The polyphosphate yield of this process would be determined not only by the production, but also by the (hydrolytic) destruction rate of polyphosphate before it could reach the deep ocean. A detailed discussion has to take into account the following considerations (*8*), among others: Phosphate would condense out of rock vapor after much of the silicate had condensed. So, rock rain would concentrate phosphate in the remaining air. The rock rain drops would fall through the surface layer and would be quenched in seconds in the ocean. Water rain would not fall until later, when the atmosphere became cooler than the critical point. This water rain would initially be buoyant on saline water and cool slowly.

In a reduced rock vapor with metallic iron, P is not volatile; it condenses in solid solution, and then as Fe_3P. This would happen in a major impact, when metallic iron is present. Phosphorous becomes a lithosphile at lower temperatures as phosphate. If iron drops quench, then P might react at low temperature. On the other hand, iron phosphide in Fe metal drops may be a good starting material for interesting prebiotic reactions. In a more oxidizing impact of silicate without metallic iron, phosphate may become concentrated more in the final vapor. [The moon is somewhat depleted in P relative to the Earth, so the final vapor that was lost to space was somewhat enriched in P (*9*)].

Finally, a further point has to be taken into account: Keefe and Miller (*4*) pointed out that if the partial pressure of water vapor exceeds 6 bar, the entropy-driven condensation reaction of phosphate into polyphosphate and water would be driven in the reverse direction. This limits the size of the impactor useful for producing polyphosphates to about 90-km diameter (*8*). Much bigger blasts in earlier times (even bigger than ocean blaster) would have destroyed any complex molecules, including polyphosphates, [the water vapor atmosphere lasts 3000 years (*7*)], but could still be beneficial for the later origin of life by reworking the upper crust thoroughly and "leaching out" the phosphate fraction. Because phosphate probably remained airborne longer than the rock fraction (*8*), it would be more concentrated in the upper layers of the Earth's crust after re-condensation. There it could be mobilized again by not so massive and deep penetrating impacts. Such large impactors, however, would have an iron core. So the above-described process has to compete with iron droplets in a large impact. Most of the Earth's P today is in the core (*8*).

The admittedly optimistic scenario described above could be a counterargument to Miller's computation (which was intended as a reductio ad absurdum) that even if the phosphate of the upper 1 km of Earth's crust could be extracted, the resulting solution in the ocean would be only 0.03 M (*4*). Of course, the circumstances described above would be difficult to simulate in a laboratory, but it would be interesting if the outcome of such experiments supported the hypothesis that those "killer impacts," through repeated "fractionation" and enrichment of polyphosphates in the future biosphere, got life started in the first place (*10*).

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REFERENCES AND NOTES

1. C. P. McKay and W. J. Borucki, *Science* **276**, 390 (1997).
2. W. Gilbert, *Nature* **319**, 618 (1986).
3. J. P. Ferris and D. A. Usher, in *Biochemistry*, G. Zubay, Ed. (MacMillan, New York, 1988) pp. 1129–1134.
4. A. D. Keefe and S. L. Miller, *J. Mol. Evol.* **41**, 693 (1995).
5. Y. Yamagata, H. Watanabe, M. Saitoh, T. Namba, *Nature* **352**, 516 (1991).
6. B. Fegley Jr., R. G. Prinn, H. Hartmann, G. H. Watkins, *ibid.* **319**, 305 (1986).
7. N. H. Sleep, K. J. Zahnle, J. F. Kasting, H. J. Morowitz, *ibid.* **342**, 139 (1989).
8. N. H. Sleep, personal communication.
9. A. E. Ringwood, *Origin of the Earth and the Moon* (Springer-Verlag, New York, 1979).
10. The rapid cooling of the re-condensed rock vapor would also probably lead to increased fracturing of the rock droplets. A big surface area would be provided. Glass reacts quickly, and could assist in the polymerization of oligonucleotides, as shown by the experiments of J. P. Ferris *et al.* [*Nature* **81**, 59 (1996)]. Also, Fe metal droplets will react and become FeS_2 or FeS templates with P readily available (*8*). Thus, there could be a connection between this process and the iron-sulfur-world scenario for the origin of life [G. Wachtershauser, *Progr. Biophys. Mol. Biol.* **58**, 85 (1992)].
11. I am thankful to N. H. Sleep for answering numerous questions.

