Journal of Magnetic Resonance **140,** 371–378 (1999)
Article ID jmre.1999.1851, available online at http://www.idealibrary.com on IDEAL®

Construction and Implementation of NMR Quantum Logic Gates for Two Spin Systems

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Received November 24, 1998; revised April 7, 1999

The implementation of small prototype quantum computers has been studied through ensemble quantum computing via NMR measurements. In such laboratory studies it is convenient to have access to a wide array of logic gates. Here a systematic approach to reduce the logic gate to an NMR pulse sequence is introduced. This approach views the truth table for a quantum logic operation as a permutation matrix that corresponds to a propagator for an NMR transition. This propagator is then used as the starting point for the derivation of a pulse sequence. Pulse sequences for all the permutations of a four level system are reported along with implementations of representative examples on a two spin-$\frac{1}{2}$ system, ^{13}C-labeled chloroform. © 1999 Academic Press

INTRODUCTION

If built, a quantum computer will be capable of performing select computations much more efficiently than a classical computer. Such a quantum computer relies on quantum parallelism whereby one operates on quantum superpositions rather than classical binary states (*1–3*).

Ensemble quantum computation has been shown to be an especially useful prototype system for a small quantum computer. To date, a universal set of logic gates (*4*), pseudo-pure states (*4, 5*), quantum database searching algorithms (*6, 7*), and error correction (*8*) have all been implemented on NMR ensemble quantum computers.

The permutation gates form a particularly important subset of the logic gates (when combined with the one-bit gates they form a complete set of logic gates) (*9*). Gates of this form include the well-known controlled-NOT (c-NOT), Toffoli, and Fredkin gates and can be easily mapped to a classical truth table. While it is true that equivalent gates may be composed from a series of c-NOT and Fredkin gates, in the present implementation of ensemble quantum computing via NMR it is often convenient to reduce such a series of gates to the simplest implementation. Although this reduction does not scale well for an actual quantum computer, it is helpful in the present testing of prototype quantum computers. This form of compilation keeps the overall time of the operation short compared to the decoherence time of the system. In addition, gates developed for coherent quantum systems need to preserve the phase of the system; it is desirable to avoid introducing and tracking phase rotations of qubits.

In this work the link amongst the truth table, permutation matrix, and propagator for a logic gate will be explored. The propagator for a logic gate can be expanded into a form that can readily be reduced to an implementable pulse sequence. A recipe for deriving pulse sequences that are consistent with the propagator, but not necessarily unique, is presented. This methodology was developed and demonstrated on a two spin system because it can provide a complete picture: since the number of gates grows faster than exponential with the number of spins, the two spin system is the only one that can be explored conveniently and in its full complexity. Extension to larger spin systems is straightforward; the formalism behind this, geometric algebra, has been used in treating some quantum computing experiments (*10*) as well as for the derivation of an effective Hamiltonian on a two spin system (*11*). A complete description of the formalism will be discussed in more detail in future work.

TRUTH TABLES AS PERMUTATION OPERATIONS

A convenient description of a logic gate is its truth table. A simple example is the c-NOT gate in which one bit is flipped conditional on the state of the other bit (Table 1). In NMR where the nuclear spin is the qubit, information is encoded in the z-state of the nuclear spin (in the case of spin $\frac{1}{2}$). Thus, true is spin-down or the state $|1\rangle$, and false is spin-up or the state $|0\rangle$.

When the logic table shown in Table 1 is written in these terms it can easily be seen that a transformation of spin eigenstates has taken place,

$$\begin{aligned} |00\rangle &\rightarrow |00\rangle \\ |01\rangle &\rightarrow |01\rangle \\ |10\rangle &\rightarrow |11\rangle \\ |11\rangle &\rightarrow |10\rangle \end{aligned} \quad . \qquad [1]$$

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TABLE 1
Logic Table for c-NOT Gate

A_{input}	B_{input}	A_{output}	B_{output}
F (up)	F (up)	F (up)	F (up)
F (up)	T (down)	F (up)	T (down)
T (down)	F (up)	T (down)	T (down)
T (down)	T (down)	T (down)	F (up)

