

Implementation of a three-quantum-bit search algorithm

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We report the experimental implementation of Grover's quantum search algorithm on a quantum computer with three quantum bits. The computer consists of molecules of ¹³C-labeled CHFBr₂, in which the three weakly coupled spin-1/2 nuclei behave as the bits and are initialized, manipulated, and read out using magnetic resonance techniques. This quantum computation is made possible by the introduction of two techniques which significantly reduce the complexity of the experiment and by the surprising degree of cancellation of systematic errors which have previously limited the total possible number of quantum gates. © 2000 American Institute of Physics.

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Elementary quantum computations¹⁻³ have recently been demonstrated experimentally⁴ using coupled nuclear spins as quantum bits (qubits) and solution nuclear magnetic resonance (NMR) techniques to prepare, manipulate, and detect the spins.^{5,6} Aside from the well-understood scaling limitations due to the use of a high-temperature (almost random) system instead of a low-temperature (low entropy) polarized spin system,^{5,7} the crucial limitation in applying this method to implement larger quantum algorithms has been systematic errors in the quantum gates. These gates are implemented by applying pulses of radio frequency (rf) electromagnetic fields of precise duration and phase, which are in practice highly inhomogeneous over the sample volume, causing the gate fidelity⁸ to be less than 95%. Producing a homogeneous field is difficult because of the sample geometry and the necessity of keeping the field transverse to the 11.8 T alignment field. If such systematic errors simply accumulated, these observations would imply that fewer than 90 gates⁹ applied to any one spin could ever be cascaded in these systems.

One technique which has been proposed for controlling errors in quantum gates is quantum error correction,¹⁰ and in fact, it is known that if the error probability per gate is smaller than a certain threshold,¹¹ and in addition the architecture of the computer satisfies certain criteria, then quantum computation could be carried out robustly and indefinitely, despite the errors. Unfortunately, this threshold is currently estimated to be below 10⁻⁴, which is virtually unreachable with current NMR quantum computation techniques and present levels of systematic errors. Now, the principle attribute of traditional error correction techniques is their ability to correct completely random errors which originate from fundamentally irreversible decoherence phenomena;¹² in principle, systematic errors, which are inherently reversible—at least on an appropriate time scale—should be much easier to control, given knowledge about their origin.

Here, we report on the experimental realization of a

three-qubit quantum search algorithm, and the observation of 28 full cycles of the theoretically predicted oscillatory behavior for the algorithm. This was made possible by the application of two techniques to reduce the number of gates required for the implementation and by the control and cancellation of systematic errors. More than 280 two-qubit quantum gates involving 1350 rf pulses were successfully cascaded, which exceeds not only the number of gates used in all previous NMR quantum computing experiments but also the limitation of 90 gates, imposed by cumulative systematic errors.

The experiments were carried out with molecules containing $n=3$ weakly coupled spin-1/2 nuclei, subject to a strong magnetic field \vec{B}_0 . Each spin represents one qubit, with the ground and excited state serving as $|0\rangle$ and $|1\rangle$. The Hamiltonian is well approximated by ($\hbar=1$)⁶

$$\mathcal{H} = - \sum_i \omega_i I_{zi} + \sum_{i<j} 2\pi J_{ij} I_{zi} I_{zj} + \mathcal{H}_{\text{env}}, \quad (1)$$

where the first term represents the free precession of each spin i about $-\vec{B}_0$, with I_{zi} the angular momentum operator in the \hat{z} direction and ω_i the Larmor frequency of spin i . The second term describes a scalar spin-spin coupling of J_{ij} between spins i and j and \mathcal{H}_{env} represents coupling to the environment, which causes decoherence. A resonant rf field rotating in the $\hat{x}-\hat{y}$ plane can be gated on to perform single-spin rotations.