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The Usefulness of NMR Quantum Computing

Quantum computing—the manipulation of a quantum mechanical system to do information processing—has attracted considerable recent attention, largely triggered by Shor's proposed algorithm for finding prime factors in polynomial instead of exponential time (*1*). The importance of this problem has also led to numerous attempts to realize quantum computers, including systems such as trapped ions and quantum dots. In their Research Article, Gershenfeld and Chuang (*2*) propose the use of a much less exotic system—nuclear magnetic resonance (NMR) of molecules in a room-temperature solution. They demonstrate that such a "bulk spin-resonance" system is capable in principle of doing quantum computation, and they discuss the generation of 6 to 10 quantum bits ("qubits"), which would be a daunting, but not impossible task with today's technology. Of course, solution NMR was used in the 1950s to study equally small molecules, yet today we study proteins with thousands of spins. If an NMR quantum computer were ultimately scalable to larger numbers of qubits (say 100), the implications for computational science would be exciting.

There is doubt, however, that solution NMR quantum computing will ever be useful. Ensembles of uncoupled two-level systems (magnetic resonance or any other form) have quite classical dynamics, as shown by Feynman (*3*). Thus the clock cycles for any nonclassical dynamics, including all of the computing operations in the report (*2*) and in any other conceivable treatment, require times on the order of the reciprocal of the spin-spin couplings ($\approx$200 Hz for directly bonded atoms, $\approx$10 Hz for protons on nearest-neighbor carbons) per step. Many such steps would be needed for logic operations between two separated spins. Dipolar couplings (for example, in solids) can increase the couplings by another factor of 10, but then the eigenstates are not the simple spin product states, and each logical manipulation will be much more complex. The slowest limit of speed estimated by Gershenfeld and Chuang (*2*) (10 logic gates per second) is thus grossly overoptimistic for a reasonably sized molecule.

Speed is not an important problem for demonstration experiments; perhaps new quantum algorithms will be found that compensate for the enormous slowdown. However, NMR is the premier spectroscopic example, not of quantum mechanics, but of quantum *statistical* mechanics including ensemble averaging. For a macroscopic sample (say $N \approx 10^{22}$ spins) the evolution is essentially deterministic. For example, all modern spectrometers routinely measure I_x and I_y simultaneously, despite the Uncertainty Principle. Fluctuations from the expectation value scale as $1/\sqrt{N}$, or about 10^{11} $\hbar$ (10^{-11} of the magnetization, but as I show below, this is still not good enough for solution NMR quantum computing). In addition, in NMR the energy difference between the two spin states of each atom is small, which implies that the possible signal in a quantum computing experiment suffers a severe degradation for systems that might be big enough, in principle, to contain a useful number of qubits (Fig. 1). For example, in a 100-spin system at room temperature, the expected signal for an ideal quantum computer is 28 orders of magnitude smaller than the room temperature magnetization.

Why is the scaling such a problem? Because the quantum computing signal relies on the fraction of the molecules starting in a single specific eigenstate in the equilibrium density matrix ρ_{eq}. After the evolution through an assumed ideal set of quantum gates onto a target state, the computing signal has to be detected (converted into observable magnetization). Because the observable operators are traceless, this reduces the signal further: Only the largest population *difference* in ρ_{eq} (the difference between the all-α and all-β states) can be made observable. It can be shown that the best way to do this is to overlap the population with the largest matrix element of I_z, so the ideal observable signal is

$$S_{\text{quantum}} = [(\rho_{eq})_{\max} - (\rho_{eq})_{\min}][\gamma\hbar(I_z)_{\max}] \qquad (1)$$

This upper limit is actually quite similar to doing N-quantum selective excitation (4) in a totally asymmetric N-spin system. This has been done for $N \geq 6$ only in high symmetry cases such as benzene or solid adamantane. For the quantum computing problem, symmetry hurts instead of helps—it reduces the number of possible qubits.

