Abstract. Much of the current understanding of logic gates for quantum computation relies on the application of one- and two-qubit gates in order to implement a universal set of logic gates, as well as other gates. Such ideas stem from the notion that the Hamiltonians available for quantum computation are one or two-body processes. However, present day NMR implementations of quantum information processing (QIP) rely on the internal Hamiltonian of a liquid state system in which there are many two-body processes that occur simultaneously. Such use of the internal Hamiltonian allows for the creation of ‘multiqubit’ logic gates, i.e. logic gates that operate on many qubits simultaneously and are more efficient than a sequence of one- and two-qubit rotations that effect the same operation. Such larger qubit operations offer a universal set of gates (even when not all couplings within the internal Hamiltonian are readily accessible) as well as more convenient and efficient implementations of the Hadamard transform, the controlled-NOT gate, and a quantum Fourier transform that scales linearly (assuming all couplings can be turned on and off at will).

1. Introduction

Quantum computing relies on the principle of quantum superposition to obtain enormous computational advantages over classical computational schemes [1]–[5]. Nuclear magnetic resonance (NMR) implementations of quantum computing are governed by an internal Hamiltonian, $H_{\text{int}}$, that dictates the behaviour of the system. Implicit in such implementations of
quantum computation is the ability to control this internal Hamiltonian and thereby manipulate the system in some fashion that is akin to computation. There are essentially two main strategies to accomplish this. In one approach, $H_{\text{int}}$ can be set to zero, and an ‘engineered’ Hamiltonian used for the control and implementation of logic gates. Conversely, $H_{\text{int}}$ can be utilized to both address the qubits and implement logic gates. In the first case, implementations of logic gates are formulated as one- and two-qubit rotations as this is the most natural form of an external Hamiltonian. In the second case, however, because $H_{\text{int}}$ simultaneously affects all qubits involved in the computation, it is more convenient to implement logic gates that operate on multiple qubits. That is, the use of $H_{\text{int}}$ to both address and manipulate the qubits allows for logic gates that can operate on many qubits simultaneously, rather than one or two qubits at a time.

Unconcerned with the limits of real systems (e.g. decoherence), the first studies of quantum logic gates concerned themselves with universality and scaling rather than parallelization. Deutsch [6] showed that a set of three-qubit logic gates is universal for quantum computation (i.e. this set of logic gates could reach any portion of the Hilbert space from any other portion of the Hilbert space). DiVincenzo [7] noted that this use of three-qubit logic gates was exceedingly difficult in many possible implementations of quantum computation (i.e. it is difficult to directly engineer three-body Hamiltonians) and gates that operated on one or two qubits at a time were much easier, and more natural, to consider. DiVincenzo therefore showed a set of two-qubit logic gates that were still universal. Barenco [8] expanded on this result and showed that a single two-qubit gate could be universal for quantum computation. Today, much of the present work with quantum logic gates relies on the notion that logic gates are to be applied to individual or pairs of qubits.

In a sense, this was also the paradigm in the first NMR quantum computation experiments [9]–[12], where a universal set of logic gates was demonstrated via the application of a one-bit gate and a two-spin controlled-NOT (c-NOT) gate to a two-spin system. Such implementations of QIP require substantial manipulation to operate correctly on all the qubits: when the internal Hamiltonian is used as the source of separating qubits as well as the means of introducing conditional gates, then of necessity every qubit must be addressed during each interval—the internal Hamiltonian being time-independent.

It is therefore possible to take advantage of the full complexity of the internal Hamiltonian and use the scalar coupling that exists between pairs of spins to construct ‘multiqubit’ logic gates, i.e. gates that operate on many qubits simultaneously and are therefore more efficient to implement than a series of one- and two-qubit logic gates. This line of reasoning was combined with methods from geometric algebra [13] to build generalized controlled-NOT (so called c^n-NOT) logic gates for any size of spin system [14] and draws on the work of Haeberlen and Waugh [15] with the development of average Hamiltonian theory in NMR.

