Implementation of the Quantum Fourier Transform

Y. S. Weinstein,[1] M. A. Pravia,[1] E. M. Fortunato,[1] S. Lloyd,[2,*] and D. G. Cory[1]

[1]*Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*

[2]*d'Arbeloff Laboratory for Information Systems and Technology, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*

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A quantum Fourier transform (QFT) has been implemented on a three qubit nuclear magnetic resonance (NMR) quantum computer to extract the periodicity of an input state. Implementation of a QFT provides a first step towards the realization of Shor's factoring and other quantum algorithms. The experimental implementation of the QFT on a periodic state is presented along with a quantitative measure of its efficiency measured through state tomography. Experimentally realizing the QFT is a clear demonstration of the ability of NMR to control quantum systems.

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Quantum computers are devices that process information in a way that preserves quantum coherence. Unlike a classical bit, a quantum bit, or "qubit," can be in a superposition of 0 and 1 at once. This nonclassical feature of quantum information allows quantum computers to perform certain computations faster than classical computers. For example, quantum computers, if constructed, could factor large numbers more rapidly [1], search databases more quickly [2], and simulate quantum systems more efficiently [3] than is possible using current classical algorithms [4–10].

A key subroutine of algorithms for factoring and simulation [11–13] is the quantum Fourier transform (QFT) [14–16]. The QFT can be used to extract periodic features of wave functions or to switch from "position" to "momentum" representations and is defined as follows:

$$\mathrm{QFT}_q|x\rangle = \frac{1}{\sqrt{q}} \sum_{x'=0}^{q-1} e^{2\pi i x x'/q}|x'\rangle . \tag{1}$$

Here, q is the dimension of the system's Hilbert space. This paper reports the experimental demonstration of a quantum Fourier transform using nuclear magnetic resonance (NMR).

The dimension of a Hilbert space for n qubits is $q = 2^n$. Thus, the two qubit QFT corresponds to the unitary operator,

$$\mathrm{QFT}_4 = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}. \tag{2}$$

The operator separates the input states by 0° in the first row and column, and then by 90°, 180°, and 270°, multiples of $\frac{\pi}{2}$.

Equation (2) shows that the QFT, which was modeled after the discrete Fourier transform and is itself discrete, has effects similar to that of the classical discrete Fourier transform. In particular, if $f(x)$ is periodic with period r, then $\tilde{f}(p)$ will exhibit a peak at $p = q/r$. This is the key to Shor's algorithm which allows a quantum computer to factor very large numbers in polynomial time. The classical Fourier transform reveals the periodicity in functions; the QFT reveals periodicity of wave functions.

As formulated by Coppersmith [14], the QFT can be constructed from two basic unitary operations, the H_j or Hadamard gate, operating on the jth qubit

$$H_j = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{3}$$

and B_{jk}, a conditional phase shift, operating on the jth and kth qubits

$$B_{jk} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\theta_{jk}} \end{pmatrix}, \tag{4}$$

where $\theta_{jk} = \pi/2^{k-j}$.

To implement the QFT on L qubits, this series of gates

$$B_{j,1}B_{j,2},\ldots,B_{j,j-1}H_j , \tag{5}$$

must be implemented on each qubit, j, as j is indexed from 1 to L. A bit reversal will then complete the QFT.

This sequence of quantum logic gates can be realized via NMR. The idea of using nuclear spins as the basic unit of a quantum computer was proposed by Lloyd [17], and detailed schemes for using NMR as a method of quantum computing were implemented by Cory *et al.* [18], Gershenfeld and Chuang [19], and Jones [20]. In NMR a series of radio frequency pulses are used to control the excess magnetization of an ensemble of quantum states. In addition, a bilinear coupling term in the Hamiltonian allows for conditional phases to be achieved and thus the preparation of entangled states.

The internal Hamiltonian of a 3 qubit (spin) system with only weak coupling is

$$H = \begin{array}{c}\omega_1 I_z^1 + \omega_2 I_z^2 + \omega_3 I_z^3 + \\ 2\pi(J_{12} I_z^1 I_z^2 + J_{13} I_z^1 I_z^3 + J_{23} I_z^2 I_z^3),\end{array} \tag{6}$$

where $I_i = \sigma_i/2$ are rescaled Pauli matrices. The three bit, $q = 8$, QFT was implemented via NMR using the three carbon-13 spins of an alanine sample. The resonant

frequency of carbon-13 on a 300 MHz spectrometer is approximately 75.468 MHz. Frequency differences between the spins are 9456.5 Hz between spins 1 and 2, 2594.3 Hz between spins 2 and 3, and 12 050.8 Hz between spins 1 and 3. Coupling constants between the three spins are $J_{12} = 54.1$, $J_{23} = 35.0$, and $J_{13} = -1.3$. Relaxation time T_1 for the three carbon spins in alanine are all longer than 1.5 s while the T_2 relaxation times are longer than 400 ms.