A (classical) computer can evaluate equation (1) by an explicit sum over states for moderate values of N. It can also be simplified in the high temperature limit $Nh\nu/kT \ll 1$:

$$S_{\text{quantum}} = N2^{-N}\gamma\hbar\sinh(Nh\nu/2kT)/\cosh^{N}(h\nu/2kT) \qquad (2)$$

This can be compared to the magnetization after one pulse in a normal NMR experiment:

$$S_{\text{quantum}}/M_z = 2^{-N+1}\sinh(Nh\nu/2kT)/[\sinh(h\nu/2kT)\cosh^{N-1}(h\nu/2kT)] \qquad (3)$$
$$\approx N2^{-N}\,(\lim Nh\nu/kT \ll 1)$$

It is apparent that the scaling to a useful number of spins is extremely unfavorable. To fully understand the scope of this problem, note that 99.99999999% of the time a generously sized room-temperature sample (10^{22} spins) contains *no* 100-spin molecules in the ground state $\alpha_1\alpha_2 \ldots \alpha_n$, or in any other single one of its 2^{100} quantum states. Furthermore, the all-β state is only 1% less probable than the all-α state in a 600-MHz spectrometer. Thus, for every 100 times one molecule accidentally gets in the "right" (all-α) initial state, there will be 99 occurrences of the "wrong" (all-β) initial state, giving exactly the negative of the desired signal. Finally, the "random" component of the magnetization ($\approx 10^{11}\ \hbar$, as discussed earlier) is 10^{22} times larger than the expected signal and evolves at the same frequency.

Gershenfeld and Chuang state that the signal grows exponentially with decreasing temperature, but exponential growth does not start until $h\nu/kT \gg 1$ ($\ll 1K$ even for ^1H in large magnets). The sample then will not be a liquid; lines will be broadened and intermolecular couplings will complicate logic gates enormously. It is possible to polarize nuclear spins from electronic spins using laser excitation, but doing this efficiently requires isolated atoms with sharp electronic transitions (for example, ^{129}Xe or ^3He in contact with Rb atoms in the gas phase (5). Spin-polarized ^{129}Xe can polarize room-temperature ^1H in solution (6), but the fractional polarization is fundamentally limited by the nature of the interaction. Solid ^3He at mK temperatures has sharp resonance lines due to spin diffusion (the linewidths are on the order of 1 Hz, similar to liquids), but in this case there are no scalar couplings. Finally, perhaps someday we will have 100-kT magnets with the required 10-nT inhomogeneity, but in that case the field itself will surely align the solute and reintroduce dipolar couplings (as happens now in proteins).

These problems are not found with other potential implementations of quantum computing. For transitions with $h\nu \gg kT$ the initial state can be prepared essentially without loss, no matter how many systems are coupled. This means, for example, that electron spin resonance (ESR) spectroscopy in modern superconducting magnets (resonance frequencies around 300 GHz) can get into the right regime at liquid helium temperatures; one could conceive of quantum computing with multiple-radical molecules in an inert matrix, using dipolar couplings plus g value differences that are far larger than J couplings and chemical shifts, respectively, in NMR. It seems more likely, however, that if quantum computing will ever be practical, it will be with "designer materials" such as precisely spaced quantum dots or free radicals positioned on a surface by force microscopy.

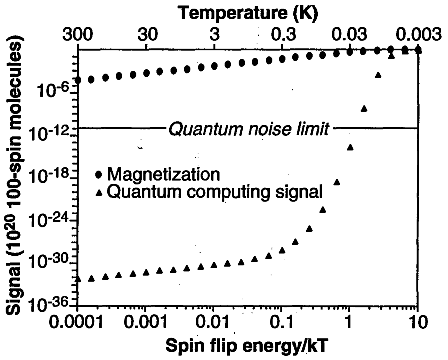

Fig. 1. Observable magnetization and the ideal quantum computing signal as a function of temperature for a 100-spin system. At room temperature, the signal is about 8×10^{-34} of the magnetization. Even for ^1H in a large magnet, the ideal signal is small until $T \ll 1K$, at which point the sample would surely not be a solution. Temperature: protons, 14.7 *T* magnet (600-MHz spectrometer) assumed.

