Robust logic gates and realistic quantum computation

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The composite rotation approach has been used to develop a range of robust quantum logic gates, including single qubit gates and two qubit gates, which are resistant to systematic errors in their implementation. Single qubit gates based on the BB1 family of composite rotations have been experimentally demonstrated in a variety of systems, but little study has been made of their application in extended computations, and there has been no experimental study of the corresponding robust two qubit gates to date. Here we describe an application of robust gates to nuclear magnetic resonance studies of approximate quantum counting. We find that the BB1 family of robust gates is indeed useful, but that the related NB1, PB1, B4, and P4 families of tailored logic gates are less useful than initially expected.

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I. INTRODUCTION

Quantum information processing [1] has made substantial progress in recent years, but formidable problems remain in the implementation of a general purpose quantum computer. The development of quantum error correction [2–4] was a key step, as it allows quantum computers to function in the presence of random errors. More recently the method of composite rotations (also called composite pulses), developed for nuclear magnetic resonance (NMR) experiments [5–8], has been used to design quantum logic gates which are robust against *systematic* errors in the control fields used to implement them [9,10].

Composite pulses are closely related to the more general field of optimal quantum control, which has been widely studied and finds applications in many fields. In the context of conventional NMR experiments there has been much study of the design of time-optimal pulse sequences [11], which enable unitary transformations to be performed while minimizing losses from decoherence. For applications in NMR quantum computing there has been particular interest in the use of strongly modulated composite pulses [12–14], which are designed to perform particular selective operations in the presence of a complex multispin Hamiltonian, and which can also be designed to be robust against systematic errors in control fields. Although often discussed separately there are clear similarities between these approaches [15]. Similar methods have also been developed in ion trap implementations of quantum computing [16].

Henceforth we only consider a particularly simple group of composite gates, based on the composite pulses originally developed for conventional NMR experiments. These pulses differ from the more general approaches mentioned above in two significant ways. First they provide a simple analytic set of solutions, which allow simple rotations to be converted directly into composite rotations, rather than a recipe for finding a numeric solution for a particular problem. Second, the implementation of these composite gates is particularly simple. For example, in NMR systems they only require control of the phase and duration of a small number of rf pulses at a single fixed frequency and power, while strongly modulated composite pulses also require the frequency and power to be varied. For this reason, these pulses are easy to implement experimentally.

Single qubit gates developed using this approach have been demonstrated experimentally in a range of systems, including NMR [9,10], electron spin resonance (ESR) [17,18], and the quantronium superconducting quantum interference device [19], but there has not yet been much study of their use in an extended quantum algorithm. A related family of robust two qubit gates has also been described [20,21], but these particular gates have not so far been studied experimentally. Here we described the application of single and two qubit logic gates based on the BB1, NB1, and PB1 families of composite pulses to an implementation of approximate quantum counting using NMR studies of a heteronuclear spin system.

II. BB1, NB1, AND PB1 FAMILIES

Composite pulses are designed to perform quantum operations in the presence of systematic errors. Note that it is not necessary to know the size of the error involved, but it is necessary to know its general form. They have been extensively developed in conventional NMR studies [7], principally to correct *pulse length errors*, that is errors in the strength of the field used to induce a rotation, and *off-resonance errors*, that is imperfections arising when an oscillating field is not quite in resonance with the transition it is supposed to drive. Most of these composite pulses are not suitable for use in quantum information processing, but a small group of them, sometimes called fully compensating pulses, are well suited. These pulses work on any initial state, and can in principle be used to replace naive gates without any further modifications.

