Experimental Realization of Discrete Fourier Transformation on NMR Quantum Computer

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Abstract

We report experimental implementation of discrete Fourier transformation (DFT) on a nuclear magnetic resonance (NMR) quantum computer. Experimental results agree with theoretical results. Using the pulse sequences we introduced, DFT can be realized on any L-bit quantum number in principle.

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1 INTRODUCTION

With the discovery of an apparent separation between the classical and quantum classifications of computational complexity[1], and of fault-tolerant schemes for quantum computation[2], quantum information theory plays an important role in computer science. In 1994, Shor[3] introduced the quantum factoring algorithm, which achieves an exponential speed-up relative to classical algorithms. Shor’s crucial insight was that the discrete Fourier transformation (DFT) can be evaluated in polynomial time on a quantum computer. In order to realize Shor’s algorithm, performing DFT becomes most important. In this paper, we introduce a version to realize DFT by using NMR
spectrometer and simulator and give our experiment and simulation results realizing two qubit DFT.

The discrete Fourier transformation modulo q(DFT_q) is a unitary transformation in q-dimension (q = 2^L). It is defined relative to chosen basis |0⟩, · · · , |q − 1⟩ by\(^3\):

\[
\text{DFT}_q : |a⟩ \rightarrow \frac{1}{\sqrt{q}} \sum_{c=0}^{q-1} \exp(2\pi iac/q) |c⟩ \tag{1}
\]

Coppersmith\(^4\) suggested the efficient algorithm for DFT on application of quantum mechanical operators and gave an improvement in which evaluation of L-bit Fourier transformation is accomplished by composing L one-qubit operations and \(\frac{1}{2}L(L−1)\) two-qubit operations. So the implementation of DFT is based on realizing one-qubit operator \(A_j\) which acts on the state of the \(j\)-qubit and two-qubit operator \(B_{jk}\) which acts on the states of qubit \(j\) and \(k\). The explicit form of the operator \(A_j\) is\(^3\):

\[
A_j = 2^{-1/2}(|0⟩_j|0⟩_j + |0⟩_j|1⟩_j + |1⟩_j|0⟩_j - |1⟩_j|1⟩_j) \quad (j = 0, \ldots, L−1) \tag{2}
\]

The explicit form of the operator \(B_{jk}\) is\(^3\):

\[
B_{jk} = |0⟩_j|0⟩_k + |0⟩_j|1⟩_k + |1⟩_j|0⟩_k + e^{i\theta_{jk}} |1⟩_j|1⟩_k \quad (\theta_{jk} = \frac{\pi}{2^{j−1}}) \tag{3}
\]

The matrix representation of \(B_{jk}\) affects only state \(|1⟩_j|1⟩_k⟩\).

We use a network to illustrate how to use operators \(A_j\) and \(B_{jk}\) to compose 5-qubit transformation in Figure 1. The operators corresponding to the network are:

\[
(A_0)(B_{34}A_3)(B_{24}B_{23}A_2)(B_{14}B_{13}B_{12}A_1)(B_{04}B_{03}B_{02}B_{01}A_0)
\]

### 2 IMPLEMENTING THE DFT IN NMR

In this paper we realize DFT by using NMR. The prime thing we should do is to perform \(A_j\) and \(B_{jk}\) by using radiofrequency pulses and spin-spin interaction. Using NMR to perform quantum computer, we should choose
AX couple system. The Hamiltonian for this system can be approximated as:
\[ H = 2\omega_{AB}J_{ZA}J_{ZB} + \omega_{A}J_{ZA} + \omega_{B}J_{ZB} + H_{\text{env}} \] (4)

We denote the rotation \( \varphi_{X}^{(k)} = \exp(i\varphi I_{x}) \) for a \( \varphi \) rotation about the \( \hat{x} \)-axis and \( \varphi_{Y}^{(k)} = \exp(i\varphi I_{y}) \) for a \( \varphi \) rotation about the \( \hat{y} \)-axis, \( j \) or \( k \) means which nucleus is operated on, and \( \tau \) is the time within which the system undergoes the unitary transformation \( \exp(2\pi i J_{ZA}J_{ZB}t) \) in the doubly rotating frame.

