Implementation of a Quantum Search Algorithm on a Nuclear Magnetic Resonance Quantum Computer

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The simulation of quantum mechanical systems with classical computers appears to be a computationally intractable problem. In 1982 Feynman\textsuperscript{1} reversed this observation, suggesting that quantum mechanical systems have an information processing capability much greater than that of corresponding classical systems, and thus could be used to implement a new type of powerful computer. In 1985 Deutsch\textsuperscript{2} described a quantum mechanical Turing machine, showing that quantum computers could indeed be constructed. Since then there has been extensive research in this field, but while the theory is fairly well understood actually building a quantum computer has proved extremely difficult, and only two methods have been used to demonstrate quantum logic gates: ion traps\textsuperscript{3,4} and nuclear magnetic resonance (NMR)\textsuperscript{5,6}. NMR quantum computers have previously been used to demonstrate quantum algorithms to solve the two bit Deutsch problem\textsuperscript{7,8}. Here we show how such a computer can be used to implement a fast quantum search algorithm initially developed by Grover\textsuperscript{9,10}.

Among other applications Grover’s algorithms enable an extremely rapid search over the domain of a binary function to find elements for which this function is satisfied (that is, the function has the value 1). This approach is simpler if the number of satisfying values is known beforehand, and is particularly simple when precisely one quarter of the elements in the domain satisfy the function\textsuperscript{11}. The algorithm can be demonstrated using a computer with two quantum bits (qubits) to search a two bit domain in which one of the four elements satisfies the function. A classical search of this domain would require between 1 and 3
evaluations of the function to find the satisfying element, while a quantum search can find this element with only one function evaluation. In the more general case of searching a domain of size $N$ for one of $k$ satisfying elements the classical search requires about $\frac{1}{2}(N/k)$ function evaluations, while the quantum search requires only $O(\sqrt{N/k})$.

A quantum circuit for implementing a quantum search in a two qubit system is shown in Fig. 1. This algorithm uses a single function evaluation to label the single state which satisfies the function, followed by a series of gates which drive the system into this particular state. There are four possible functions $f$ with a unique satisfying element, and these functions are conveniently labelled by the bit pattern of the satisfying element. The algorithm starts with the quantum computer in state $|00\rangle$ and ends with the computer in a state corresponding to the bit pattern of the unique element, and so this element can be immediately identified by determining the final state of each qubit.

This algorithm was implemented using our two qubit NMR quantum computer, described in Ref. [7]. This computer uses the two spin states of $^1$H nuclei in a magnetic field as qubits, while radio frequency (RF) fields and spin–spin couplings between the nuclei are used to implement quantum logic gates. Our molecule, partially deuterated cytosine, contains two $^1$H nuclei, and thus can be used to implement a two qubit computer. The pseudo-Hadamard gates ($h$) were implemented using 90° pulses, while the function evaluation was performed using the pulse sequence shown in Fig. 2. The phases of five of the pulses depend on which of the four possible functions is to be implemented, and these phases should be set as shown in the figure caption. The final gate, $U_{00}$, is easily implemented, as it is identical to $U_{f00}$.

The algorithm should start with the computer in state $|00\rangle$, but with an NMR quantum computer it is not practical to begin in a true $|00\rangle$ state. Using the methods of Cory et al., it is, however, possible to create an effective pure state, which behaves in an equivalent manner. Similarly it is not practical to determine the final state directly, but an equivalent measurement can be made by exciting the spin system with a further 90° pulse, and observing the phases of the resulting NMR signals. The absolute phase of an NMR signal depends in a complex manner on a variety of experimental details, and so it is not possible to interpret absolute phases, but this can be overcome by measuring a reference signal, obtained by applying a 90° pulse directly to the initial state.

The results of this approach are shown in Fig. 3. Five spectra are shown: a reference spectrum acquired using a single 90° pulse, and spectra acquired from the same computer implementing the search algorithm for each of the four possible functions, $f$. Each spectrum consists of two closely spaced pairs of lines: each pair of lines corresponds to a single qubit, while the barely visible splitting within each pair arises from the spin–spin coupling, $J$, used to implement the two qubit gates. To improve the appearance of the spectra the final 90° detection pulse was
preceded by a magnetic field gradient pulse, which acts to dephase the majority of any error terms which might occur.

The reference spectrum corresponds to the computer being in state $|00\rangle$, and the phase of this spectrum was adjusted so that both lines are in positive absorption phase (that is, pointing upwards). The same phase correction was then applied to the other four spectra, allowing positive absorption lines to be interpreted as qubits in state $|0\rangle$, while negative absorption lines can be interpreted as qubits in state $|1\rangle$. The left hand pair of lines arises from the first spin, and thus corresponds to the first qubit, while the right hand pair of lines corresponds to the second qubit. Thus, for example, spectrum (c) corresponds to the state $|01\rangle$. Examining the four spectra (b)–(e), it is clear that our implementation of a quantum search using the function $f_{ab}$ leaves the computer largely in a final state $|ab\rangle$, much as expected.