Perhaps the most useful family of fully compensating pulses developed to date is the BB1 family of pulses which are robust against pulse length errors. The ideal unitary transformation for a θ_ϕ pulse is

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$$U(\theta,\phi)=\exp[-i\theta(I_x\cos\phi+I_y\sin\phi)] \tag{1}$$

but in a real physical system the actual operation will not have this perfect form. In the presence of pulse length errors the real operation has the form

$$V(\theta,\phi)=\exp[-i(1+f)\theta(I_x\cos\phi+I_y\sin\phi)], \tag{2}$$

where f is the fractional error in the pulse length or field power. Defining the propagator fidelity as

$$F=|\mathrm{Tr}(VU^\dagger)|/\mathrm{Tr}(UU^\dagger) \tag{3}$$

gives the result

$$F=\cos\left(\frac{f\theta}{2}\right)\approx 1-\frac{f^2\theta^2}{8} \tag{4}$$

for a simple θ_ϕ pulse. The BB1 family of robust pulses is obtained by replacing the simple pulse θ_ϕ by the composite pulse sequence

$$(\theta/2)_\phi(\pi)_{\phi+\psi}(2\pi)_{\phi+3\psi}(\pi)_{\phi+\psi}(\theta/2)_\phi, \tag{5}$$

where $\psi=\arccos(-\theta/4\pi)$. This composite pulse has a fidelity of

$$F\approx 1-f^6\frac{(32\pi^4\theta^2+14\pi^2\theta^4-\theta^6)}{9216} \tag{6}$$

showing that for small errors the BB1 pulse is far less error prone than a simple pulse.

The NB1 family of pulses is obtained in a similar way; in this case the simple pulse is replaced by

$$(\theta/2)_\phi(\pi)_{\phi+\psi}(2\pi)_{\phi-\psi}(\pi)_{\phi+\psi}(\theta/2)_\phi \tag{7}$$

which has the same structure as BB1, differing only in the phases. This sequence is *more* error-prone than a simple θ_ϕ pulse, and so cannot be used to suppress errors. It does, however, have the interesting property that when $|f|\approx 1$ the resulting composite pulse is a good approximation to the identity operation. Thus is the case of very low pulse powers ($f\approx -1$) an NB1 pulse "does nothing": in effect, evolution under weak fields is suppressed.

The PB1 family of pulses offers a compromise between these two extremes. The simple pulse is replaced by

$$(\theta/2)_\phi(2\pi)_{\phi+\psi'}(4\pi)_{\phi-\psi'}(2\pi)_{\phi+\psi'}(\theta/2)_\phi, \tag{8}$$

where $\psi'=\arccos(-\theta/8\pi)$. These pulses are both robust to small errors *and* able to suppress weak fields, suggesting that PB1 is the best general purpose family of pulses, although the BB1 and NB1 families perform their respective tasks more effectively.

Since these families were described, a range of similar pulses have been discovered, most notably the arbitrary precision pulses of Brown and co-workers [22,23]. In their notation BB1 is called B2 and PB1 is called P2; these are the first members of a series of families of pulses with ever greater error tolerance. These sequences swiftly become extremely long, and here we consider only the next two members, B4 and P4. The B4 composite pulse takes the form

$$\begin{aligned}&(\theta/2)_\phi[(\pi)_{\phi+\psi}(2\pi)_{\phi+3\psi}(\pi)_{\phi+\psi}]^4-2\pi_{\phi+\psi}\\&\quad\times(-4\pi)_{\phi-\psi}(-2\pi)_{\phi+\psi}[(\pi)_{\phi+\psi}(2\pi)_{\phi+3\psi}(\pi)_{\phi+\psi}]^4(\theta/2)_\phi,\end{aligned} \tag{9}$$

where $\psi=\arccos(-\theta/24\pi)$ and the superscript 4 indicates that the section enclosed by square brackets is repeated four times. The central three pulses have negative rotation angles; these can be partially canceled with surrounding pulses, and the remaining rotations can be implemented as positive rotations around axes with phase angles offset by π. The P4 composite pulse is similar, taking the form

$$\begin{aligned}&(\theta/2)_\phi[(2\pi)_{\phi+\psi'}(4\pi)_{\phi-\psi'}(2\pi)_{\phi+\psi'}]^4(-4\pi)_{\phi+\psi'}(-8\pi)_{\phi-\psi'}\\&\quad\times(-4\pi)_{\phi+\psi'}[(2\pi)_{\phi+\psi'}(4\pi)_{\phi-\psi'}(2\pi)_{\phi+\psi'}]^4(\theta/2)_\phi,\end{aligned} \tag{10}$$

where $\psi'=\arccos(-\theta/48\pi)$. Note that the forms for these pulses originally published by Brown *et al.* [22] are slightly incorrect [23].