2. Three-bit universal gates in NMR

An internal Hamiltonian for an $n$-spin system under weak coupling is of the form

$$H_{\text{int}} = \sum_{i} \frac{1}{2} \omega i \sigma_{z} i + \sum_{(i \neq j)} \frac{1}{2} \pi J_{ij} \sigma_{z} i \sigma_{z} j$$ (1)

where $\sigma_{z}$ is the Pauli spin matrix, $\omega$ is the Larmor precession frequency in radians, and $J$ is the scalar coupling in hertz. Implicit in this expansion is the fact that nature gives the NMR experimentalist every possible combination of couplings amongst all pairs of spins within the

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system (i.e. the second term in the above expression), although some may not be practically accessible (e.g. the coupling constants, $J$, may be too small to allow for some operations). Given such a Hamiltonian, it is clear that an NMR experiment necessarily allows for interaction among multiple spins simultaneously. It is therefore advantageous to design and implement logic gates which take advantage of this feature of the internal Hamiltonian.

Deutsch’s method for the creation of an arbitrary unitary transformation relies on the following three-bit operations [6]

$$U_\lambda = \begin{pmatrix} 1 & \cos(\lambda) & \sin(\lambda) \\ i\sin(\lambda) & \cos(\lambda) & 0 \\ i\sin(\lambda) & 0 & \cos(\lambda) \end{pmatrix} \quad V_\lambda = \begin{pmatrix} 1 & \cos(\lambda) & \sin(\lambda) \\ 0 & -\sin(\lambda) & \cos(\lambda) \\ 0 & \sin(\lambda) & \cos(\lambda) \end{pmatrix} \quad W_\lambda = \begin{pmatrix} 1 & e^{-i\lambda} & 0 \\ 0 & 0 & e^{i\lambda} \end{pmatrix} \quad X_\lambda = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\lambda} \end{pmatrix}$$

(where the 1 represents the upper $6 \times 6$ unity matrix) to create any arbitrary unitary operation. These operations can be expressed in exponential form as

$$U_\lambda = e^{iE_1^1 E_2^2 \sigma_3^3 \lambda}$$
$$V_\lambda = e^{iE_1^1 E_2^2 \sigma_3^3 \lambda}$$
$$W_\lambda = e^{-iE_1^1 E_2^2 \sigma_3^3 \lambda}$$
$$X_\lambda = e^{-iE_1^2 E_2^3 \sigma_3^3 \lambda}$$

where $E_{1,2} = \frac{1}{2} (1 \pm \sigma_3^3)$. Using previously outlined methods from geometric algebra [16] it is possible to generate pulse sequences to implement any of the above operations. For example, the expression for $U_\lambda$ can be expanded into (re-indexing for convenience later)

$$U_\lambda = e^{i\sigma_3^1 \lambda/4} \cdot e^{-i\sigma_3^1 \sigma_3^2 \lambda/4} \cdot e^{-i\sigma_3^2 \sigma_3^3 \lambda/4} \cdot e^{-i\sigma_3^1 \sigma_3^2 \sigma_3^3 \lambda/4}$$
$$= e^{i\sigma_3^1 \lambda/4} \cdot e^{-i\sigma_3^1 \sigma_3^2 \lambda/4} \cdot e^{-i\sigma_3^2 \sigma_3^3 \lambda/4} \cdot e^{-i\sigma_3^1 \sigma_3^2 \sigma_3^3 \lambda/4}$$
$$\cdot e^{-i\sigma_3^1 \sigma_3^2 \sigma_3^3 \lambda/4}$$

a series of rotations that can be translated into an NMR pulse sequence directly [9]. Note that the term $\sigma_3^1 \sigma_3^2 \sigma_3^3$ is implemented as a series of two-body interactions, as outlined in [14]. Rather than perform operations that address only one spin or a pair of spins at a time, it is possible to take advantage of commuting terms within the expansion such that several operations occur in parallel. For example, the second and third terms in the above expression can be rewritten