To perform \( A_{j} \) is actually to perform a Walsh-Hadamard transformation, which rotates each quantum qubit from \( |0\rangle \) to \( (|0\rangle + |1\rangle)/\sqrt{2} \). the pulse sequences is\[5]: \((\frac{\pi}{2})_{X} - (\frac{\pi}{2})_{Y} \)

To perform \( B_{jk} \), we use radiofrequency pulses and spin-spin interaction like:
\[ (-\frac{\pi}{2})_{Y}(-\frac{\pi}{2})_{Y} - (-\varphi)_{X}^{j}(-\varphi)_{X}^{k} - (\frac{\pi}{2})_{Y} - (\frac{\pi}{2})_{X}^{j} - (\frac{\pi}{2})_{X}^{k} - (\frac{\pi}{2})_{Y}^{j} - (\frac{\pi}{2})_{Y}^{k} \]
\( (\varphi = \frac{\pi}{2^{j-k+1}}, \tau = \frac{1}{2\omega_{A}J_{ZB}}) \)

Using the pulse sequences and spin-spin interaction we introduced above, we can implement DFT to any quantum number with \( L \)-qubit in principle.

3 EXPERIMENTAL AND SIMULATION RESULTS

In order to demonstrate the results described above, we have constructed an NMR quantum computer capable of implementing the DFT. In this section, we give NMR experimental and NMR simulation results after doing DFT on state \( |0,1\rangle \) by using the two radiofrequency pulse sequences corresponding to the operator \( A_{j} \) and \( B_{jk} \) respectively. Data of the NMR experiment were taken at room temperature with a Bruker ARX-500 spectrometer and the signals were obtained with single-shot measurement.

In the experiment we chose \( H_{2}PO_{3} \) as our sample, labeled \( ^{31}P \) as \( j \)-qubit and \( ^{1}H \) as \( k \)-qubit. The observed J-coupling between \( ^{1}H \) and \( ^{31}P \) was 647.451Hz. First, we produced effective pure state \( |00\rangle \) by using "temporal averaging"\[3]. The pulses we used were\[7]:

\textit{E: NONE}

\textit{P1:} \((\frac{\pi}{2})_{X}^{H} - \frac{1}{2}J - (\frac{\pi}{2})_{Y}^{P} - (\frac{\pi}{2})_{X}^{H} - \frac{1}{2}J - (\frac{\pi}{2})_{Y}^{H}\)

\textit{P2:} \((\frac{\pi}{2})_{X}^{H} - \frac{1}{2}J - (\frac{\pi}{2})_{X}^{P} - \frac{1}{2}J - (\frac{\pi}{2})_{Y}^{H}\)

Since we wanted to perform DFT on the state \( |01\rangle \), so after the preparation of the state \( |00\rangle \), we should operate the pulse sequence: \((\frac{\pi}{2})_{Y}^{H} - \frac{1}{2}J - (\frac{\pi}{2})_{X}^{H}\)
and $^1H$ to obtain the state $|01\rangle$.

Second, we performed state Fourier transformation on $|01\rangle$. We list the pulses and spin-spin interaction are as follows:

$$ (\pi)^P_X - (-\frac{\pi}{2})^P_Y - \frac{\pi}{2}^P_Y (\frac{\pi}{2})^H_X (\frac{\pi}{4})^H_X \frac{\pi}{4}^H_X - (-\frac{\pi}{2})^P_Y (\frac{\pi}{2})^H_X - \frac{\pi}{2}^H_X - (\pi)^P_X - (\frac{\pi}{2})^H_X $$

The first two pulses and the last two pulses correspond to the operator $A_j$ and $A_k$ respectively, the rest pulses correspond to $B_{jk}$. After these operations, the initial state $|01\rangle$ was transformed into state:

$$ \frac{1}{2} (|00\rangle - |01\rangle + |10\rangle - i |11\rangle). $$

Compared with the definition of DFT (1) which means that after doing DFT operation, the state $|01\rangle$ should become

$$ |01\rangle \rightarrow \frac{1}{2} ( |00\rangle + e^{i\frac{\pi}{2}} |01\rangle + e^{ix} |10\rangle + e^{i\frac{\pi}{4}} |11\rangle) $$

$$ = \frac{1}{2} ( |00\rangle + i |01\rangle - |10\rangle - i |11\rangle) $$

and the density matrix is:

$$ \begin{pmatrix} 1 & -i & -1 & i \\ i & 1 & -i & -1 \\ -1 & i & 1 & -i \\ i & -1 & i & 1 \end{pmatrix}, $$