Under ideal conditions B4 and P4 perform slightly better than their simpler counterparts, but the gain is slight and more detailed simulations [24] indicate that these pulses are highly sensitive to the presence of off-resonance and phase errors. This is confirmed by our experience, described below, that the performance of B4 and P4 is in practice quite poor. Thus the original three families offer perhaps the best combination of simplicity and effectiveness, and we concentrate on them in most of what follows. It might seem that, as previously suggested, PB1 is the best general purpose family of pulses, but this turns out not to be the case.

III. QUANTUM COUNTING EXPERIMENT

Most studies of these particular robust quantum logic gates to date have been either theoretical or have involved only simple demonstrations of single logic gates. Although these are of some interest, it is also important to investigate more complex situations, such as quantum algorithms containing large numbers of logic gates. Quantum counting provides an ideal testing ground as it permits large numbers of logic gates to be implemented in a simple physical system.

Quantum counting is closely related to Grover's quantum search [25–27]. Consider a function $f(x)$ which maps n-bit strings to a single output bit, such that $f(x)=0$ or 1. In general there are $N=2^n$ possible input values, with k values for which $f(x)=1$. Grover's quantum search allows one of these k items to be located, while quantum counting [28,29] allows the value of k to be estimated. The counting algorithm estimates an eigenvalue of the Grover iterate $G=HU_0H^{-1}U_f^-$, which forms the basis of the searching algorithm, where H is the n-bit Hadamard transform, U_0 maps $|000\cdots0\rangle$ to $-|000\cdots0\rangle$ and leaves the remaining basis states alone, and U_f^- maps $|x\rangle$ to $(-1)^{f(x)+1}|x\rangle$. For further details see Ref. [29].

A quantum circuit which implements this algorithm on a two qubit NMR quantum computer is shown in Fig. 1. As usual, pairs of Hadamard gates have been replaced by NMR pseudo-Hadamard gates and their inverse [29,30]. This circuit can be used to count the number of solutions to $f(x)=1$ over a one-bit search space, but similar circuits exist for larger search spaces.

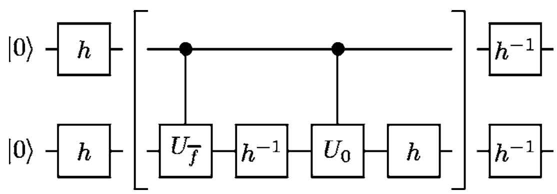

FIG. 1. A quantum circuit for implementing quantum counting on a two qubit NMR quantum computer; the central sequence of gates, surrounded by brackets, is applied r times. A similar circuit can be constructed for a larger search space by replacing the (lower) target bit by a register and replacing gates applied to the target by multibit versions. Gates marked h implement the NMR pseudo-Hadamard operation, while those marked h^{-1} implement the inverse operation.

IV. SINGLE QUBIT GATES

To investigate the effects of systematic errors on single qubit gates we implemented this circuit in an NMR experiment using a solution of ^{13}C labeled sodium formate in D_2O [31]. The formate anion HCO_2^- provides an isolated two spin system, comprising a ^{1}H and a ^{13}C nucleus, with a large coupling between the nuclei. This coupling arises from the scalar coupling interaction, and in a heteronuclear spin system takes the weak-coupling form, usually written as $\pi J 2 I_z S_z$ in NMR product operator notation [5]. (This coupling is sometimes said to have the Ising form, although this name more properly refers to extended networks of such couplings.) In a heteronuclear spin system the RF transmitters can be place in perfect resonance with each qubit, and so off-resonance effects can be essentially ignored. The major remaining source of systematic error is pulse length errors arising from inhomogeneity of the rf fields.