$$e^{-i\sigma_3^1 \sigma_3^2 \lambda/4} \cdot e^{-i\sigma_3^1 \sigma_3^2 \lambda/4}$$
$$= e^{-i\sigma_3^1 \pi/4} \cdot e^{-i\sigma_3^1 \sigma_3^2 \lambda/4} \cdot e^{i\sigma_3^1 \pi/4} \cdot e^{-i\sigma_3^1 \sigma_3^2 \lambda/4}$$
$$\cdot e^{-i\sigma_3^1 \sigma_3^2 \pi/4} \cdot e^{i\sigma_3^1 \sigma_3^2 \pi/4} \cdot e^{i\sigma_3^1 \sigma_3^2 \pi/4}$$

and the terms that resulted from the scalar coupling periods can also be combined to yield the sequence

$$U_\lambda = e^{i\sigma_3^1 \lambda/4} \cdot e^{-i\sigma_3^1 \pi/4} \cdot e^{-i(\sigma_3^1 \sigma_3^2 + \sigma_3^1 \sigma_3^3) \lambda/4} \cdot e^{i\sigma_3^1 \pi/4} \cdot e^{-i(\sigma_3^1 \sigma_3^2 + \sigma_3^1 \sigma_3^3) \pi/4} \cdot e^{-i\sigma_3^1 \lambda/4} \cdot e^{i(\sigma_3^1 \sigma_3^2 + \sigma_3^1 \sigma_3^3) \pi/4}$$

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where now the implementation of the logic gate takes advantage of the internal Hamiltonian of the spin system so that multiple couplings proceed simultaneously, and the overall time to implement the sequence has been reduced. The application of \( n \)-bit operations in NMR allows, in essence, a truncation of the application of a series of logic gates. It is clear from (3) that the \( U_\lambda \) gate may be implemented by a series of NOT- and XOR-type gates \([17]\). However, in NMR implementations of QIP, a single XOR gate is implemented with at least four operations (three RF pulses and a delay time), thereby making the sequential application of NOT and XOR gates less efficient than the multiqubit implementation of \( U_\lambda \) shown in (5).

It is similarly possible to generate the remainder of Deutsch’s set (\( W_\lambda, V_\lambda, X_\lambda \)) and achieve a universal set of gates in NMR using the originally posited three-qubit interactions.

### 3. Incomplete sets of couplings in actual experiments

The above treatment works well in a variety of NMR settings, but is still naive. Because all possible couplings between pairs of spins are present, the size of the couplings vary such that some are virtually inaccessible. For example, alanine (a three-spin compound) has coupling between the outermost (labelled 1 and 3) spins, \( J_{13} \), of only 1.1 Hz, while \( J_{12} = 3.6 \) Hz and \( J_{23} = 5.4 \) Hz. However, as long as there is a ‘coupling pathway’ (a set of couplings between various pairs of spins such that no spin is effectively completely uncoupled from all other spins) it is still possible to construct all components of a universal gate \([1]\), albeit with linear overhead. The expression derived in (5) could not be directly applied to a compound such as alanine because the coupling between the first and third spins is much less than the other couplings. Thus, it is necessary to assemble an interaction between the first and third spins using a pathway that connects the first with the second and the second with the third. A simple INEPT \([18]\) coherence transfer experiment (long known in NMR spectroscopy) can transfer information through an indirect path. For example, an indirect coupling between the first and third spins can be implemented as follows

\[
e^{i\sigma_1^z\sigma_3^z\alpha} = e^{-i\sigma_1^z\pi/4} \cdot e^{-i\sigma_3^z\pi/4} \cdot e^{-i(\sigma_1^x + \sigma_3^x)\pi/2} \cdot e^{-i\sigma_1^z\pi/4} \cdot e^{-i\sigma_3^z\pi/4} \cdot e^{-i(\sigma_1^x + \sigma_3^x)\pi/2} \cdot e^{-i\sigma_1^z\pi/4} \cdot e^{-i\sigma_3^z\pi/4}.
\]

(6)

Analyses similar to the above have been used in the implementation of the Deutsch–Jozsa algorithm via NMR \([19]\).