The action of the c-NOT logic gate is to swap two of the spin populations. Logic gates such as these, which can be expressed as a truth table and which are unitary, are necessarily *permutation matrices,* wherein each column and row contains exactly a single 1, while the rest of the matrix is zeroes (*12*, *13*). These permutations are propagators for specific NMR transitions (since a transition is just a permutation of the spin populations around the energy level diagram). Thus, the truth table, the permutation matrix, and the propagator all describe the same logical operation and can be used interchangeably. The propagator describing the c-NOT is therefore

$$P = U = \begin{array}{c} \\ |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{array} \begin{array}{c} \begin{array}{cccc} \langle 00| & \langle 01| & \langle 10| & \langle 11| \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{array}. \qquad [2]$$

PERMUTATION OPERATIONS FOR TWO SPIN SYSTEMS

Since the implementation of the logic gate on a physical system is of interest, it is useful to make this mapping concrete by referring to the energy level diagram of a two spin system (Fig. 1). A weakly coupled two spin-$\frac{1}{2}$ system has an internal Hamiltonian of $H_{\text{int}} = \frac{1}{2}\omega_{\text{A}}\sigma_Z^A + \frac{1}{2}\omega_{\text{B}}\sigma_Z^B + \frac{1}{2}\pi J\sigma_Z^A\sigma_Z^B$.

The highlighted transformation in Fig. 1 can be implemented by a selective RF pulse (*14*, *15*). The effective propagator may be approximated as

$$U = e^{-i\omega t(1/4)(\sigma_X^B - \sigma_Z^A\sigma_X^B)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos\left(\frac{\omega t}{2}\right) & -i\sin\left(\frac{\omega t}{2}\right) \\ 0 & 0 & -i\sin\left(\frac{\omega t}{2}\right) & \cos\left(\frac{\omega t}{2}\right) \end{pmatrix}. \qquad [3]$$

The true propagator is more complex (*11*) but has been shown to reduce to the above form to within an arbitrarily small error. For the case $\omega t = \pi$, the propagator, U, becomes

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \end{pmatrix}. \qquad [4]$$

To within a phase, the unitary operation in Eq. [4] which exchanges the spin populations in levels 2 and 3 is a permutation matrix. While the description so far has involved only classical elements (truth tables), logic gates for quantum computation must operate "correctly" on superposition states. It is inconvenient to have and track additional phase terms like those that appear in Eq. [4]. For convenience, a propagator like the permutation matrix given in Eq. [2] is desired, where there are no additional phase terms.

Rather than characterize these gates based on truth tables, it is more compact to use the well-known symmetry relations of the permutation group. A permutation, P, that swaps the spin populations in the energy levels denoted as 2 and 3 in Fig. 1 is designated as $P = (2\ 3)$. This expression is a cyclic permutation of 2 and 3; thus (0 3 2 1) is a cyclic permutation of all four members of the energy level diagram.

In general, with n objects there are $n!$ permutations. The set of these $n!$ permutations forms a *group* called the symmetric group of degree n and is denoted by S_n (*16*). The two spin case with four energy levels and four different spin populations describes the group S_4. There are 4!, or 24, different permutations, each corresponding to a different transformation in the energy level diagram.

It is helpful to divide the members of the permutation group on the basis of their *conjugacy class.* A conjugacy class of order k is an operation that switches k different energy levels. In the case of a two spin system there are conjugacy classes defining different operations: the identity operation and oper-

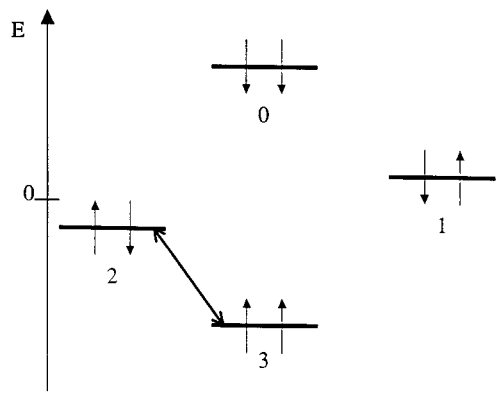

FIG. 1. Energy level diagram for a coupled two spin system with the internal Hamiltonian, $H_{\text{int}} = \frac{1}{2}\omega_{\text{A}}\sigma_Z^A + \frac{1}{2}\omega_{\text{B}}\sigma_Z^B + \frac{1}{2}\pi J\sigma_Z^A\sigma_Z^B$. Such a system has four different energy levels, labeled {0, 1, 2, 3}. Quantum logic operations can be thought of as permutations that permute the populations of various energy levels. In the above example, a c-NOT gate exchanges the populations of energy levels 2 and 3. Thus the propagator, the permutation matrix, and the truth table all represent the same information.

