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1. Introduction

The quantum Fourier transform (QFT) is a key ingredient in quantum algorithms. We have


different implementations of the quantum Fourier transform in experimental situations.
where each qubit is in a state \( |p(\phi_j\rangle) = (|0\rangle + e^{2\pi i \phi_j}|1\rangle)/\sqrt{2} \). The phases are determined by

\[
\phi_j = \sum_{k=0}^{n-1-j} a_k 2^{j+k-n}
\]

Equation (3) serves as the basis for implementing the QFT by one- and two-qubit operations. One implementation \([19, 20, 21]\) uses single-qubit Hadamard rotations gates \( H_j \) and two-qubit controlled-phase gate \( B_{j,k} \) that act on the qubits \( j \) and \( k \) and are given by

\[
B_{j,k} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & e^{i\theta_{jk}}
\end{pmatrix}
\]

where \( \theta_{jk} = \pi 2^{j-k} \) is a conditional phase shift applied only if both qubits are in the state \( |1\rangle \). In terms of these gates, the quantum circuit for \( n \) qubits is

\[
QFT_n = (H_1 B_{1,2} \ldots B_{1,n})(H_2 B_{2,3} \ldots B_{2,n})\ldots
\]

\[
\ldots(H_{n-1} B_{n-1,n})(H_n)
\]

(4)

with the sequence of operations being performed from right to left. With this implementation, the bit values of the result appear in reversed order. If a sequence reversal is required, this can be achieved by a sequence of SWAP operations on pairs of qubits.

We shall denote this decomposition of the QFT, as ‘serial’. For \( n \) qubits, it requires a total of \( n H_j \) gates, \( n(n-1)/2 B_{j,k} \) gates, and \( n/2 \) SWAP operations, leading to a computational complexity of \( O(n^2) \).

Individual Hadamard operations are qubit-selective and hence costlier than a total Hadamard operator that is applied on all qubits simultaneously. It would be thus desirable to have a decomposition of the QFT that involves a non-selective Hadamard transformation [9].

A more useful (for NMR) decomposition of the QFT can be obtained by noting that the Hadamard operator is self-inverse and that a Hadamard rotation of the controlled-phase gate can be decomposed as a root of a controlled-NOT gate,

\[
H_k B_{j,k} H_k^{-1} = e^{i\pi 2^{j-k}} (U_{CNOT})_{j,k}^{1/2}
\]

where \( j \) is the control and \( k \) the target qubit. The global phase factor does not influence measurement results and is henceforth ignored. Further, using

\[
[H_i; B_{j,k}] = 0, \ i \neq j, k,
\]

the sequence of operations in Eqn. (4) can be modified to

\[
QFT_n = [H_T][U_1 U_2 \ldots U_{n-2} U_{n-1}]
\]

(5)

where

\[
H_T = H_1 H_2 H_3 \ldots H_{n-1} H_n
\]

is the total non-selective Hadamard operator on all qubits, i.e. a single \( \pi/2 \) radio frequency pulse.

The \( U \) gates in Eqn. (5) are

\[
U_1 = H_2 B_{2,3}^{-1} = (U_{CNOT})_{2,3}^{1/2}
\]

\[
U_{n-2} = H_{n-1}(B_{1,n-1} B_{2,n-2} \ldots B_{n-2,n-1}) H_{n-1}^{-1} = (U_{CNOT})_{1,n-1}^{1/2} (U_{CNOT})_{2,n-2}^{1/2} (U_{CNOT})_{n-2,n-1}^{1/2}
\]

\[
U_{n-1} = H_n(B_1 B_2 \ldots B_{n-1,n}) H_n^{-1} = (U_{CNOT})_{1,n}^{1/2} (U_{CNOT})_{2,n}^{1/2} (U_{CNOT})_{n-1,n}^{1/2}
\]

(6)

They correspond to single spin rotations conditioned on the status of all the other spins involved in the operation. Since they are single spin rotations, they can be implemented as single radio frequency pulses. The conditioning on the state of the other spins is achieved by making them selective on specific transitions. As an example, for a system of three qubits, the operation \( U_{n-1} \) in this case is given by a fourth-root of a controlled-NOT gate on qubits one and three, followed by a square-root of a controlled-NOT gate on qubits two and three, with the third qubit being the target qubit in both cases. These gates thus involve three transitions of the third qubit: 100 \( \rightarrow \) 101, 110 \( \rightarrow \) 111, and 010 \( \rightarrow \) 011. Since these are unconnected transitions, rotations in the subspace of