### 4. The implementation of other gates as multiqubit operations

The primitives of the universal gates \( U_\lambda, W_\lambda, V_\lambda \) and \( X_\lambda \) are not the only gates that lend themselves to more natural implementations as multiqubit transformations. Another example of such a gate is the Hadamard transform, which takes the state \( |0\rangle \) into the superposition of states \( \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \).

Normally the implementation of a multispin Hadamard transform is viewed as a series of one-spin Hadamard transforms. The NMR implementation of a one-spin Hadamard transformation is a rotation about an axis located 45° between the \( x \) and \( z \) axes

\[
H_1 = e^{-i\frac{\pi}{4} |\rangle\langle (1-(\sigma_1^x + \sigma_3^x))/\sqrt{2}|}.
\]

(7)
A multispin Hadamard transform is the tensor product of the individual spin transforms, \( H_N = H_1 \otimes \ldots \otimes H_n \). However, since each Hadamard is necessarily on a different spin, the individual operations all commute and may be brought into one common exponential operator

\[
H_{1, \ldots, n} = e^{-i \frac{\pi}{2} \left( 1 - (\sigma_1^x + \sigma_2^x + \ldots + \sigma_n^x) + (\sigma_1^y + \sigma_2^y + \ldots + \sigma_n^y) \right) / \sqrt{2}} \tag{8}
\]

that can be implemented in NMR via ‘hard’ compound pulses in a number of operations constant in the size of the input, \([\pi/4]_{y}^{1,2,\ldots,n} - [\pi]_{x}^{1,2,\ldots,n} - [\pi/4]_{-y}^{1,2,\ldots,n}\). It should be noted that such implementations are reliable only when the spectral width of the various nuclei is small with respect to the maximum RF power that can be applied.

The Hadamard is a special case where all terms commute and can be expressed as a single product. However, even in cases where it is not possible to express all operations as a single operator, NMR implementations of quantum logic gates are still often more convenient in terms of multiqubit operations. An example of this is the generalized controlled-NOT (or \( c^N \)-NOT) gate, a generalization of the XOR and Toffoli gates to larger qubit systems. Such a gate can be expressed as

\[
U_{c^N-\text{NOT}} = \sigma_x^1 \left( E_2^2 E_3^3 \cdots E_n^n \right) + \left( 1 - E_2^2 E_3^3 \cdots E_n^n \right) \tag{9}
\]

which is an instruction to rotate the first qubit, conditional upon the \( n - 1 \) other qubits in the system being 1. Using this formalism the \( c^2 \)-NOT, or Toffoli, gate is expressed as

\[
U_{c^2-\text{NOT}} = e^{-i(\sigma_1^x)(E_2^2 E_3^3)\pi/2} \cdot e^{-i(\sigma_1^y)(E_2^2 E_3^3)\pi/4} \cdot e^{-i(\sigma_1^z)(E_2^2 E_3^3)\pi/8} \cdot e^{-i(\sigma_2^x)(E_2^2 E_3^3)\pi/8} \cdot e^{-i(\sigma_2^y)(E_2^2 E_3^3)\pi/4} \cdot e^{-i(\sigma_2^z)(E_2^2 E_3^3)\pi/4} \tag{10}
\]

Using manipulations like those in the previous section, the \( c^2 \)-NOT gate can be expanded into

\[
U_{c^2-\text{NOT}} = U_{pc} \cdot e^{i \sigma_1^x \pi/8} \cdot e^{-i \sigma_1^y (\sigma_1^x + \sigma_3^x) \pi/8} \cdot e^{-i \sigma_1^z (\sigma_1^x + \sigma_3^x) \pi/4} \cdot e^{-i \sigma_2^x (\sigma_1^x + \sigma_3^x) \pi/4} \cdot e^{-i \sigma_2^y (\sigma_1^x + \sigma_3^x) \pi/4} \cdot e^{-i \sigma_2^z (\sigma_1^x + \sigma_3^x) \pi/4} \tag{11}
\]

where \( U_{pc} \) is the phase correction

\[
U_{pc} = e^{-i \pi/8} \cdot e^{i \sigma_2^x \pi/8} \cdot e^{i \sigma_2^y \pi/8} \cdot e^{-i \sigma_2^z \pi/8} \cdot e^{-i \sigma_3^x \pi/8} \cdot e^{-i \sigma_3^y \pi/8} \cdot e^{-i \sigma_3^z \pi/8} \cdot e^{-i \sigma_4^x \pi/8} \cdot e^{-i \sigma_4^y \pi/8} \cdot e^{-i \sigma_4^z \pi/8} \tag{12}
\]