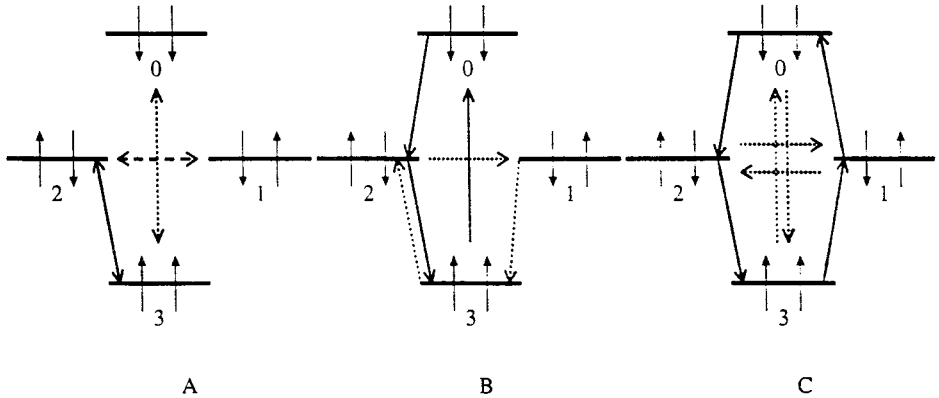

FIG. 2. Energy level diagrams for 2-, 3-, and 4-element operations. (A) Two-element operations showing zero (dashed), single (solid), and double (dotted) quantum transitions. (B) 3-element operations. Note that the arrows are now unidirectional, indicating that populations are no longer being swapped, but are being rotated around a "loop." (C) Four-element operations. The solid lines indicate single quantum "loops" while the dotted lines show zero and double quantum transitions.

ations which swap two, three, and four elements. For S_4, operations which swap two and three elements are two- and three-cycles, respectively, while four element swaps can be accomplished by both four-cycle operations and operations which are the product of two *disjoint* (i.e., neither two-cycle has elements in common) two-cycles.

The conjugacy classes of the 24 permutations are associated with transitions on an energy level diagram (Fig. 2). The identity operation simply leaves the spin populations exactly as they are. In a two-cycle operation, two spin populations are swapped with one another, while the others are left alone. Analysis of the energy level diagram shows that two-cycles may involve zero, single, or double quantum transitions. Three-cycle operations swap three different spin populations and will involve either a zero or a double quantum transition. Four element swap operations permute all of the spin populations. There are four-cycles that involve single quantum "loops" that exchange populations around the energy level diagram. In addition, there are operations that swap four elements, but may be described as the product of two disjoint two-cycles where each two-cycle has no members in common. Methods for dealing with this will be discussed shortly.

USING THE TOOLS OF GEOMETRIC ALGEBRA TO CONSTRUCT PULSE SEQUENCES

The tools of geometric algebra (*10*) provide a useful means of constructing pulse sequences for quantum logic operations from the permutation matrix (note that the systematic derivation of a pulse sequence in this manner is analogous to the work of Briand and Sorensen found in Refs. (*19*) and (*20*)). The method is based on the use of primitive idempotents. Primitive idempotents, $E_{\pm}$, satisfy the following properties:

$$E_+ + E_- = 1, \quad (E_\pm)^2 = E_\pm, \quad E_+E_- = 0. \qquad [5]$$

A useful property of these idempotents is that they help simplify exponential operations as follows:

$$e^{A\cdot E_\pm} = e^A E_\pm + E_\mp \quad (\text{provided that } [A, E_\pm] = 0). \qquad [6]$$

For spin-$\frac{1}{2}$ particles, the idempotents of interest are

$$E^i_\pm = \frac{1}{2}(1 \pm \sigma^i_Z) \quad E^{i,j}_\pm = \frac{1}{2}(1 \pm \sigma^i_Z\sigma^j_Z), \qquad [7]$$

where σ are the Pauli matrices. Note that E^A_+ is thus the density matrix for the A spin in the up state, E^B_- is the density matrix for the B spin in the down state, etc. It should be noted that such operators have been useful in other NMR quantum computing experiments (*17*).

