Experimental Implementation of Fast Quantum Searching

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Using nuclear magnetic resonance techniques with a solution of chloroform molecules we implement Grover's search algorithm for a system with four states. By performing a tomographic reconstruction of the density matrix during the computation good agreement is seen between theory and experiment. This provides the first complete experimental demonstration of loading an initial state into a quantum computer, performing a computation requiring fewer steps than on a classical computer, and then reading out the final state. [S0031-9007(98)05850-5]

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The study of computation in quantum systems began with the recognition of the theoretical possibility [1–3]. This was followed by a series of results leading up to proofs that a quantum computer requires fewer operations than a classical computer for problems including factoring [4] and searching [5,6]. Appreciation of the power of quantum computing was quickly tempered by the realization that preserving quantum coherence made the implementation of practical quantum computers appear to be unlikely [7–9].

Two recent developments have changed that conclusion. The first is the recognition that quantum error correction can be used to compute with imperfect computers [10,11]. And the second is that it is possible to decrease the influence of decoherence by computing with mixed-state ensembles rather than isolated systems in a pure state. This can be done by introducing extra degrees of freedom [12] using quantum spins [13], space [14], or time [15] to embed within the overall system a subsystem which transforms like a pure state. We apply these ideas here in the first experimental realization of a significant quantum computing algorithm, using nuclear magnetic resonance (NMR) techniques to perform Grover's quantum search algorithm [5,6].

Classically, searching for a particular entry in an unordered list of N elements requires $\mathcal{O}(N)$ attempts. The list could be stored as a table, such as finding a name to go along with a phone number in a phone book, or computed as needed, like testing possible combinations to unlock a padlock. Grover's surprising result is that a quantum computer can obtain the result with certainty in $\mathcal{O}(\sqrt{N})$ attempts.

The simplest interesting application of Grover's algorithm is the $N = 4$ case, which can be posed as follows: on the set $x = \{0, 1, 2, 3\}$ a function $f(x) = 1$ except at some x_0, where $f(x_0) = -1$. How many evaluations of f are required to determine x_0? In the worst case, x_0 has a uniform probability of being either 0, 1, 2, or 3, and so the average number of evaluations required classically is $9/4 = 2.25$. With a quantum computer using Grover's algorithm, this is reduced to a *single* evaluation. We have experimentally implemented this case using molecules of chloroform as a quantum computer, and confirmed the periodic behavior expected of the algorithm.

The algorithm works by representing x as a pair of two-state quantum systems. We take these to be the spins of the carbon and hydrogen nuclei, writing $|\uparrow\rangle = |1\rangle$ and $|\downarrow\rangle = |0\rangle$. The function $f(x)$ is implemented as a unitary transform that flips the phase of the x_0 element. If the operator corresponding to $x_0 = 3$ is applied to the superposition $|\psi_0\rangle = (|00\rangle + |01\rangle + |10\rangle + |11\rangle)/2$ the result is $(|00\rangle + |01\rangle + |10\rangle - |11\rangle)/2$. Measurement of this state is not useful because each answer occurs with equal probability. Grover's algorithm amplifies the correct answer by following the conditional flip with a second operation that inverts each state about the mean. Applied to a superposition $\sum_k \alpha_k|k\rangle$ this step gives a new state $\sum_k \beta_k|k\rangle$ with $\beta_k = -\alpha_k + 2\langle\alpha\rangle$, where $\langle\alpha\rangle$ is the mean value of α_k. For $N = 4$ and $x_0 = 3$ the result of the conditional flip followed by the inversion about the mean is the state $|\psi_1\rangle = |11\rangle$, providing the answer immediately. For general N, about $\pi\sqrt{N}/4$ repetitions of these two steps are required to find x_0 [16].

Further iteration of the flip and inversion operations leads to a periodicity in the state. Let U be the unitary transform which does these two operations, so that $|\psi_n\rangle = U^n|\psi_0\rangle$ is the state after the nth iteration. Boyer *et al.* have shown that the amplitude $\langle x_0|\psi_n\rangle \approx \sin[(2n + 1)\theta]$, where $\theta = \arcsin(1/\sqrt{N})$; this periodicity arises from the finite size of the system and the unitarity of U. For $N = 4$ the theoretical expectation is the sequence $|11\rangle = |\psi_1\rangle = -|\psi_4\rangle = |\psi_7\rangle = -|\psi_{10}\rangle \ldots$, a period of 6 (or 3 if the overall sign is disregarded).