There are however small but significant errors in the calculation, which result in distortions in the final spectra. While most of these distortions are removed by the field gradient pulse, their effects remain visible as variations in the heights of the NMR lines. These errors arise from a variety of causes, but the most significant is errors in the NMR pulse sequence used to implement the calculation. These pulse sequences require a large number of selective pulses, that is pulses which only affect one of the two spins making up the computer. In practice it is difficult to achieve the desired effect at one spin while leaving the other entirely unaffected, resulting in errors in the final result. Interestingly the distortions are much worse in some cases than in others: they are particularly bad in the spectrum obtained when the function is $f_{01}$. Understanding this variability may lead to techniques for reducing the distortion in all cases.

Implementing Grover’s algorithm is a major step forward for NMR quantum computing (since this letter was first submitted an implementation of Grover’s algorithm using heteronuclear NMR has been published\textsuperscript{12}, but is by no means the limit of what can be achieved. Preliminary studies have been made of systems containing three qubits\textsuperscript{13} and it should be possible to build larger NMR quantum computers, allowing the implementation of more complex algorithms.

References

1 Feynman, R. P. Simulating Physics with Computers. \textit{Int. J. Theor. Phys.} \textbf{21}, 467–488 (1982).

2 Deutsch, D. Quantum-Theory, the Church-Turing Principle and the Universal Quantum Computer. \textit{Proc. R. Soc. Lond. A} \textbf{400}, 97–117 (1985).

3 Cirac, J. I. & Zoller, P. Quantum Computations with Cold Trapped Ions. \textit{Phys. Rev. Lett.} \textbf{74}, 4091–4094 (1995).
4 Monroe, C., Meekhof, D. M., King, B. E., Itano, W. M. & Wineland, D. J. Demonstration of a Fundamental Quantum Logic Gate. *Phys. Rev. Lett.* **75**, 4714–4715 (1995).

5 Cory, D. G., Fahmy, A. F. & Havel, T. F. Ensemble quantum computing by NMR spectroscopy. *Proc. Natl. Acad. Sci. USA* **94**, 1634–1639 (1997).

6 Gershenfeld, N. A. & Chuang, I. L. Bulk Spin-Resonance Quantum Computation. *Science* **275**, 350–356 (1997).

7 Jones, J. A. & Mosca, M. Implementation of a Quantum Algorithm to Solve Deutsch’s Problem on a Nuclear Magnetic Resonance Quantum Computer. *J. Chem. Phys.*, in press. See also LANL e-print quant-ph/9801027.

8 Chuang, I. L., Vandersypen, L. M. K., Zhou, X., Leung, D. W., & Lloyd, S. Experimental realization of a quantum algorithm. *Nature*, in press. See also LANL e-print quant-ph/9801037.

9 Grover, L. K. A fast quantum mechanical algorithm for database search. *Proceedings of the 28th Annual ACM Symposium on Theory of Computation*, 212–219 (1996).

10 Grover, L. K. Quantum Mechanics Helps in Searching for a Needle in a Haystack. *Phys. Rev. Lett.* **79**, 325–328 (1997).

11 Boyer, M., Brassard, G., Høyer, P., & Tapp, A. Tight bounds on quantum searching. *Proceedings of fourth workshop on Physics and Computation—PhysComp’96*, 36–41 (1996).

12 Chuang, I. L., Gershenfeld, N. & Kubinec, M. Experimental Implementation of Fast Quantum Searching. *Phys. Rev. Lett.* **80**, 3408-3411 (1998).

13 Laflamme, R., Knill, E., Zurek, W. H., Catasti, P. & Mariappan, S. V. S. NMR GHZ. *Proc. Roy. Soc. Lond.*, in press.

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Figure 1: A quantum circuit for the implementation of a quantum search algorithm on a two qubit computer. Gates marked $h$ (pseudo-Hadamard gates) act to take a single eigenstate to a uniform superposition of the four possible eigenstates, while gates marked $h^{-1}$ implement the inverse operation. The first two qubit gate $U_{f_{ab}}$ corresponds to an evaluation of the function $f_{ab}$, replacing an eigenstate $|ij\rangle$ by $-|ij\rangle$ if $i = a$ and $j = b$, while $U_{00}$ simply replaces $|00\rangle$ by $-|00\rangle$.

Figure 2: NMR pulse sequence used to implement $U_{f_{ab}}$. Narrow boxes correspond to 90° pulses, while wide boxes are 180° pulses; the upper and lower lines refer to the nuclear spins corresponding to the first and second qubits respectively. The time period $\tau$, during which no pulses are applied, is set equal to $1/4J$, where $J$ is the size of the spin–spin coupling between the nuclei. The phase of each pulse is written above it, and for five of the pulses this phase depends on which of the four functions $f_{ab}$ is to be implemented. These phases should be set as follows: $f_{00}$, $\theta = +y$, $\phi = +x$, $\psi = -y$; $f_{01}$, $\theta = +y$, $\phi = -x$, $\psi = +y$; $f_{10}$, $\theta = -y$, $\phi = -x$, $\psi = -y$; $f_{11}$, $\theta = -y$, $\phi = +x$, $\psi = +y$. 
Figure 3: Experimental spectra from our NMR quantum computer. Spectrum (a) is a reference spectrum, used to determine the absolute phases of the NMR signals, while spectra (b)–(e) were acquired from the same computer implementing the quantum search algorithm using each of the four possible functions: (b) $f_{00}$, (c) $f_{01}$, (d) $f_{10}$, (e) $f_{11}$. These four spectra were processed using the reference phase obtained from spectrum (a), and so the phases of the signals can be interpreted as states of the corresponding qubits, as described in the main text.