulse ((a), (c), (e)) and a Tycko-type composite pulse ((b), (d), (f)) for a system with a fairly large resonance offset. The black dot shows the final position on the Bloch sphere, and the pale ring shows the target position, from a starting state of I_x ((a), (b)), I_y ((c), (d)) or I_z ((e), (f)). The three rotations within the composite pulse sequences are shown in different colours. These plots correspond to a spin system with a resonance offset of 2 ppm in a 750 MHz magnet with an RF field strength of 10 kHz. See also the animated versions of these figures. Trajectories for compensated and other pulse sequences can be generated by a java applet available at http://www.qubit.org/people/holly/grapefruit.html.

$$\theta_1 = \pm \arcsin \left(\frac{-\sin\theta \left(1 + \cos\theta - \sqrt{(1+\cos\theta)(7+\cos\theta)}\right)}{4(1+\cos\theta)} \right) + 2n\pi \quad (14)$$

but these solutions are equal in the region $0 \le \theta_{target} \le \pi$ for the positive root and a consistent choice of signs‡. We follow Tycko and choose $n = 1$ so that $2\pi \le \theta_1 \le 4\pi$. The final rotation angles are

$$\begin{aligned} \theta_1 &= \arccos \left(\frac{(1-\cos\theta)^2 + \sqrt{(1-\cos\theta)(7+\cos\theta)}\sin\theta}{4(1-\cos\theta)} \right) + 2\pi \\ \theta_2 &= \theta_1 + \theta_3 - \theta \\ \theta_3 &= \theta_1 - 2\pi. \end{aligned} \quad (15)$$

Within this family, the quality of the pulses is remarkably insensitive to the actual details of the pulse sequence. As long as equation (11) is strictly satisfied, any sequence with angles vaguely like those given by equation (15) will produce broad-band rotations.

RF inhomogeneity is a less fundamental and less interesting source of error than off-resonance effects because it can be reduced by various experimental improvements. The most obvious means is to use better coil designs, but using smaller samples in Shigemi tubes [30] or RF selection techniques [31] is also effective. For these reasons inhomogeneity errors were not considered in the above derivation, but it is nonetheless important to check that our composite pulse family is at least relatively insensitive to RF errors. We do this by taking $V = V_{rf} = \delta\omega_1 (I_x \cos\phi(t) + I_y \sin\phi(t))$, where $\delta\omega_1$ is a measure of the field inhomogeneity, and evaluating $V^{(0)}$ for the ϕ_i specified above. This gives

$$V_x^{(0)} = \delta\omega_1 \quad (16)$$

$$V_y^{(0)} = 0 \quad (17)$$

$$V_z^{(0)} = 0. \quad (18)$$

The error dependence of $V^{(0)}$ for the composite sequence (in the absence of off-resonance effects) is no worse than that of a single pulse, which is acceptable. In the presence of both inhomogeneity and off-resonance errors, evaluating the insensitivity of the sequence becomes more complicated, and it is simplest to assess it graphically by plotting the fidelity of our sequence as a function of RF inhomogeneity and resonance offset. (The fidelity is a measure of how close the composite pulse is to an ideal single pulse; for a description of how it is calculated in a way which is independent of the starting conditions, see reference [20]). Figure 6 shows fidelity plots for Tycko's original 90° composite pulse, and a new pulse derived using our analytic method. For the purpose of comparison, fidelity plots for the equivalent uncompensated pulses are included as well. As can be seen, the RF sensitivity of the new sequences is similar to that of uncompensated sequences, but the sensitivity to off-resonance effects is much smaller.

This insensitivity can also be visualized directly by calculating trajectories of the Bloch vector for single and composite pulses, shown in figure 7. A large resonance offset was chosen so that the mechanism of the pulse's action was clear. The composed pulse is significantly more accurate than the uncompensated one.

‡ This is easily checked by examining the Taylor expansions about 0, and less easily checked by evaluating the difference between equations (13) and (14) using an identity for $\arcsin\alpha - \arccos\beta$.

5. 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.

Acknowledgments

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