The first method to reduce the number of one- and two-spin gates used to realize any given n -qubit unitary operation starts with a library of efficient implementations for often-used building blocks. For example, four equivalent realizations of a Z rotation using a rf coil in the transverse plane, are $Z \equiv YX\bar{Y} \equiv \bar{Y}\bar{X}Y \equiv X\bar{Y}X \equiv X\bar{Y}\bar{X}$, where X and \bar{X} denote $+90^\circ$ and -90° rotations about the \hat{x} axis. And $\text{CNOT}_{ij} \equiv X_j Y_j \tau_{ij} Z_i \bar{Y}_j \equiv \bar{X}_j \bar{Y}_j \tau_{ij} \bar{Z}_i Y_j \equiv Y_j \tau_{ij} Z_i \bar{Y}_j X_j \equiv \bar{Y}_j \tau_{ij} \bar{Z}_i Y_j \bar{X}_j$, where τ_{ij} describes a time evolution of $1/2J_{ij}$, during which all couplings except J_{ij} are refocused⁵ (CNOT_{ij} represents a controlled-NOT which flips spin j if and only if the control spin i is $|1\rangle$). For any given quantum circuit, e.g., Fig. 1 (after

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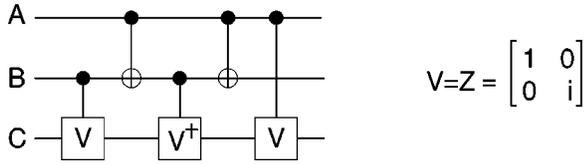


FIG. 1. Quantum circuit for a three-qubit Toffoli gate which flips the phase of the $|1\rangle|1\rangle|1\rangle$ term. Vertical lines connecting two horizontal lines represent two-qubit gates, which perform the unitary operation shown on the target qubit if and only if the control qubit (indicated by a black dot) is $|1\rangle$ (an open circle represents a NOT gate). Time goes from left to right.

Ref. 13), specific implementations of the building blocks can then be laid out such that adjacent pulses invert each other, so they can be omitted. The simplification process can exploit the commutation of Z rotations with time evolutions (the Hamiltonian), and of rf pulses on different spins with each other. Furthermore, NMR permits a direct implementation of many useful gates such as the controlled V (Fig. 1), which can be realized by $\tau_{ij}/2$ and a few single-spin rotations. If only CNOTs and one-qubit gates were used to implement the controlled V s (as in Ref. 13) and if no pulses were canceled out, $70.5 \pi/2$ pulses and 8 evolutions of $1/2J$ would be required for the Toffoli gate (Fig. 1). This was reduced to 19 pulses, 2 evolutions of $1/2J$, and 3 of $1/4J$, by using the simplification methodology.¹⁴

The second method to reduce the complexity concerns the initialization of the qubits to the ground state, generally the first step in quantum algorithms. The density matrix ρ_{eq} of the system of Eq. (1) in equilibrium at room temperature is highly mixed ($\hbar \omega_i \ll k_B T$, with $k_B T$ the thermal energy). The use of room temperature nuclear spins is made possible by converting the equilibrium state into an “effective pure state”⁵ (one population deviates from a uniform background). We propose the preparation of an effective pure ground state ρ_g by a new variant of temporal averaging.¹⁵ The original scheme involves the summation of $2^n - 1$ density matrices, each of which is obtained from ρ_{eq} by cyclicly permuting all populations except the ground state population;¹⁵ but this gets rather involved for $n \geq 3$. A much simpler approach is to take a weighted sum of (diagonal) density matrices ρ_l which are obtained from ρ_{eq} by performing just a few CNOTs to rearrange the $2^n - 1$ populations. The weights w_l are determined by solving a set of linear equations $\sum_l w_l \text{diag}(\rho_l) = \text{diag}(\rho_g)$. This approach may still require up to $2^n - 1$ experiments to get exactly ρ_g , but allows one also to approximate ρ_g using far fewer experiments. All the data shown below were obtained using just three experiments, resulting in an expected variance of the $2^n - 1$ populations of only 7% of their average value. These modifications thus increase both the simplicity and scalability of temporal labeling.