(7)

The third step: we should reverse the qubit. That is, for example, for the case of three qubits, $|ijk\rangle \rightarrow |kji\rangle$. The third step is composed of three C-NOT operations, The network is shown in Figure 2. The radiofrequency pulses corresponding to the three C-NOT operators are:

1. $(\frac{\pi}{2})^H_Y - \frac{\pi}{4}^P_Y - (-\frac{\pi}{2})^P_Y (\frac{\pi}{2})^H_X (\frac{\pi}{4})^H_X - \frac{\pi}{4}^H_X - (\pi)^P_X - (\frac{\pi}{2})^H_X$
2. $(\frac{\pi}{2})^P_Y - \frac{\pi}{4}^P_Y - (-\frac{\pi}{2})^Y (\frac{\pi}{2})^H_X (\frac{\pi}{4})^H_X - \frac{\pi}{4}^H_X - (\pi)^P_X - (\frac{\pi}{2})^H_X$
3. $(\frac{\pi}{2})^H_Y - \frac{\pi}{4}^P_Y - (-\frac{\pi}{2})^Y (\frac{\pi}{2})^H_X (\frac{\pi}{4})^H_X - \frac{\pi}{4}^H_X - (\pi)^P_X - (\frac{\pi}{2})^H_X$

Actually, the quantum-mechanical operation "reverse the qubit" is not applied. Instead of this, one measures the state after DFT and reads the result of the measurement in the opposite order $\mathbb{F}$.

After these three steps, we had finished the operation of DFT on the initial state $|01\rangle$. In order to illustrate the result we got, we need to obtain all the elements in the two-spin density matrix of the ultimate state by using state tomography $\mathbb{F}$. Before we did the experiment, we had simulated the experiment by using NMR simulator. The results are shown in Figure 3a, it can be regarded as a theoretical result. The matrix representation of the

$$ \begin{pmatrix} 1 & -i & -1 & i \\ i & 1 & -i & -1 \\ -1 & i & 1 & -i \\ -i & -1 & i & 1 \end{pmatrix}, $$

which is the same as we expected.

An advantage of doing NMR simulator is that it can represent the physics problem in spite of considering experimental errors (chemical shift, the affec-
tion of environmental and so on). So using NMR simulator can be considered as a quantum computer to simulate some quantum mechanical problem.

The experimental results are shown in Figure 3b, we measured and got real and imaginary components of the integral area from each peak, then we used all the integral areas we’d got to reconstruct that density matrix. Compared with the theoretical results, the experimental results agree with those deduced from theory. The relative errors are 24.8% and 4.7%. They primarily due to the imperfect calibration of the rotation, and are also caused by inhomogeneity of the magnetic field or magnetization and least-squares fitting used in the tomography procedure. Using other NMR techniques, such as phase cycling, the errors can be minimized.

4 CONCLUSION

We have demonstrated that the discrete Fourier transition can be implemented by means of NMR spectrometer and simulator and the experiment agrees with the theory well. Using the method we introduced, we can perform DFT on any quantum number with $L$-qubit. Performing DFT successfully gives a probability to realize Shor’s algorithm by using NMR. Fourier analysis is a versatile tools in the laboratory\cite{10}, so we might expect that the fast DFT should be an important application to physics.

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Figure 1: Quantum network for the quantum discrete Fourier transform

Performing on a five-qubit register, gate $B_k$ performing the conditional phase shift by $2 \pi / 2^k$

Figure 2: The network of performing operation "reverse the qubit".
Figure 3. Theoretical (simulator) and experimental (spectrometer) deviation density matrices after operated DFT on state $|01\rangle$. The unit of magnitude is arbitrary and the unit of phase is $\pi$. Relative errors were obtained according to: $||\rho_{\text{theory}} - \rho_{\text{exp}}|| / ||\rho_{\text{theory}}||$