![Diagram (a)](image1)

![Diagram (b)](image2)
these transitions can be achieved simultaneously. Many pulsed irradiation schemes for such precise selective excitation exist in NMR, mostly involving shaping the excitation profile of the rf waveform [22]. The entire QFT operation in this decomposition therefore reduces to a sequence of \( n \) radio frequency pulses. It scales linearly with the number of qubits, and we will denote it as the “parallel” implementation.

III. TIME-COST OF THE QFT

The main issue in the experimental implementation of quantum algorithms is not the number of logical operations per se, but the actual time-cost of each logical operation/quantum gate. The \( U \) transformations in Eqn. (5) are no longer two-qubit phase-shift gates but correspond to square- and higher-roots of controlled-NOT operations on specific qubits. They can be implemented experimentally using multiqubit gates that perform manipulations on qubits simultaneously. Since the NMR Hamiltonian has terms connecting multiple pairs of qubits, such multiqubit gates can be directly implemented. The quantum circuits for both serial and parallel implementations of the QFT are shown in Figure 1.

The most expensive operation in the serial implementation of the QFT is the controlled-phase shift gate \( B_{jk} \). The ideal time-cost is computed assuming all gates take the same amount of time. However experimentally, the controlled-phase shift gate requires a time \( \tau_{jk} \) proportional to the desired phase rotation angle \( \theta_{jk} \) (related to the “distance” \( (k - j) \) of the qubits), and inversely proportional to the interaction \( J_{jk} \) between the qubits. The magnitude of the interaction \( J_{jk} \) and hence the time cost depends on the specific experimental quantum computing technology under consideration. For liquid-state NMR, \( J_{jk} \) is the electron-mediated scalar coupling between the qubits. For our calculations, we assume the \( J_{jk} \)'s to be of the same order of magnitude for all qubits, represented by a universal constant coupling \( J \). The actual time cost of the serial decomposition of the QFT, involving only one-qubit Hadamards and the two-qubit phase-controlled gate is

\[
T_{\text{sseq}} = n\delta + \sum_{j=0}^{n-1} \sum_{k=j+1}^{n} \tau_{jk} = n\delta + \kappa \sum_{j=0}^{n-1} \sum_{k=j+1}^{n} 2^{j-k} = n\delta + \kappa(n - 1 + 2^{-n}) \approx O(n) \tag{7}
\]

where \( \delta \) is the time-cost of each single-qubit Hadamard rotation and \( \kappa = \pi / J \). Using multiqubit gates in the parallel implementation of the QFT reduces the actual time-cost of the algorithm. Quite apart from the saving obtained by using a non-selective Hadamard transformation in the beginning on all the qubits, each \( U \) gate can be thought of as having components from one or more \( B_{jk} \) gates. The actual time-cost of the parallel QFT is

\[
T_{\text{Ypar}} = \kappa \sum_{j=0}^{n-1} \sum_{k=j+1}^{n} \tau_{jk} \tag{8}
\]

Since for multiqubit gates, the system evolves under more than one coupling period simultaneously, only the largest of these need be counted for contribution to the time-cost and the inner sum in Eqn. (8) vanishes to give

\[
T_{\text{Ypar}} = \kappa \sum_{j=0}^{n-1} 2^{-1} = \kappa n / 2 \approx O(n) \tag{9}
\]

The analysis does not include the degradation of each gate due to dephasing nor does it take into account the SWAP operations, since the latter can in most cases be avoided by a relabeling of qubits. Implementing the Approximate QFT [19] would require fewer controlled-phase gates but would correspondingly reduce the accuracy.

IV. NMR IMPLEMENTATIONS OF THE QFT

Experiments were performed on a degassed, flame-sealed sample of \( ^{13} \)C-labeled chloroform, with \( ^{13} \)C and \( ^{1} \)H as the two qubits and a coupling constant of \( J_{12} \approx 215 \) Hz. Qubit-selective 90 degree pulses are of the order of 10\( \mu \)s. The unitary transformations required for the parallel decomposition of the QFT can be implemented either by transition-selective pulses or by J-coupling intervals sandwiched between qubit-selective pulses. A low-power rectangular pulse of length 6.5 ms was used to selectively excite individual transitions for the selective implementation of the QFT. For heteronuclear systems, RF pulses are applied on two different channels, leading to a reduction in the duration of selective pulses.