Using the definitions of E_+, E_-, and σ_X, the propagator in Eq. [2] can be written in a simple form.

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$
$$= E^A_+E^B_+ + E^A_-E^B_+ + \sigma^B_X E^A_+E^B_- + \sigma^B_X E^A_-E^B_-. \qquad [8]$$

The upper left hand element of the matrix, $|00\rangle$, is $E^A_+E^B_+$, the next element, $|10\rangle$, is $E^A_-E^B_+$, etc. By taking advantage of the rules in Eq. [5], namely that $E^i_+ + E^i_- = 1$, the right hand side of Eq. [8] simplifies to

$$U = \sigma^B_X E^A_- + E^A_+. \qquad [9]$$

In this form, there is a simple interpretation of the propagator, U. The right hand side of Eq. [9] can be read as an instruction

TABLE 2
Two-Cycle Operations

Transition	Propagator	Idempotent expression
(1 2)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$E_+^{A,B} + \sigma_X^A \sigma_X^B E_-^{A,B}$
(0 3)	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	$E_-^{A,B} + \sigma_X^A \sigma_X^B E_+^{A,B}$
(2 3)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$E_+^A + \sigma_X^B E_-^A$
(1 3)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	$E_+^B + \sigma_X^A E_-^B$
(0 1)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$E_-^A + \sigma_X^B E_+^A$
(0 2)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$E_-^B + \sigma_X^A E_+^B$

to rotate the B spin about the x axis if the A spin is down and to do the identity operation (i.e., nothing) if the A spin is up. The expression given in Eq. [9] could have been written directly from the truth table. Table 2 gives the idempotent expressions for the two-cycle operations.

The expression of the problem in terms of idempotents also makes the generation of the pulse sequence quite straightforward. The propagator for the c-NOT should be manipulated into elements which can be physically applied (e.g., RF pulses and evolutions under the internal Hamiltonian). This is accomplished by first rewriting the propagator as

$$U = E_+^A + (\iota)(-\iota)\sigma_X^B E_-^A, \qquad [10]$$

which can then be factorized into

$$U = (-\iota\sigma_X^B E_-^A + E_+^A)(\iota E_-^A + E_+^A). \qquad [11]$$

Using the fact that the idempotents may be expressed as exponentials as given in Eq. [6], the above expression becomes

$$U = e^{-\iota\sigma_X^B E_-^A \pi/2} \cdot e^{\iota E_-^A \pi/2}. \qquad [12]$$

This expression may be expanded as

$$U = e^{\iota\pi/4} \cdot e^{-\iota\sigma_X^B \pi/4} \cdot e^{-\iota\sigma_Z^A \pi/4} \cdot e^{\iota\sigma_Z^A \sigma_X^B \pi/4}. \qquad [13]$$

This is an exact expression for the propagator and is also a pulse sequence for its implementation. It should be noted that all of these terms commute, so that they may applied in any order. When implemented, and the order is decided upon, the pulse sequence will be read from right to left since the above expression constitutes the left hand side propagator.

In order to implement this propagator on the spectrometer it should be noted that

$$e^{-\iota\sigma_Z^A \pi/4} = e^{-\iota\sigma_X^A \pi/4} \cdot e^{-\iota\sigma_Y^A \pi/4} \cdot e^{\iota\sigma_X^A \pi/4}, \qquad [14]$$