We used these methods to implement the eight instances of the three-qubit Grover algorithm. This algorithm achieves a quadratic speed-up over classical algorithms when searching in an unsorted database with N entries:³ given an unknown function $f(x)$ with the promise that $f(x_0) = -1$ for a unique x_0 , and $f(x) = 1$ elsewhere, a classical search needs $\mathcal{O}(N)$ (4.375 for $N = 8$) attempts to find x_0 , while $\mathcal{O}(\sqrt{N})$ (2 for $N = 8$) queries suffice using Grover’s quantum algorithm.³ For $N = 8$, the algorithm requires four Toffoli

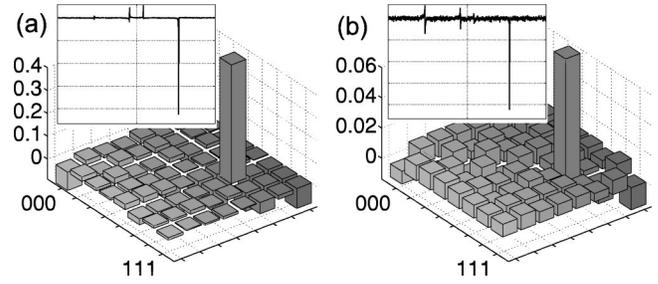


FIG. 2. Experimental deviation density matrices ρ_{exp} for $|x_0\rangle = |1\rangle|0\rangle|1\rangle$, shown in magnitude with the sign of the real part (all imaginary components were small), after 2(a) and 28(b) Grover iterations. The diagonal elements give the population difference with respect to the average. The off-diagonal elements represent coherences between the basis states. Inset: The corresponding ^{13}C spectra (^{13}C was the least significant qubit). The receiver phase and readout pulse are set such that the spectrum be absorptive and positive for a spin in $|0\rangle$.

gates,¹³ plus several one-qubit gates. Earlier experiments^{4,7} required at most one Toffoli gate and a few two-qubit gates.

We selected ^{13}C -labeled CHFBBr_2 ¹⁶ for our experiments. The Hamiltonian of the ^1H – ^{19}F – ^{13}C spin system is of the form of Eq. (1) with $J_{\text{HC}} = 224$ Hz, $J_{\text{HF}} = 50$ Hz, and $J_{\text{FC}} = -311$ Hz. The scalar interaction with the Br nuclei is averaged out and only contributes to \mathcal{H}_{env} .⁶ Experiments were carried out at IBM using an 11.7 T Oxford Instruments magnet and a Varian Unity Inova spectrometer with a triple resonance (H–F–X) probe from Nalorac. The output state of each spin i , $|0\rangle$ or $|1\rangle$, can be determined from the phase of the signal induced in the rf coil after applying an X_i readout pulse. In fact, the spectrum of the signal of any one spin suffices to determine the output state of all the spins given that they are in an effective pure energy eigenstate and that they are all mutually coupled: each spectrum then contains only a single line, the frequency of which, combined with the knowledge of the J_{ij} , reveals the state of the remaining spins [Fig. 2(a), inset]. We also reconstructed the complete output deviation (traceless) density matrix⁵ using quantum state tomography¹⁷ [Fig. 2(a)].

The agreement between experimental results and theoretical predictions is very good, considering that about 100 pulses were used and that the systematic error rate exceeds 5% per rf pulse (the measured signal loss due to rf field inhomogeneity after applying X_i). This suggests that the systematic errors cancel each other out to some degree. We examined this in more detail in a series of experiments with increasingly longer pulse sequences executing up to 28 Grover iterations (repeated executions of the two main steps of Grover’s algorithm).³ Theoretically, the probability of $|x_0\rangle$ oscillates as a function of the number of iterations k , reaching a first maximum for $k = \mathcal{O}(\sqrt{N})$.³ Figure 3(a) shows that the diagonal entry d_{x_0} of ρ_{exp} oscillates as predicted but the oscillation is damped as a result of errors, with a time constant T_d of 12.8 iterations. However, T_d would have been smaller than 1.5 if the errors due to just the rf field inhomogeneity were cumulative [Fig. 3(a), solid line]. Remarkably, after a considerable initial loss, d_{x_0} decays at a rate close to the ^{13}C T_2 decay rate⁶ (dashed line), which can be regarded as a lower bound on the overall error rate. A more complete measure to quantify the error and benchmark results is the relative error $\epsilon_r = \|\rho_{\text{exp}} - \rho_{\text{th}}\|_2 / \|\rho_{\text{th}}\|_2$, where ρ_{exp} and ρ_{th}