Our experiments used a 0.5 milliliter, 200 millimolar sample of Carbon-13 labeled chloroform (Cambridge Isotopes) in d_6 acetone. Data were taken at room temperature with a Bruker DRX 500 MHz spectrometer. The coherence times were measured to be $T_1 = 20$ sec

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and $T_2 = 0.4$ sec for the proton, and $T_1 = 21$ sec and $T_2 = 0.3$ sec for the carbon (the large ratio is due to C-Cl relaxation), and the coupling was measured to be $J = 215$ Hz. All resonance lines from other nuclei and the solvent were far from the region of interest in this experiment. In the rotating frame of the proton (at about 500 MHz) and carbon (at about 125 MHz), the Hamiltonian for this system can be approximated as [17]

$$\mathcal{H} = 2\pi\hbar J I_{zA} I_{zB} + P_{\phi A}(t) I_{\phi A} + P_{\phi B}(t) I_{\phi B} + \mathcal{H}_{\text{env}}, \tag{1}$$

where $I_{\phi A}$ and $I_{\phi B}$ are the angular momentum operators in the $\hat{\phi}$ direction for the proton (A) and carbon (B), and $\mathcal{H}_{\text{env}}$ represents the coupling to the environment, responsible for the decoherence. $P_{\phi A}$ and $P_{\phi B}$ describe the strength of radio-frequency (rf) pulses which are applied on resonance to perform single-spin rotations to each of the two spins. These rotations will be denoted as $X \equiv \exp(i\pi I_x/2)$ for a 90° rotation about the $\hat{x}$ axis, and $\bar{Y} \equiv \exp(-i\pi I_y/2)$ for a 90° rotation about $-\hat{y}$, with a subscript specifying the affected spin.

We used temporal labeling [15] to obtain the signal from the pure initial state

$$|\psi_{\text{in}}\rangle = |00\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{2}$$

by repeating the experiment three times, cyclically permuting the $|01\rangle$, $|10\rangle$, and $|11\rangle$ state populations before the computation and then summing the results.

The calculation starts with a Walsh-Hadamard transform W, which rotates each quantum bit (qubit) from $|0\rangle$ to $(|0\rangle + |1\rangle)/\sqrt{2}$, to prepare the uniform superposition state

$$|\psi_0\rangle = W|\psi_{\text{in}}\rangle = \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}. \tag{3}$$

Note that $W = H_A \otimes H_B$, where $H = X^2\bar{Y}$ (pulses applied from right to left) is a single-spin Hadamard transform.

The operator corresponding to the application of $f(x)$ for $x_0 = 3$ is as

$$C = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \tag{4}$$

This conditional sign flip, testing for a Boolean string that satisfies the AND function, is implemented by using the coupled-spin evolution which occurs when no rf power is applied. During a time t the system undergoes the unitary transformation $\exp(2\pi i J I_{zA} I_{zB} t)$ in the doubly rotating frame. Denoting a $t = 1/2J$ (2.3 millisecond) period evolution as the operator τ, we find that $C = Y_A \bar{X}_A \bar{Y}_A Y_B \bar{X}_B \bar{Y}_B \tau$ (up to an irrelevant overall phase factor).

An arbitrary logical function can be tested by a network of controlled-NOT and rotation gates [13,18], leaving the result in a scratch pad qubit. This qubit can then be used as the source for a controlled phase-shift gate to implement the conditional sign flip, if necessary reversing the test procedure to erase the scratch pad. In our experiment these operations could be collapsed into a single step without requiring an extra qubit.

The operator D that inverts the states about their mean can be implemented by a Walsh-Hadamard transform W, a conditional phase shift P, and another W:

$$D = WPW = W\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

$$W = \frac{1}{2}\begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix} \tag{5}$$

This corresponds to the pulse sequence $P = Y_A X_A \bar{Y}_A Y_B X_B \bar{Y}_B \tau$.

Let $U = DC$ be the complete iteration. The state after one cycle is

$$|\psi_1\rangle = UW|\psi_0\rangle = |11\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}. \tag{6}$$

A measurements of the system's state will now give with certainty the correct answer, $|11\rangle$. For further iterations, $|\psi_n\rangle = U^n|\psi_0\rangle$,

$$|\psi_2\rangle = \frac{1}{2}\begin{bmatrix} -1 \\ -1 \\ -1 \\ 1 \end{bmatrix} \quad |\psi_3\rangle = \frac{1}{2}\begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$$

$$|\psi_4\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \end{bmatrix}. \tag{7}$$

We see that a maximum in the amplitude of the x_0 state $|11\rangle$ recurs every third iteration.