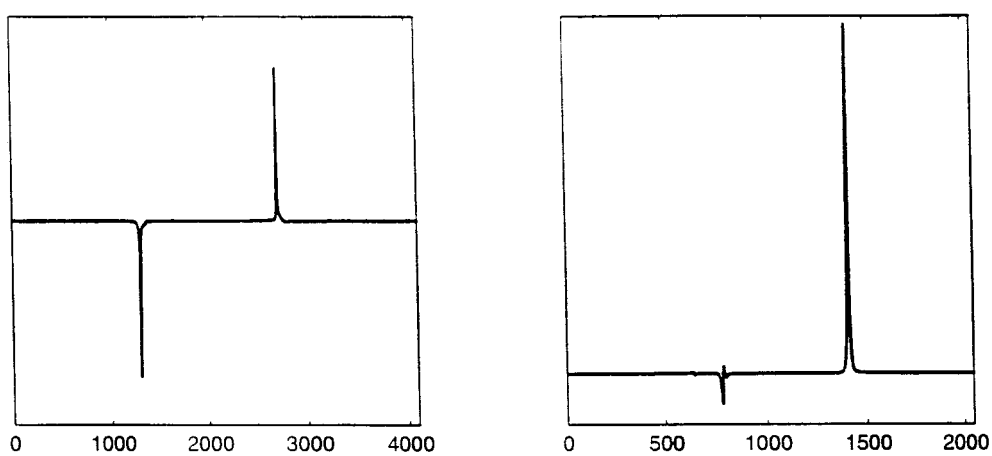

FIG. 3. Results of applying the transition (2 3) to the equilibrium state of chloroform, which performs the transformation $\frac{1}{2}(\sigma_Z^A + \sigma_Z^B) \rightarrow \frac{1}{2}(\sigma_Z^A \sigma_Z^B + \sigma_Z^B)$. The spectrum on the left is after a $\pi/2$ readout pulse on the A spin. It is an antiphase spectrum corresponding to the antiphase state $\frac{1}{2}(\sigma_X^A \sigma_Z^B + \sigma_Z^B)$ as expected. The spectrum on the right is after a $\pi/2$ readout pulse on the B spin. The single peak corresponds to the state $\frac{1}{2}(\sigma_Z^A \sigma_X^B + \sigma_X^B)$, which is as expected.

TABLE 3
Three-Cycle Operations

Operation	Propagator	Idempotent expression
(0 2 3)	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$(E_-^B + \sigma_X^A E_+^B)(E_+^A + \sigma_X^B E_-^A)$
(0 3 1)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	$(E_-^{A,B} + \sigma_X^A \sigma_X^B E_+^{A,B})(E_+^B + \sigma_X^A E_-^B)$
(0 3 2)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	$(E_-^{A,B} + \sigma_X^A \sigma_X^B E_+^{A,B})(E_+^A + \sigma_X^B E_-^A)$
(0 1 3)	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	$(E_-^A + \sigma_X^B E_+^A)(E_+^B + \sigma_X^A E_-^B)$
(0 1 2)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$(E_-^A + \sigma_X^B E_+^A)(E_+^{A,B} + \sigma_X^A \sigma_X^B E_-^{A,B})$
(0 2 1)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$(E_-^B + \sigma_X^A E_+^B)(E_+^{A,B} + \sigma_X^A \sigma_X^B E_-^{A,B})$
(1 3 2)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	$(E_+^B + \sigma_X^A E_-^B)(E_+^A + \sigma_X^B E_-^A)$
(1 2 3)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$(E_+^{A,B} + \sigma_X^A \sigma_X^B E_-^{A,B})(E_+^A + \sigma_X^B E_-^A)$

and

$$e^{\iota\sigma_Z^A\sigma_X^B\pi/4} = e^{-\iota\sigma_Y^B\pi/4} \cdot e^{\iota\sigma_Z^A\sigma_Z^B\pi/4} \cdot e^{\iota\sigma_Y^B\pi/4}. \quad [15]$$

By combing like terms the propagator, U, becomes

$$U = e^{-\iota(\sigma_X^A+\sigma_X^B)\pi/4} \cdot e^{-\iota(\sigma_Y^A+\sigma_Y^B)\pi/4} \cdot e^{\iota\sigma_X^A\pi/4} \cdot e^{\iota\sigma_Z^A\sigma_Z^B\pi/4} \cdot e^{\iota\sigma_Y^B\pi/4}. \quad [16]$$

This is easily seen as an NMR pulse sequence (recall, though, that the above propagator is to be applied from right to left),

$$\left(\frac{\pi}{2}\right)_{-Y}^{B} - \left(\frac{1}{2J}\right)_{\mathrm{SC}} - \left(\frac{\pi}{2}\right)_{-X}^{A} - \left(\frac{\pi}{2}\right)_{Y}^{A+B} - \left(\frac{\pi}{2}\right)_{X}^{A+B}, \quad [17]$$

where $(\frac{1}{2}J)_{\mathrm{SC}}$ is a period of length $\frac{1}{2}J$ where only scalar coupling takes place and the chemical shift terms have been refocused. A convenient means of implementing this is a pulse that simultaneously rotates the two coupled spins (*18*). The $\sigma_Z^A\sigma_Z^B$ rotation can be rewritten

$$e^{\iota\theta\sigma_Z^A\sigma_Z^B} = e^{(\iota/2)(\theta\sigma_Z^A\sigma_Z^B+\omega_A\sigma_Z^A+\omega_B\sigma_Z^B)} \cdot e^{(\iota/2)(\theta\sigma_Z^A\sigma_Z^B-\omega_A\sigma_Z^A-\omega_B\sigma_Z^B)}. \quad [18]$$

