QUANTUM COMPUTING

Fast Searches with Nuclear Magnetic Resonance Computers

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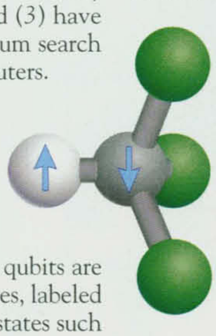
Quantum computers could revolutionize many branches of science through their ability to tackle problems too large for any classical computer. Although the theory is well understood [see the accompanying commentary by Grover on page 228 (*1*)], actually building a quantum computer has proved extremely difficult, and until recently it has only been possible to demonstrate the very simplest operations. In the last few years, however, the development of computers based on nuclear magnetic resonance (NMR) spectroscopy has been extremely rapid. Researchers at IBM, Massachusetts Institute of Technology, and the University of California at Berkeley (*2*) and in my laboratory in Oxford (*3*) have now demonstrated powerful quantum search algorithms with small NMR computers.

All current designs are built out of the same basic components, quantum bits (qubits) and quantum logic gates. Qubits are the quantum analogs of classical bits, but whereas bits can only take two different values, 0 and 1, qubits are not confined to their two basic states, labeled $|0\rangle$ and $|1\rangle$, but can also exist in states such as $|0\rangle + |1\rangle$, called superpositions. A qubit in this state is not simply in state $|0\rangle$ or $|1\rangle$, nor is it in an intermediate state; rather the qubit is in both states simultaneously. Quantum logic gates act on qubits, just as classical logic gates act on classical bits, but quantum gates also work with superpositions and so can perform multiple logic operations at the same time.

A qubit can be implemented with any two-state quantum mechanical system. In NMR computers, the two spin states of a spin-1/2 atomic nucleus in a magnetic field are used. Different atoms in a molecule can be distinguished, and so a molecule can be used as a quantum computer, with each spin-1/2 nucleus providing a single qubit. Simple logic gates that only affect a single qubit are easily implemented with radio frequency fields. These fields interact strongly with nuclear spins, allowing them to be controlled with great precision. To perform interesting computations, however, more complex gates are needed, which allow the state of one qubit to affect other qubits in the computer. This requires some form of interaction between nuclear spins, so that one spin can sense the state of other spins in the molecule. This is easily achieved, because the naturally occurring spin-spin coupling interaction has the desired form.

The NMR signal from a single molecule is far too weak to be detected, and so it is necessary to use a large number of identical copies to amplify the signal. This is not difficult because even a few milligrams of a chemical compound will contain the required number of molecules. It is, however, impossible to ensure that all the copies start the calculation in the same initial state, and so different copies will in effect perform different calculations, making it extremely difficult to extract the desired result. This inability to prepare NMR computers in a well-defined initial state prevented their use for many years.



Molecular bits. The ^{1}H and ^{13}C nuclei in isotopically labeled chloroform behave like small magnets and interact with an external magnetic field. Nuclear spins aligned with the field correspond to qubits in state $|0\rangle$, whereas those aligned against the field correspond to qubits in state $|1\rangle$. The molecule depicted here represents a computer in the state $|0,1\rangle$. The three chlorine nuclei, shown in green, can be ignored.

In 1997, two separate solutions (*4*) to this problem were published. Both reports described how to "distill" an effectively pure starting state from a complex mixture and thus run the calculation of interest (the signals from other starting states can be arranged to cancel, so that they make no overall contribution to the final result). Since then, two different two-qubit NMR computers have been built: one by Chuang and co-workers (*2*), based on the ^{1}H and ^{13}C nuclei in isotopically labeled chloroform (see figure), and one by my research group in Oxford using two ^{1}H nuclei in cytosine (*3*). Both systems have been used to implement a simple quantum algorithm to solve Deutsch's problem (*5*), which calculates the value of a function for two different inputs and allows the two values to be compared. This comparison is achieved with only a single function evaluation, which is applied to both inputs simultaneously.

Deutsch's problem is of great historical interest, but it has few practical implications. By contrast, Grover's quantum search algorithms (*1*) have great practical importance. The simplest version, searching for a single item among four possibilities, can be implemented on a two-qubit computer and is thus within the range of current NMR systems. Chuang and co-workers have described a complete implementation of this algorithm on their chloroform computer (*2*). Their results show that it is possible to locate the desired item in one step, as predicted, and that it is also possible to determine that there is indeed only one item to be found. We have performed a similar but less complete implementation of this algorithm on our cytosine computer in Oxford (*3*).

Implementing a quantum search algorithm is a major step forward for NMR quantum computers but is by no means the limit of their development. The next step is to implement more complex algorithms on larger systems [preliminary results on three-qubit systems (*6*) have already been demonstrated]. Some commentators (*7*) have claimed that it will not be possible to build NMR computers with large numbers of qubits, because the efficiency of the distillation process used to obtain an initial pure state falls off rapidly with the number of qubits. This criticism is almost certainly correct but in practice is unlikely to prove a substantial limitation in the near future. Other problems, related to the difficulty of selectively addressing individual spins, will make it difficult to build NMR computers with more than about six qubits. This would, however, provide the ability to investigate many important problems. It is also much larger than any quantum computer likely to be built with the use of other approaches in the near future. NMR is likely to remain a leading technology for quantum computers for many years to come.

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References and Notes

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7. See, for example, W. S. Warren, *Science* **277**, 1688 (1997).

8. I thank A. Ekert, M. Mosca, and R. H. Hansen for helpful discussions.