Barenco et al [17] found that the implementation of a generalized \( c^n \)-NOT gate, without use of ancilla qubits, would take \((2 \times 2^n - 1) - 2\) XOR gates and \((2 \times 2^{n-1})\) one-bit rotations, or six gates for the \( c^2 \)-NOT gate (it should be noted that only the exact implementation without ancilla scales in this manner [17] offers efficient approximate implementations), while the NMR method presented here is implemented in a number of operations equivalent to two such one- and two-bit gates. Note that this treatment assumes that the scalar coupling values between the various spins are equal; in the realistic case that they are not, and there will need to be additional rotations to equalize the coupling constants.

While \( c^N \)-NOT gates and the like are often initially expressed as multiqubit rotations and then scaled down to one- and two-bit rotations for purposes of implementation, the quantum Fourier transform (QFT) is a more difficult example, in that the well understood implementation of the QFT [21] relies on a series of one- and two-bit rotations as a starting point. The NMR implementation of the QFT [21] has also been composed and implemented in this fashion. However, there is a straightforward version of the QFT that can be constructed using some of the aforementioned multiqubit simplifications. In fact, such an implementation gives a version of the QFT that scales linearly, assuming that all couplings are accessible, much like the parallel version presented by Coppersmith [20]. It is important to note, however, that the most straightforward NMR implementation may scale as much as cubically because refocusing all couplings during each operation is quadratic [22].

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The QFT can be composed from one-bit Hadamard transformations and two-bit conditional phase rotations

\[
\text{QFT}_{1,2,\ldots,n} = U_1 \cdot U_2 \ldots U_n = (H_1 \cdot C_{1,2} \ldots C_{1,n})(H_2 \cdot C_{2,3} \ldots C_{2,n}) \ldots (H_{n-1} \cdot C_{n-1,n})(H_n)
\]

(13)

where \(C_{j,k} = e^{i\theta_{j,k} E_j E_k}\) and \(\theta_{j,k} = \pi/2^{k-j}\). Note first that each factor \(U\) can be rearranged such that the Hadamard transforms occur first

\[
U_1 = H_1 \cdot e^{i\theta_{1,2} E_1 E_2} \cdot e^{i\theta_{1,3} E_1 E_3} \ldots e^{i\theta_{1,n} E_1 E_n}
\]

\[
= H_1 \cdot e^{i\theta_{1,2} E_1 E_2} \ldots e^{i\theta_{1,n} E_1 E_n} \cdot H_1^* \cdot H_1
\]

\[
= e^{iH_1 \cdot E_1 \cdot H_1^* (\theta_{1,2} E_2 + \ldots + \theta_{1,n} E_n)} \cdot H_1
\]

\[
= e^{\frac{i}{2} (\theta_{1,2} E_2 + \ldots + \theta_{1,n} E_n)} \cdot e^{-\frac{i}{2} \sigma_z^n (\theta_{1,2} E_2 + \ldots + \theta_{1,n} E_n)} \cdot H_1
\]

(14)

In addition, the commutativity of the various conditional phase rotations allows them to be expressed in one common exponential operator. Moreover, since \(H_1\) will have no effect on \(U_2\), and \(H_2\) will have no effect on \(U_3\), etc, all the Hadamard transforms may be brought to one side and combined into one single operation

\[
\text{QFT}_{1,2,\ldots,n} = e^{\frac{i}{2} (\theta_{1,2} E_2 + \ldots + \theta_{1,n} E_n + \theta_{2,3} E_3 + \ldots + \theta_{2,n} E_n + \ldots + \theta_{n-1,n} E_n)}
\]

\[
\cdot e^{-\frac{i}{2} \sigma_z^n (\theta_{n-1,n} E_n)} \cdot e^{-\frac{i}{2} \sigma_z^{n-1} (\theta_{n-2,n} E_n)} \cdot \ldots \cdot H_{1,2,\ldots,n}
\]

(15)

Thus it is possible to implement the QFT in a number of operations that scales linearly with the number of inputs [13] (the above derivation is essentially the same as that found in [13] but corrects several typographical errors).