This is equivalent to,

$$= e^{\iota Ht/2} \cdot e^{\iota(\sigma_X^A+\sigma_X^B)\pi/2} \cdot e^{\iota Ht/2} \cdot e^{-\iota(\sigma_X^A+\sigma_X^B)\pi/2}, \quad [19]$$

where H is the internal Hamiltonian of the system. Thus, the pulse sequence to implement the above $(\frac{1}{2}\mathrm{J})_{\mathrm{SC}}$ is

$$\left(\frac{1}{4J}\right) - (\pi)_X^{A+B} - \left(\frac{1}{4J}\right) - (\pi)_{-X}^{A+B}. \quad [20]$$

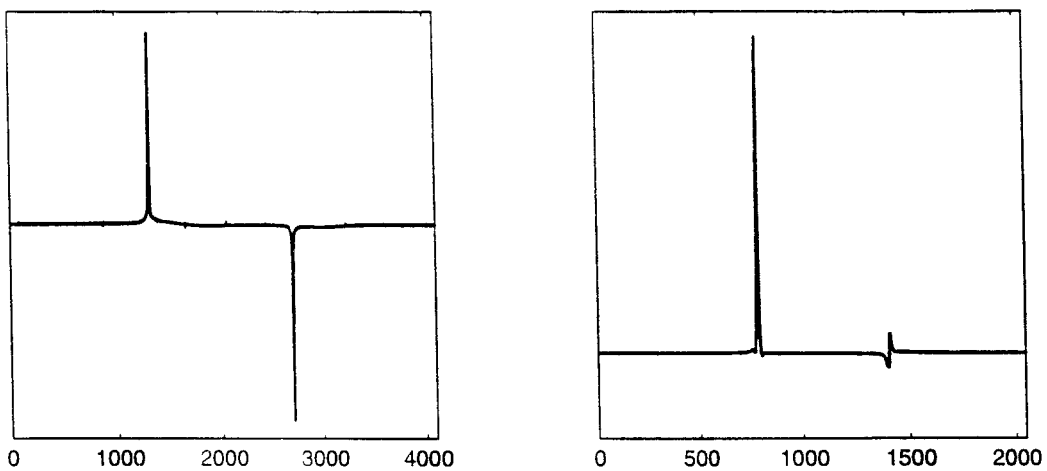

FIG. 4. Results of applying the transition (0 3 2) to the equilibrium state of chloroform, which performs the transformation $\frac{1}{2}(\sigma_Z^A + \sigma_Z^B) \rightarrow \frac{1}{2}(\sigma_Z^A\sigma_Z^B - \sigma_Z^B)$. The spectrum on the left was acquired after application of a $\pi/2$ readout pulse on the A spin and corresponds to the state $\frac{1}{2}(\sigma_X^A\sigma_Z^B - \sigma_Z^B)$. The spectrum on the right was acquired after a $\pi/2$ pulse on the B spin and yields the state $\frac{1}{2}(\sigma_Z^A\sigma_X^B - \sigma_X^B)$.

TABLE 4
Four-Element Operations

Operation	Propagator	Idempotent expression
(0 3) (1 2)	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	$\sigma_X^A \sigma_X^B$
(0 1) (2 3)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	σ_X^A
(0 2) (1 3)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	σ_X^B
(1 3 0 2)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	$\sigma_X^B E_+^{A,B} + \sigma_X^A E_-^{A,B}$
(2 0 3 1)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\sigma_X^A E_+^{A,B} + \sigma_X^B E_-^{A,B}$
(3 2 0 1)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	$\sigma_X^A(\sigma_X^B E_-^A + E_+^A)$
(3 0 1 2)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	$\sigma_X^B(\sigma_X^A E_+^B + E_-^B)$
(2 3 1 0)	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	$\sigma_X^A(E_+^A + \sigma_X^B E_-^A)$
(1 2 3 0)	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\sigma_X^B(E_+^B + \sigma_X^A E_-^B)$

Several points about the above derivation deserve mention. First, the above formulation is not entirely surprising since it is the expression of the transition Hamiltonian given by Sorensen *et al.* and Hatanaka *et al.* (*14, 15*) with an additional global phase term, and a z-rotation on the A spin. This z-rotation explains the phase differences between the propagator given in Eq. [4] and the permutation matrix from Eq. [2]. The expansion of the propagator into idempotents has just given an expression that lends itself more to the language of quantum computation.