We begin by demonstrating the effect of using robust quantum logic gates to implement a pseudo-Hadamard gate (a 90°_y rotation) on the ^{1}H qubit which begins in an equilibrium state. In addition to the pulse length errors which arise naturally from inhomogeneity, additional errors can be introduced by deliberately mis-setting the pulse length. The effect of doing this is shown in Fig. 2. Each subfigure contains a set of spectra corresponding to pulse length errors in the range ±100%, while the six subfigures correspond to naive pulses and the five families of composite pulses described previously.

As expected the naive pulse gives a signal whose intensity is a cosine function of the fractional error. The BB1 family is much more robust to pulse length errors, while the NB1 family is more sensitive to errors than the naive pulse, and gives much smaller excitations than the naive pulse for errors close to ±100%. The PB1 family shows the expected compromise behavior, with a broad central maximum for small errors, and broad minima around errors of ±100%. Note that the performance is better for errors around −100%, which is the experimentally important case of very weak fields, than for the theoretically equivalent but experimentally unimportant case of errors close to +100%; this reflects the intrinsic inhomogeneity of the rf field. The performance of the B4 composite pulse is broadly similar to that of the much simpler BB1 sequence, while the performance of P4 is clearly rather poor.

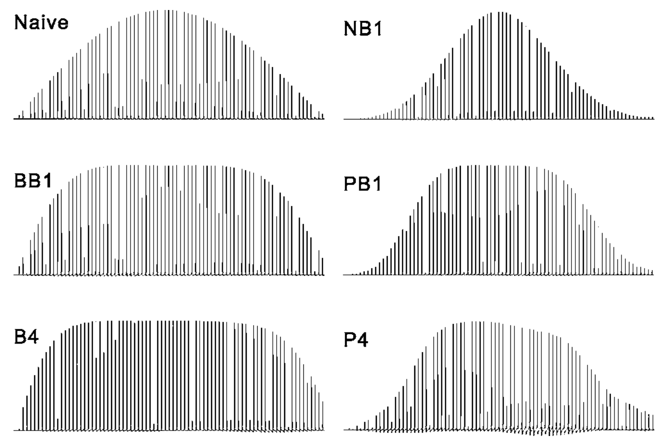

FIG. 2. The effects of pulse length errors on a single qubit pseudo-Hadamard gate (a 90°_y rotation). The figures show the effect of applying this gate to a spin in the thermal equilibrium state, which is equivalent to a pseudopure state $|0\rangle$, followed by observation of the NMR spectrum, effectively measuring the off-diagonal components of the single-spin density matrix. For further details see the main text.

This shows that the robust logic gates can have the desired effects when used to implement a single logic gate, with BB1 and PB1 offering the best performance, but it is also important to investigate how they work in more complex situations. This was done by implementing the quantum counting circuit with the results shown in Fig. 3. Only naive and BB1 single qubit gates were used. The improvement obtained by using BB1 single qubit gates is clear, with much of the signal loss that would naively be ascribed to decoherence clearly arising from pulse length errors. BB1 single qubit gates are therefore used throughout the remainder of this paper.

V. TWO QUBIT GATES

A very similar approach can also be used to tackle systematic errors in coupling gates, which provide the basic two qubit gate for NMR quantum computation [30]. Evolution under a scalar coupling can be thought of as a rotation about the $2I_zS_z$ axis, and errors in the coupling constant J correspond to errors in a rotation angle about this axis. Such er-

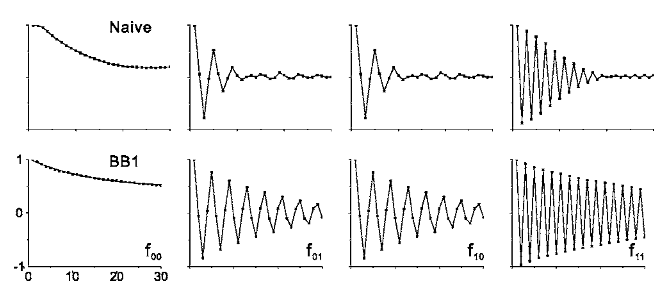

FIG. 3. An implementation of approximate quantum counting with naive and BB1 single qubit gates. The use of BB1 single qubit gates greatly reduces the apparent decoherence rate, indicating that much of the signal loss actually arises from pulse length errors, and that BB1 is effective in correcting for this in a complex sequence.