Using the methods outlined in the previous section it is possible to implement the QFT more directly, while still maintaining a linear scaling. Using the expression in (15), and taking advantage of cancellations and commuting terms, the general QFT can be rewritten as

\[
\text{QFT}_N = e^{\frac{i}{2} (\theta_{1,2} E_2 + \ldots + \theta_{1,n} E_n + \ldots + \theta_{n,1} E_n)}
\]

\[
\cdot e^{-\frac{i}{2} \sigma_z^n (\theta_{1,2} + \ldots + \theta_{1,n})} \cdot \cdot e^{-i\sigma_z^n \pi/4} \cdot e^{-\frac{i}{2} (\theta_{1,2} \sigma_z^2 + \theta_{1,3} \sigma_z^2 + \ldots + \theta_{1,n} \sigma_z^2 \cdot \cdot e^{i\sigma_z^n \pi/4} \cdot \cdot e^{\frac{i}{2} (\theta_{1,2} \sigma_z^2 + \theta_{1,3} \sigma_z^2 + \ldots + \theta_{1,n} \sigma_z^2 \cdot \cdot e^{i\sigma_z^n \pi/4} \cdot \cdot e^{-\frac{i}{2} \sigma_z^{n-1} \cdot \cdot e^{-i\sigma_z^{n-1} \pi/4} \cdot \cdot e^{-\frac{i}{2} (\theta_{n-1,n} \sigma_z^{n-1} \cdot \cdot e^{i\sigma_z^{n-1} \pi/4} \cdot \cdot H_{1,2,\ldots,n}}
\]

(16)

where each additional qubit adds only four new terms to the expansion: three RF pulses and an additional coupling period. While each additional qubit adds another coupling term that must occur during a given scalar coupling period, this does not require an additional operation because several couplings can take place simultaneously. For example, using these methods the three-qubit QFT can be implemented with the pulse sequence

\[
\left[\begin{array}{c}
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ x \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ x \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ x \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ x \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ y \\
\frac{\pi}{4}\ y
\end{array}\right]
\]

where the \(1/4 J_{12}\) and \(1/8 J_{13}\) coupling periods occur simultaneously, such that the total coupling time of the sequence is only \(1/4 J_{23} + 1/4 J_{12}\). This will be the case with the addition of each new spin: the overall time of the sequence will increase by \(n/4 J\) (i.e. for four spins the overall time is expressed as \(1/4 J_{14} + 1/4 J_{23} + 1/4 J_{12}\), etc) because additional coupling periods can take
place simultaneously. However, the $J$ coupling periods for spins that are successively further and further apart are larger and larger so that growth is not necessarily linear. Conversely, the serial method presented by Coppersmith could be implemented as

$$D = \frac{\pi}{4} \left( [\pi]_x^2 - [\pi]_y^2 - [\pi]_x^3 - [\pi]_y^3 - \frac{1}{4J_{12}} - [\pi]_x^3 - [\pi]_y^3 - \frac{1}{4J_{13}} - [\pi]_x^3 - [\pi]_y^3 - \frac{1}{4J_{23}} - [\pi]_x^3 - [\pi]_y^3 \right)$$

where each coupling period happens serially, and the total coupling time is $1/4J_{12} + 1/8J_{13} + 1/4J_{23}$. Note that in this implementation the overall time of the sequence increases roughly as $n/2J$ with additional spins (i.e. for four spins the overall time is expressed as $1/4J_{12} + 1/8J_{13} + 1/4J_{23} + 1/16J_{14} + 1/8J_{24} + 1/4J_{34}$, etc) giving the multiqubit expression an extra factor of two in time savings. Furthermore, because the magnitude of the scalar coupling between two distant spins increases even faster, there is an even greater advantage in not having to go through each coupling period individually, giving an even greater time saving with multiqubit implementations.