Each version of the QFT was implemented on a temporally averaged pseudopure state [23], obtained from the thermal equilibrium ensemble as the sum of three experiments

\[
\{\{90_x\}\}^C \frac{1}{2 J_{12}} \{\{90_y\}\}^C \{\{90_x\}\}^H \frac{1}{2 J_{12}} \{\{90_y\}\}^H \{\{90_x\}\}^H \frac{1}{2 J_{12}} \{\{90_y\}\}^H
\]

The details of the pulse sequences used to implement the serial, parallel and the selective-pulse (parallel) decompositions of the QFT, are given in Table I. The final SWAP operation was not executed; instead the readout in the reverse order was achieved by “relabeling” the qubits at the end of each experiment.

The results of all three implementations of the QFT are shown in Figure 2, using three-dimensional bar graphs to represent components of the final density matrix. Since only single-quantum terms are observable in NMR, it is
necessary to perform a series of experiments that rotate unobservable terms into observable ones, in order to sample the entire density matrix. The density matrix after each implementation of the QFT was reconstructed by standard quantum state tomography procedures, using a set of nine experiments and qubit-selective readouts [24, 25].

The precision of the QFT implementation can be estimated by measuring its “fidelity”, defined for mixed density matrices (such as the ones encountered in NMR) [7]

\[ F = \frac{Tr(\rho_t \rho_{exp})}{\sqrt{Tr(\rho_t)^2}} \] \[
\times \sqrt{\frac{Tr(\rho_{exp}^2)}{Tr(\rho_{init}^2)}} \] \]

The first term in the expression measures the correlation between the experimental deviation density matrix \( \rho_{exp} \) and the theoretical deviation density matrix \( \rho_t \) (obtained by “applying” the unitary operator corresponding to the ideal QFT transformation, to the initial density matrix \( \rho_{init} \)). The second term is the weighting factor to take into account the overall signal loss due to decoherence during the experiment.

The fidelities measured for the serial, parallel and selective-pulse versions of the QFT are 79%, 80% and 85% respectively. The reduction in fidelity is mainly due to imperfections in pulse calibration as well as system decoherence. It is not surprising that the serial and parallel versions are equally accurate for the case of two qubits. The savings in time and the increase in accuracy of the parallel QFT will be realised only for a larger number of qubits. The better performance of the selective scheme is due to the fact that with a direct implementation of the square-root of the controlled-NOT gate does not require refocusing schemes [26, 27]. However, in systems with a larger number of qubits such selective pulse schemes might not be feasible, the major stumbling blocks in such cases being decoherence during the pulses and the overlap of transitions in crowded spectra.

V. OTHER SPIN-BASED ARCHITECTURES

Recently, several approaches have been suggested for the design of solid-state spin-based quantum computers. Kane’s proposal [15] using single donor spins in Si, addresses the problem of scalability but has the disadvantages inherent in single-spin measurements. Ladd et al.’s solid-state NMR quantum computing device on the other hand, is made entirely of silicon, with the qubits being spin-1/2 nuclei located in isolated atomic chains [16]. Suter et. al. [17] proposed an alternative architecture with each logical qubit being represented by two physical qubits - an active electron spin to manipulate quantum information and a passive nuclear spin to store information. A logical qubit is addressed using magnetic field gradients and SWAP gates, realised as a cascade of three transition-selective pulses, are used to convert between active and passive states. A basic two-qubit gate relies on the dipolar interaction between electron spins and requires four additional SWAP gates, two to switch between active and passive states and two back-SWAPs to switch off the interaction between the neighbouring qubits. The hyperfine interaction is of the order of a few MHz and the electron dipolar interaction strength is around 10-50 MHz. An estimate of the actual time-cost of the QFT for such a solid-state spin quantum computer yields

\[ T_{ser} = n\delta + \sum_{j=0}^{n-1} \sum_{k=0}^{n-j} (\tau_{jk} + 2*\tau_{SWAP}) \]