Second, the global phase term is not as unimportant as it may seem. Although it would not have any bearing on a two spin experiment, in a computationally significant experiment it will be the case that these two spin operations are being performed within a larger population of spins (there are no computationally significant two-bit computations). These two spin operations are now embedded within a larger density matrix, and the phase term is no longer global. In such an instance the dependent phase terms must be correctly applied.

Finally, the pulse sequence derived above is not unique, and any number of sequences can be derived from the idempotent expansion. Using the expression of the logic in terms of geometric algebra yields a concrete physical implementation of a logic gate that can depend on the system under study. For example, in some compounds the use of hard pulses may be simpler and the derivation of the pulse sequence can reflect this.

Results of applying the pulse sequence given in Eq. [17] to the equilibrium state of ^{13}C-labeled chloroform are shown in Fig. 3. The c-NOT operation has the effect of taking the equilibrium state $\frac{1}{2}(\sigma_Z^A + \sigma_Z^B)$ into $\frac{1}{2}(\sigma_Z^A\sigma_Z^B + \sigma_Z^B)$. A readout on the carbon spins (the A spins) gives the expected antiphase doublet, while a readout on the hydrogen spins (the B spins) gives the expected single peak at double the intensity.

CONSTRUCTION OF HIGHER ORDER OPERATIONS FROM THE TWO-ELEMENT OPERATIONS

Methods from group theory provide a means whereby the higher order cycles, in this case the three-cycle and four element operations, can be constructed from two-cycle operations.

Construction of the Three-Cycle Operations

As was mentioned above, the three-cycle operations are of the form (0 1 3), etc. Such a permutation can be constructed from two two-cycles by breaking up the three-cycle as (0 1 3) = (0 1) (1 3). Thus the pulse sequence for (0 1 3) is obtained by appending the pulse sequence for the two-cycle (0 1) to the two-cycle (1 3), both of which are found in Table 2.

There is still a degree of flexibility whereby the two sequences that are the easiest to implement for a given compound can be merged. Since each two-cycle is its own inverse, the product of two two-cycles $(a\ b)\ (b\ c)$ can be viewed as $(a\ b)\ (b\ c)\ (a\ b)^{-1}\ (a\ b)$. The first three terms are a rotation of sorts: $(a\ b)\ (b\ c)\ (a\ b)^{-1} = (a\ c)$. Thus, $(a\ b)\ (b\ c) = (a\ c)\ (a\ b)$, and Eq. [19] can be rewritten as any of the following:

$$(1\ 2\ 3) = (1\ 2)\ (2\ 3) = (2\ 3)\ (1\ 3) = (1\ 3)\ (1\ 2). \quad [21]$$

The expressions for the three-cycle operations are shown in Table 3.

The results of applying the transition (0 3 2) to the equilibrium state of chloroform are shown in Fig. 4. The (0 3 2) sequence operates opposite the above c-NOT operation and takes the equilibrium state $\frac{1}{2}(\sigma_Z^A + \sigma_Z^B)$ into $\frac{1}{2}(\sigma_Z^A\sigma_Z^B - \sigma_Z^B)$. A readout on the carbon spins (the A spins) gives the expected antiphase doublet (which is now opposite in phase to that of the