Like any computer program that is compiled to a microcode, the rf pulse sequence for U can be optimized to eliminate unnecessary operations. In a quantum computer this is essential to make the best use of the available coherence. Ignoring irrelevant overall phase factors, and noting that $H = \bar{X}^2\bar{Y}$ also works, we can simplify U

by removing sequential rotations which cancel each other out, to get

$$U = \bar{X}_A\bar{Y}_A\bar{X}_B\bar{Y}_B\tau X_A\bar{Y}_A X_B\bar{Y}_B\tau \qquad (x_0 = 3)\,. \quad (8)$$

The other possible cases are obtained by changing the signs of the first two X rotations,

$$U = \begin{cases} \bar{X}_A\bar{Y}_A\bar{X}_B\bar{Y}_B\tau X_A\bar{Y}_A\bar{X}_B\bar{Y}_B\tau & (x_0 = 2)\,, \\ \bar{X}_A\bar{Y}_A\bar{X}_B\bar{Y}_B\tau\bar{X}_A\bar{Y}_A X_B\bar{Y}_B\tau & (x_0 = 1)\,, \\ \bar{X}_A\bar{Y}_A\bar{X}_B\bar{Y}_B\tau\bar{X}_A\bar{Y}_A\bar{X}_B\bar{Y}_B\tau & (x_0 = 0)\,. \end{cases} \quad (9)$$

Because the magnetization that is detected in an NMR experiment is the result of a weak measurement on the ensemble, the signal strength gives the fraction of the population with the measured magnetization rather than collapsing the wave function into a measurement eigenstate. The readout can be preceded by a sequence of single spin rotations to allow all terms in the deviation density matrix $\rho_\Delta = \rho - \mathrm{tr}(\rho)/N$ to be measured [19]. Nine experiments—no rotation, rotation about $\hat{x}$, and about $\hat{y}$, for each of the two spins—were performed to do this reconstruction of the density matrix to facilitate comparison between theory and experiment.

Figure 1 shows the theoretical and measured deviation density matrices $\rho_{\Delta n} = |\psi_n\rangle\langle\psi_n| - \mathrm{tr}(|\psi_n\rangle\langle\psi_n|)/4$ for the first seven iterations of U. As expected, $\rho_{\Delta 1}$ clearly reveals the $|11\rangle$ state corresponding to $x_0 = 3$. Analogous results were obtained for experiments repeated for