In the above expressions both sequences have neglected the refocusing scheme for the coupling period, as well as the overall phase correction. It may be the case that more creative refocusing schemes are necessary in the multiqubit implementations; however, the overall reduction in the number of operations combined with sophisticated refocusing schemes [22] will mean that the number of operations in a parallel implementation of the QFT scales better than the serial one- and two-bit implementation.

5. A comment on scaling

The above analysis begs the question: does the complexity of the internal Hamiltonian allow for NMR implementations of logic gates that are always more efficient than one- and two-qubit operations? Not surprisingly, the answer is no.

First, multiqubit gates still scale exponentially for the implementation of arbitrary unitary operations. The work by Barenco et al [17] shows that an arbitrary unitary operation can be stated as

$$U = \prod_{x1,x2 \in \{0,1\}^m, x1 < x2} T(x1, x2) \cdot D$$

where $D$ is a diagonal matrix of only phase factors and the $T(x1, x2)$ operation executes a grey code, connecting pairs of basis states. In the formulation of Barenco et al the $T(x1, x2)$ operation is a series of two-bit rotations that connect pairs of basis states, while leaving the other states unchanged. With the methods outlined above, it is possible to execute the $T(x1, x2)$ operation as a multiqubit operation that can be implemented in a number of steps less than the number required from successive two-bit rotations. However, in order to create $U$, an exponential number of $T$s must be applied, which is not obviated by our currently described method. This can also be seen in the application of geometric algebra methods to the generalized $\Lambda_N(U)$ gates presented by Barenco et al, which immediately reveals similar exponential scaling.

Specific unitary operations such as the QFT scale better than (i.e. slower than) exponential using these methods. However, it is worth noting that since the internal Hamiltonians are a sum.
of one and two qubit Hamiltonians, the number of terms in the expression of $H_{\text{tot}}$ is quadratic. Thus, while the realization that several coupling periods can occur simultaneously does certainly offer a new form of parallelization for NMR quantum computation, the maximum speed-up from this form of parallelization over the usual serial processing is, at best, quadratic in overall time.

More importantly though, while the use of the internal Hamiltonian gives a certain advantage in the present implementations of QIP with NMR, it does not scale well. The internal Hamiltonian given in (1) works well for a small number of spins, in that the frequency separation between adjacent spins is much larger than the scalar coupling constant, so that there is no overlap of resonance lines. In addition, for small numbers of spins the coupling constants are large enough for a large number of operations to be performed. However, as the size of the spin system grows, such features will cease to exist: coupling between spins becomes vanishingly small, and there is a great deal of overlap among various resonances thereby making multiqubit gates impossible to implement. The same complexity that makes multiqubit implementations more efficient for small numbers of qubits seemingly makes these implementations impossible for large numbers of qubits.

6. Conclusion

We have demonstrated a method of analysing and composing logic gates in NMR quantum computing that allows for the creation of a universal set of $n$-qubit gates, as well as simpler implementations of other important quantum logic gates. Initial implementations of logic gates with liquid state NMR techniques followed methods proposed for physical systems that use an engineered Hamiltonian to manipulate qubits (i.e. one- and two-qubit rotations). However, liquid state techniques use the internal Hamiltonian to both address and manipulate qubits, thereby allowing for a greater degree of complexity in the construction and implementation of logic gates. It is most efficient to make use of this complexity and generate logic gates that operate on multiple qubits simultaneously.

Ultimately, though, it may be the case that the complexity of the internal Hamiltonian makes large-scale $n$-qubit rotations much more difficult to implement than successive one- and two-qubit operations when the size of the spin system grows large. Today, however, the use of the internal Hamiltonian to address and manipulate multiple qubits does offer an important convenience in the present construction and implementation of NMR quantum logic gates, particularly when the limits imposed by the intrinsic decoherence rates are taken into account. What is more, future implementations of QIP may also use internal Hamiltonians or have NMR-like properties, thereby making the methods outlined above useful for other QIP techniques.

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