The pulse program is conveniently derived from an idempotent or projection operator description of the propagators. The operators $E\pm$ are defined as $(1 \pm \sigma_z)/2$. The H_j matrix can be broken down into $E_+ - E_- + \sigma_x(E_+ + E_-)$. The pulse sequence [21] of the H_j gate is

$$H_j = \left(\frac{\pi}{2}\right)_y^j - (\pi)_x^j . \tag{7}$$

This pulse program reads apply a pulse that rotates spin j 90° about the y axis, followed by a pulse that rotates j 180° about the x axis. Magnetization along the positive z axis would be rotated to the positive x axis. The B_{jk} gate can be implemented using the coupling between qubits. In terms of projection operators the B_{jk} gate is $1 - E_-^1 E_-^2 + e^{i\theta} E_-^1 E_-^2$, and the following pulse sequence:

$$(\pi)_\phi^j - (\tfrac{\theta_{jk}}{2\pi J_{jk}}) - (\pi)_\phi^j - (\tfrac{\pi}{2})_y^{j,k} - (\tfrac{\theta}{2})_x^{j,k} - (\tfrac{\pi}{2})_{-y}^{j,k} . \tag{8}$$

ϕ is an arbitrary phase. The notation $\frac{\theta_{jk}}{2\pi J_{jk}}$ represents a time interval during which spin evolution occurs between spins j and k while chemical shifts and couplings between all other spins are refocused. The superscripts j, k denotes a pulse on both spins j and k. The final three pulses perform a rotation around the z axis.

Finally, the bit reversal can be implemented by a series of swap gates. Swap_{jk} gates can be done via the following pulse sequence:

$$(\tfrac{\pi}{2})_y^{j,k} - (\tfrac{1}{2J_{jk}}) - (\tfrac{\pi}{2})_{-y}^{j,k} - (\tfrac{1}{2J_{jk}}) - (\tfrac{\pi}{2})_x^{j,k} - (\tfrac{1}{2J_{jk}}) - (\tfrac{\pi}{2})_{-x}^{j,k} . \tag{9}$$

The complete gate sequence for the three qubit QFT is

$$H_1 B_{12} H_2 B_{13} B_{23} H_3 \text{swap}_{13} . \tag{10}$$

The complete pulse program for the QFT is the compilation of the pulse programs for each of the gates listed above. Pulses were combined when possible without affecting the overall unitary operator. In addition, since the J_{13} coupling is small, any J_{13} couplings were replaced by a series of J_{12} and J_{23} couplings that would perform the exact same operations, so called relayed experiments [22]. For example, the swap_{13} gate was replaced by $\text{swap}_{12}\text{swap}_{23}\text{swap}_{12}$ which enacts the exact same unitary transformation. The pulses used for the implementation were self-refocusing for all J couplings and chemical shifts.

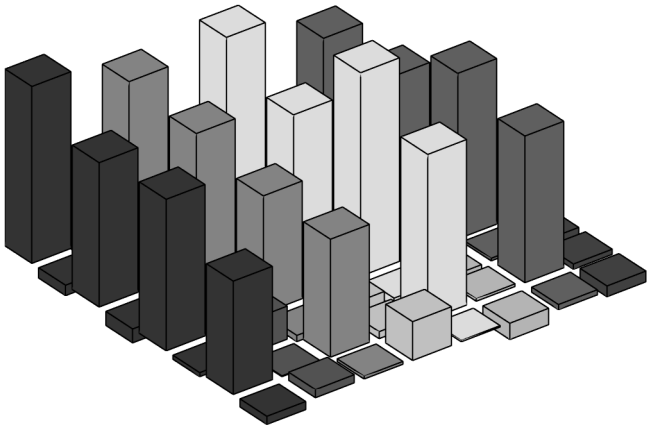

FIG. 1. Real part of the density matrix of the input state for the QFT implementation. This state, created by Hadamards on the first and second bit after the three bits were put into a pseudopure state, is a superposition of the $|000\rangle + |010\rangle + |100\rangle + |110\rangle$ states. Note that the input state has a periodicity of $r = 2$.

The implemented QFT will give the correct results to any input state. To show the ability of the QFT to extract periodicity we created a periodic input state of periodicity $r = 2$ and implemented the QFT on that state. The periodic input state was created by performing a $\frac{\pi}{2}$ pulse on the first and second bits of the $|000\rangle$ pseudopure state. The density matrix of the input state is shown in Fig. 1.

Figure 2 shows the density matrix after subsequent implementation of the QFT. Clearly, the density matrix is now periodic with a periodicity of $q/r = 4$ showing that the QFT did indeed extract the periodicity of our input state.