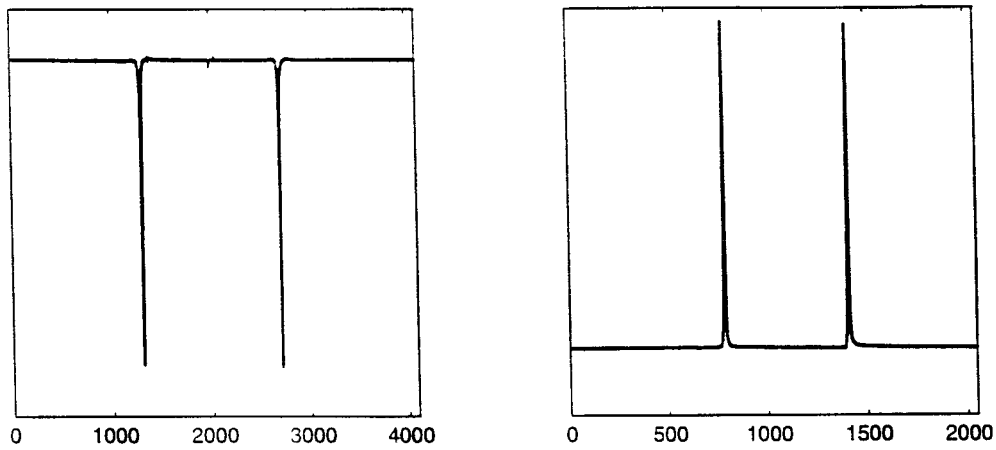

FIG. 5. Application of the transformation (0 1)(2 3) to the equilibrium state of chloroform, which performs the transformation $\frac{1}{2}(\sigma_Z^A + \sigma_Z^B) \rightarrow \frac{1}{2}(-\sigma_Z^A + \sigma_Z^B)$. The spectrum on the left was obtained after an application of a readout pulse on the A spins and corresponds to the state $\frac{1}{2}(-\sigma_X^A + \sigma_Z^B)$. The spectrum on the right, acquired after a readout pulse on the B spins corresponds to the state $\frac{1}{2}(-\sigma_Z^A + \sigma_X^B)$.

c-NOT), while a readout on the hydrogen spins (the B spins) gives a single peak at twice the intensity, but on the opposite transition from the above c-NOT.

Construction of the Four-Element Operations

The four-element operations are somewhat easier to construct. As was stated earlier, some operations are the product of two disjoint (commuting) two-cycles. A disjoint two-cycle is of the form $(a\ b)\ (c\ d)$ where neither two-cycle has an element in common with the other. In such a case, the elements of one do not affect the other. An example of this is the operation that swaps populations at 0 and 3 and populations at 1 and 2. Such an operation is expressed as (0 3) (1 2). Using the methods outlined above the operation can be expressed as

$$U = \sigma_X^A \sigma_X^B, \qquad [22]$$

which is a hard π-pulse. Note that applying the two two-cycle operations will simplify to the above expression.

As with the three-cycle operations, the four-cycles can be composed from a series of two-cycles. An example of this is the operation (0 1 2 3) which can be rewritten as (0 1) (1 2) (2 3). The same techniques of rotating the members can be used and the above is rewritten as (0 1) (2 3) (1 3). The first two terms are a disjoint two-cycle which is just the operation σ_X^A, and the expression for (1 3) was already found. Thus, the operation (0 1 2 3) is

$$U = \sigma_X^A(\sigma_X^B E_-^A + E_+^A). \qquad [23]$$

Analysis of the other nondisjoint operations shows that they, too, are an additional rotation of a two-cycle operation. These results are summarized in Table 4.

The pulse sequence for the transition (0 1)(2 3) is a π-pulse on the *A* spin. This was implemented on the chloroform sample and the results can be seen in Fig. 5. This is simply a NOT gate on the *A* spin. Thus the equilibrium state $\frac{1}{2}(\sigma_Z^A + \sigma_Z^B)$ is taken into $\frac{1}{2}(-\sigma_Z^A + \sigma_Z^B)$. The readout on the carbon spins shows that they have been inverted, while the readout on the hydrogen spins confirm that they were left alone.

CONCLUSIONS

Actual pulse sequences have been derived for all possible two spin logic gates where the gate is expressible as a both a unitary operator and a truth table. Starting with the truth table for the operation, we have used methods from geometric algebra and group theory to construct physical implementations of these gates on an NMR spectrometer. The general method for the construction of these pulse sequences can be extended to more complex spin systems. Care was taken in the design of these sequences to preserve the phases in the propagator such that any of these sequences will operate correctly on a quantum superposition. In our exploration of quantum computing on a prototype ensemble quantum computer, we have found it to be very useful to have such an array of logic gates available.

ACKNOWLEDGMENTS

This work was supported by the U.S. Army research office Grant DAAG55-97-1-0342 under the DARPA Ultrascale Computing Program. AFF thanks NSF/MCB 9527181. MDP thanks the Harvard–MIT Division of Health Sciences and Technology for academic and financial support.

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