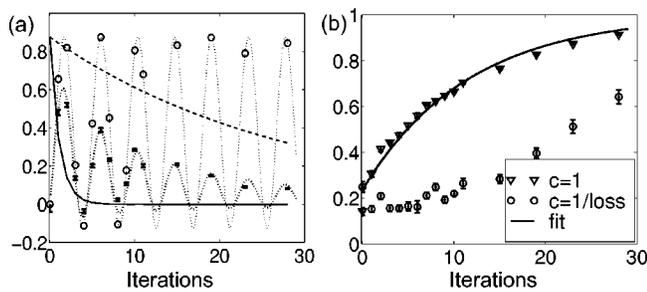


FIG. 3. (a) Experimental (error bars) and ideal (circles) amplitude of d_{x_0} , with fits (dotted) to guide the eye. Dashed line: the signal decay for ^{13}C due to intrinsic phase randomization or decoherence (for ^{13}C , $T_2 \approx 0.65$ s). Solid line: the signal strength retained after applying a continuous rf pulse of the same cumulative duration per Grover iteration as the pulses in the Grover sequence (averaged over the three spins; measured up to 4 iterations and then extrapolated). (b) The relative error ϵ_r .

are the experimental and theoretical (traceless) deviation density matrices, and $\|\cdot\|_2$ is the two norm.^{18,19} Comparison of ϵ_r with $c=1$ and c equal to the inverse of the signal loss [Fig. 3(b)] reveals that signal loss dominates over other types of error. Furthermore, the small values of ϵ_r with $c > 1$ suggest that $|x_0\rangle$ can be unambiguously identified, even after almost 1350 pulses. This is confirmed by the density matrix measured after 28 iterations, which has a surprisingly good signature [Fig. 2(b)]. Given the error of $>5\%$ per single $\pi/2$ rotation, all these observations demonstrate that substantial cancellation of errors took place in our experiments.

The error cancellation achieved was partly due to a judicious choice of the phases of the refocusing pulses, but a detailed mathematical description in terms of error operators is needed to fully exploit this effect in arbitrary pulse sequences. This difficult undertaking is made worthwhile by our observations. This conclusion is strengthened by a similar observation in Ref. 7. Also, we believe that error cancellation behavior is not a property of the Grover iterations, because we found experimentally that the choice of implementation of the building blocks dramatically affects the cancellation effectiveness. Whereas the cancellation of systematic errors makes it possible to perform surprisingly many operations, the methods for simplifying pulse sequences reduce the number of operations needed to implement a given quantum circuit. This combination permitted

the successful realization of Grover's algorithm with three spins and brings many other interesting quantum computing experiments within reach.

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¹⁶Synthesized by heating a mixture of $^{13}\text{CHBr}_3$ (2.25 g, CIL) and HgF_2 (2.8 g, Aldrich) in increments (5 °C for 15 min) from 70 to 85 °C in a Kugelrohr apparatus and condensing the product into a cooled bulb. This material was redistilled bulb-to-bulb at 65 °C to give 750 mg (99% purity) of $^{13}\text{CHFBr}_2$, which was dissolved in *d*₆-acetone.

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¹⁸The two-norm gives the absolute value of the largest eigenvalue. It is a pessimistic measure, compared to the traditional $1 - \text{Tr}(\sqrt{\rho_1}\rho_2\sqrt{\rho_1})$ (the latter is defined only for non-negative matrices, though).

¹⁹As the signal strength retained after applying a continuous rf pulse of the same cumulative duration per Grover iteration as the pulses in the Grover sequence (averaged over the three spins).