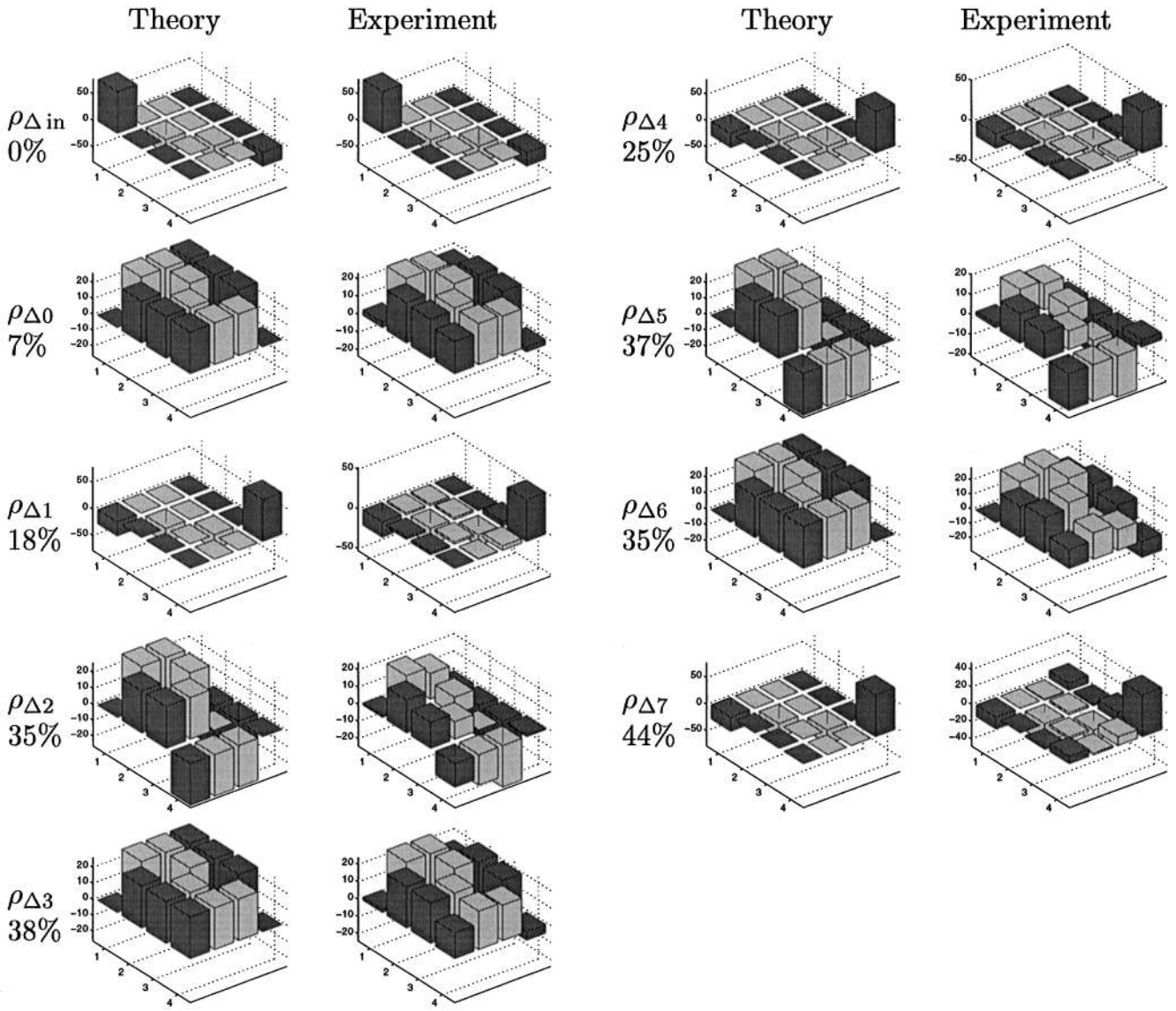

FIG. 1. Theoretical and experimental deviation density matrices (in arbitrary units) for seven steps of Grover's algorithm performed on the hydrogen and carbon spins in chloroform. Three full cycles, with a periodicity of three iterations are clearly seen. Only the real component is plotted (the imaginary portion is theoretically zero and was found to contribute less than 12% to the experimental results). Relative errors $||\rho_{\mathrm{theory}} - \rho_{\mathrm{expt}}||/||\rho_{\mathrm{theory}}||$ are shown as percentages.

the other possible values of x_0. Measuring each density matrix required $9 \times 3 = 27$ experimental repetitions, nine for the tomographic reconstruction and three for the pure state preparation. Both of these operations were performed as tests of the computation, but neither was necessary. In our experiment, starting from the thermal state the maximum population can be identified in a single iteration, with the result obtained from a single output spectrum. In the general N case, readout of $\log N$ expectation value measurements would be required, and good inputs for Grover's algorithm can be distilled in a number of steps polynomial in $\log(N)$ [15].

The longest computation, for $n = 7$, took less than 35 milliseconds, which was well within the coherence time. The periodicity of Grover's algorithm is clearly seen in Fig. 1, with good agreement between theory and experiment. The large signal-to-noise ratio (typically better than 10^4 to 1) was obtained with just single-shot measurements. Numerical simulations indicate that the 7%–44% errors are primarily due to inhomogeneity of the magnetic field, magnetization decay during the measurement, and imperfect calibration of the rotations (in order of importance).

These experimental results demonstrate the operation of a simple quantum computer that can load an initial state, perform a computation, and read out the answer. While there is a long way to go from such a demonstration to a system that can exceed the performance of the fastest classical computers, the experimental study of quantum computation has already come much farther in its short life than either early theoretical predictions or the history of mature computing technologies would have suggested. While scaling up to much larger systems poses daunting challenges, many optimizations remain to be taken advantage of, including increasing the sample size, using coherence transfer to and from electrons, and optical pumping to cool the spin system [19]. Furthermore, Grover's algorithm can be matched to convenient physical operations by performing generalized rapid search, which uses transforms other than the Walsh-Hadamard [20].

The NMR system that we have described already has all of the components of a complete computer architecture, including the rudiments of compiler optimizations. It can implement a nontrivial quantum computation; the challenge now is to accomplish a useful one.

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