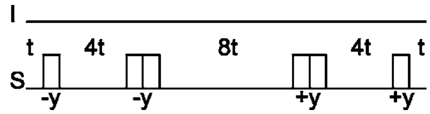

FIG. 4. Pulse sequence for a BB1 robust coupling gate to implement a controlled-NOT gate in a two spin (IS) system. Boxes correspond to single qubit rotations with rotation angles of $\psi = \arccos(-1/8) \approx 97.2°$ applied along the $\pm y$ axes as indicated; time periods correspond to free evolution under the scalar coupling, $\pi J 2 I_z S_z$, for multiples of the time $t=1/4J$. The naive coupling gate corresponds to free evolution for a time $2t$.

rors can be overcome [20,21] by rotating about a sequence of axes tilted from $2I_zS_z$ towards another axis, such as $2I_zS_x$. Defining

$$\theta_\phi \equiv \exp[-i\theta(2I_zS_z \cos\phi + 2I_zS_x \sin\phi)] \qquad (11)$$

allows the naive sequence θ_0 to be replaced by Eq. (5) as before. The tilted evolutions can be achieved by sandwiching free evolution under the coupling Hamiltonian between $\phi_{\mp y}$ pulses applied to spin S. For the case that $\theta = \pi/2$ (which forms the basis of the controlled-NOT gate) the final sequence takes the form shown in Fig. 4.

The results of using these robust two qubit gates could be investigated in much the same way as the single qubit gates shown above, but it is more interesting to consider another phenomenon, that is the ability of the NB1 and PB1 gates to suppress evolution under small scalar couplings. This was studied by implementing quantum counting on the more complex spin system provided by alanine which is ^{13}C labeled at position 2. Like the formate anion, this contains a CH spin system, comprising the labeled ^{13}C and the directly bonded ^{1}H nucleus, but unlike formate this spin system is not completely isolated, as both nuclei have small couplings to the ^{1}H nuclei in the methyl group. This additional coupling interaction could be removed by deuterating the methyl group, or by applying decoupling fields, but here we seek to suppress the coupling using robust logic gates.

We begin by studying evolution under the CH coupling, and concentrate on evolution times of $n/2J$, where n is a positive integer. This was done by applying a pseudo-Hadamard gate to the ^{13}C nucleus and then allowing the spin system to evolve under a coupling gate (either naive or composite) for an effective time $n/2J$. The results are shown in Fig. 5. The naive gate appears to perform well for small evolution times, as the evolution under the small J coupling can be largely ignored: this coupling is clearly visible in the spectra where each component of the doublet is split into a 1:3:3:1 multiplet, but all four components appear to have very similar phases. For longer evolution times, however, the detrimental effect of this additional coupling becomes clear, as the components appear with quite different phases, indicating significant evolution under the coupling.

In an attempt to overcome this we implemented NB1 coupling gates, which should suppress evolution under this small coupling. It is immediately obvious from Fig. 5 that this approach does not work, as the multiplets are far more distorted than those seen using the naive sequence. In retrospect