\[ = n\delta + 2n\Delta + \kappa \sum_{j=0}^{n-1} \sum_{k=0}^{n-j} 2^{j-k} \]

\[ = n\delta + 2n\Delta + \kappa(n - 1 + 2^{-n}) \approx O(n) \] \]

where \( \delta \) is the time-cost of each single-qubit Hadamard rotation, \( \kappa = \pi/\delta \), \( \delta \) is the strength of the dipolar interaction and \( \Delta \) is the time unit of one SWAP gate. Since the gate times for this implementation are very fast, a greater number of logical operations compared to liquid-state NMR computers, can be performed within the system decoherence limit. These solid-state proposals are also scalable to a very large number of qubits.

In conclusion, we have estimated the realistic time-costs of different decompositions of the QFT for liquid
and solid-state NMR quantum computers and have measured the accuracy of the implementations experimentally using liquid-state NMR. While all quantum computation can be implemented using the two-qubit universal controlled-NOT gate and one-qubit rotations, the number of these basic operations increases exponentially with the number of qubits. It has been suggested that for more specific QC purposes, using more complicated multiqubit gates might be computationally more efficient [28, 29]. The parallel implementation of the QFT suggested by Cory et al., using multiqubit gates, performs better than the serial implementation. The actual experimental time-costs can be improved upon using innovative techniques like multiqubit gates, creative refocusing schemes [30] and time-optimal gates designed using control theory [31, 32].

Acknowledgments

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<table>
<thead>
<tr>
<th>Implementation</th>
<th>$n = 2$</th>
<th>$n = 3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Serial QFT</td>
<td>${90_\varphi}^1 {180_\varphi}^1 \frac{1}{\sqrt{2}} {90_\varphi}^{1,2} {45_\varphi}^{1,2}$</td>
<td>${90_\varphi}^1 {180_\varphi}^1 {45_\varphi} {90_\varphi}^{1,2} {45_\varphi} {90_\varphi}^{2,3} {45_\varphi}^2 {90_\varphi}^{2,3} {45_\varphi}^2$</td>
</tr>
<tr>
<td></td>
<td>${90_\varphi}^{1,2} {90_\varphi}^{2} {180_\varphi}^{1,2} \frac{1}{\sqrt{2}}$</td>
<td>${90_\varphi}^{1,2} {180_\varphi}^{1,2} {45_\varphi}^{1,2} {90_\varphi}^{2,3} {90_\varphi}^{2,3} {45_\varphi}^2 {180_\varphi}^2 \frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>${90_\varphi}^{1,2} {90_\varphi}^{2} {180_\varphi}^{1,2} \frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>Parallel QFT</td>
<td>${90_\varphi}^{1,2} {180_\varphi}^{1,2} {90_\varphi}^{2} {180_\varphi}^{1,2} \frac{1}{\sqrt{2}}$</td>
<td>${90_\varphi}^{1,2} {180_\varphi}^{1,2} {45_\varphi}^{1,2} {90_\varphi}^{2,3} {90_\varphi}^{2,3} {45_\varphi}^2 {180_\varphi}^2 \frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>Selective-pulse (parallel QFT)</td>
<td>${90_\varphi}^{1,2} {180_\varphi}^{1,2} {90_\varphi}^{2} {45_\varphi}^{1}$</td>
<td>${90_\varphi}^{1,2} {180_\varphi}^{1,2} {90_\varphi}^{2} {45_\varphi}^{1,2} {90_\varphi}^{3} {45_\varphi}^3 {90_\varphi}^{4}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>${90_\varphi}^{1,2} {180_\varphi}^{1,2} {90_\varphi}^{2} {45_\varphi}^{1,2} {90_\varphi}^{3} {45_\varphi}^3 {90_\varphi}^{4}$</td>
</tr>
</tbody>
</table>

TABLE 1: NMR pulse schemes for different implementations the QFT on $n = 2$ and 3 qubits. Superscript $r \to s$ indicates a selective RF pulse on the transition $r \to s$. Superscripts $r$ and $r, s$ indicate spin-selective pulses on the spins $r$ and $r, s$ respectively. Subscript $z$ indicates a composite-z pulse which can be expanded as a sandwich of rf pulses $\{\theta_z\} \equiv \{90_\varphi\} \{\theta_z\} \{90_\varphi\}$. 