In order to measure the accuracy with which the QFT has been performed, we need an appropriate measure. Room temperature NMR is always very close to the fully mixed state. All the information is contained in the deviation from the fully mixed state which has a relative weight of one-millionth the weight of the fully mixed state. Therefore, the conventional measurement of entanglement fidelity [23,24] would give very close to one for any room

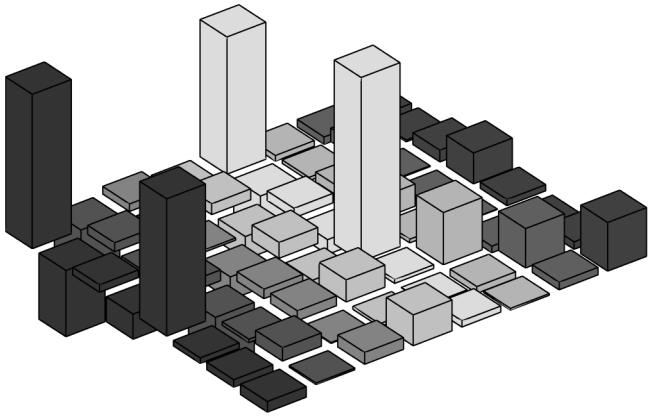

FIG. 2. Real part of the density matrix after implementation of the QFT. Notice there is now a periodicity of $q/r = 4$ in the density matrix. This shows that the QFT extracted the periodicity of the input state.

temperature NMR experiment. A measure of accuracy more appropriate for almost fully mixed density matrices is [25]

$$C = \frac{\mathrm{Tr}(\varrho_{\mathrm{theory}}\varrho_{\mathrm{exp}})}{\sqrt{\mathrm{Tr}(\varrho_{\mathrm{theory}}^2)}\sqrt{\mathrm{Tr}(\varrho_{\mathrm{exp}}^2)}}\sqrt{\frac{\mathrm{Tr}(\varrho_{\mathrm{exp}}^2)}{\mathrm{Tr}(\varrho_{\mathrm{initial}}^2)}}. \qquad (11)$$

Here, ϱ is the deviation density matrix, the density matrix, ρ, of the system, minus the large identity term (in NMR, this is called the "reduced" density matrix; it should not be confused with the reduced density matrix obtained by partially tracing the density matrix for a composite quantum system over some of its subsystems). The first term in C measures the correlation between the density matrices $\varrho_{\mathrm{theory}} = U_{\mathrm{theory}}\varrho_{\mathrm{initial}}U_{\mathrm{theory}}$, where U_{theory} is the theoretical operator, and $\varrho_{\mathrm{initial}}$ is the experimentally obtained initial reduced density matrix. This is weighted by the second term, the reduction in signal over the course of the experiment. A correlation of 1 shows that the theoretical and experimental deviation density matrices are totally correlated. If the theoretical and experimental deviation density matrices were anticorrelated $C = -1$, and if they were uncorrelated $C = 0$.

In NMR, only dipolar transverse magnetization can be detected by the dipolar coil of the NMR spectrometer. Therefore, only single spin single quantum terms are observed in the spectra. To see the other terms of the deviation density matrix, it is necessary to perform readout pulses after the experiment that will rotate the unobservable terms into observable ones. Here, the creation of the input state and the implementation of the QFT was performed a number of times each time applying a series of readout pulses to reconstruct the entire deviation density matrix. For three bits, 11 different experiments are sufficient. Of the 11 experiments, one does not require a readout pulse, while the other ten have combinations of $\frac{\pi}{2}$ pulses [26].

The accuracy of the implementation of the QFT is 80% not including the swap gate, and 62% with the swap gate. This measure reflects both imperfections in the applied pulses and delays, as well as decoherence. Spin lattice relaxation (T_1) is not an important factor over the time scale of the experiment. As a check to the accuracy of the results, we also performed the QFT on a thermal state (without a final swap), obtaining an accuracy of 87% (the greater accuracy for the thermal state arises because no input state need be created). The fact that our algorithm gives the correct results for both pseudopure and thermal states suggests that the high accuracy obtained is not due to accidental cancellation of anomalous results.

In conclusion, using NMR, the QFT has been implemented on a three bit quantum system to extract periodicity of an input state. In addition, the correlation has been measured. Although the correlation does not reach that required for fault tolerant computing [27], it is high enough to permit studies on small quantum systems including quantum simulations. A particularly straightforward use of the QFT is in quantum chaos: as Balazs and Voros [28] pointed out, a simple version of the quantum bakers map can be performed by QFTs and Schack [29] has shown how such a quantum map might be realized on a quantum computer [30].

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*Author to whom correspondence should be addressed.

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