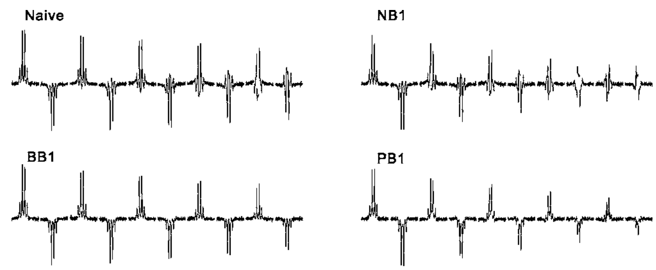

FIG. 5. Implementation of an coupling gate in the presence of extraneous couplings. For details see the main text. The ten ^{13}C spectra in each subfigure correspond to increasing periods of evolution under the coupling, and the desired pattern is a simple alternation in signal intensity between +1 and −1; deviations in the naive implementation arise from evolution under the extraneous couplings to the methyl protons. It might be expected that evolution under this small coupling would be effectively suppressed by the NB1 sequence, but this performs very poorly, and the best results are seen from the BB1 sequence.

this is unsurprising: NB1 is designed to suppress a small coupling on the assumption that this is the only coupling present. If the small coupling occurs in addition to another much larger coupling then there is no reason to believe that NB1 will suppress it.

Examination of the results from BB1 and PB1 coupling gates makes this point even more clearly. BB1 gives much cleaner spectra than the naive coupling gate, with the results of PB1 being similar but significantly poorer. Once again the explanation is clear in retrospect: although we know that the splittings visible in the spectrum arise from the combination of a large coupling and a small coupling, the pulse sequence is blind to this origin. The same pattern could in principle arise from a mixture of different molecules with a *range* of coupling constants. The BB1 robust gate is designed to give very similar behavior over this range of coupling sizes, and so all the different components of the multiplet appear in phase. The action of PB1 is similar: the quality of the spectra seen arises not from the ability of this sequence to suppress small couplings, but from its ability to tolerate a range of couplings. Over the range of couplings seen in this system the behavior of PB1 and BB1 should be very similar, and the relatively poor results observed from PB1 are probably a consequence of the fact that the PB1 sequence take almost twice as long as BB1, leading to increased problems from decoherence.

VI. SIMPLIFYING SPIN SYSTEMS

The results above show that our original idea that NB1 based composite two qubit gates could be used to suppress small couplings, in effect simplifying complex spin systems, is incorrect. However, BB1 based two qubit gates do result in the desired suppression, with PB1 sequences giving similar but slightly poorer results, suggesting that it might be possible to use these to simplify spin systems instead.

Following this idea we attempted to implement quantum counting in our labeled alanine spin system, using BB1 to suppress the small couplings between the ^{13}C qubit and the methyl protons while using the large coupling between the ^{13}C and the directly bonded ^{1}H qubit to implement logic gates. These attempts were not successful (data not shown), and once again it is clear in retrospect why this idea will not work. Although the small couplings between the ^{13}C and the methyl protons in the labeled alanine spin system can indeed be suppressed by BB1, there are also small couplings between the ^{1}H qubit and the methyl protons which will not be suppressed. These homonuclear couplings could, of course, be removed by frequency selective pulses, or by decoupling, but either approach would act to directly simplify the spin system, rendering the BB1 approach unnecessary.

VII. CONCLUSIONS

Our results confirm that simple composite pulses can indeed be used to suppress systematic errors on single qubit gates used in implementations of complex quantum algorithms. The BB1 approach is likely to prove the most useful, while PB1 may find applications in some special areas. The BB1 sequence can also be used to implement robust two qubit gates, although in this case the extra time required for the longer pulse sequence may cause difficulties. The more complex B4 and P4 sequences, although theoretically superior, do not perform well in practice.

Two qubit gates based on NB1 and PB1 could in principle be used to suppress the effects of small couplings, but this is not effective when the small couplings occur in addition to larger couplings which are used to implement gates. In this case the small couplings can be treated as small errors in the large coupling, and BB1 provides the best suppression of their effects. It might appear that this approach could be used to neglect small couplings in complex spin systems, effectively simplifying the spin system through composite pulses, but this approach will rarely if ever be effective, as corresponding homonuclear couplings cannot be suppressed by these simple composite pulse methods. More complex approaches, such as strongly modulated composite pulses, could be more effective, but such pulses need to be designed on a case by case basis.

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