In summary, quantum computing might well turn out to be capable someday of solving certain problems better than conventional techniques; but if so, bulk NMR is not likely to play any role in a practical implementation.

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REFERENCES AND NOTES

1. P. Shor, *Proceedings of the 35th Annual Symposium on Foundations of Computer Science* (IEEE Computer Society Press, New York, 1994); A. Ekert and R. Jozsa, *Rev. Mod. Phys.* **68**, 733 (1996).
2. N. A. Gershenfeld and I. L. Chuang, *Science* **275**, 350 (1997).
3. R. P. Feynman, F. L. Vernon Jr., R. W. Hellwarth, *Appl. Phys.* **49**, 28 (1957).
4. W. S. Warren, S. Sinton, D. P. Weitekamp, A. Pines, *Phys. Rev. Lett.* **43**, 1791 (1979); W. S. Warren and A. Pines, *J. Chem. Phys.* **74**, 2808 (1981).
5. See, for example, B. Driehuys *et al.*, *Appl. Phys. Lett.* **69**, 1668 (1996); A. S. Barton, G. D. Cates, W. Happer, H. Middleton, *Phys. Rev.* **A48**, 4441 (1993), and references therein.
6. G. Navon *et al.*, *Science* **257**, 1848 (1996); K. L. Sauer, R. J. Fitzgerald, W. Happer, *Chem. Phys. Lett.*, in press.
7. Supported by the National Science Foundation under grant CHE-9412948. I thank H. Rabitz and K. K. Lehmann for useful discussions.

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Response: Few researchers can match Warren's innovative contributions to NMR techniques, but he makes a number of restrictive assumptions about areas of active research that led him to draw unduly pessimistic conclusions about the usefulness of bulk spin resonance quantum computing.

First, our conclusion (which he agrees with) was that realizing a 10-qubit quantum computer is within reach of existing NMR spectrometers (*1*). While there are grounds to think that it will be possible to scale beyond that, even 10 qubits is remarkable, because just a year ago there were confident predictions that building any nontrivial quantum computer would be impossible. In the short time since its introduction, this new technique has already led to the first experimental realization of quantum gates connected into circuits (2) that have been used to run programs to experimentally test theoretical predictions of unusual quantum dynamics (3). Even in these first simple examples, the introduction of quantum computation to NMR has already proved itself to provide fruitful new ways to explore the creation and loss of coherence in complex systems.

Warren makes two fundamental points, both of which were clearly identified in our Research Article (1). First, the slowest operations come from coupling terms, which usefully range down to on the order of 10 Hz. Warren states that this rate severely limits the feasible molecule size, but we gave two reasons why this conclusion is incorrect. The first is that a quantum computer does exponential work per time step. At the speed of the fastest (publicly known) classical factoring to date, finding the factors of a 1000-digit number would take on the order of the age of the universe. A quantum computer with a 1-Hz clock cycle time could reduce this time to a matter of days. Further, a polynomial decrease in coupling strength with increasing molecule size will still lead to an exponential increase in computation speed. The second reason why the coupling frequency does not limit the molecule size is that, as with classical computation, quantum computation is possible using only local (and hence strong) interactions. Quantum cellular automata are computationally universal, and have favorable scaling properties (4).

Warren than reproduces our conclusion that, in the high-temperature limit, the signal strength falls off roughly exponentially in the number of qubits. This limits conventional spectrometers to roughly 10 qubits. But, the special features of quantum computation suggest many optimizations not possible in a general-purpose spectrometer. Starting by transferring electron polarization gives an improvement by a factor of 10^3 in signal strength (the ratio of the gyromagnetic ratios); reading out with transfer back to electrons gives another factor of 10^3 in magnetization and another factor of 10^3 in the time rate of change of flux in a pick-up coil. Because the system can be designed around a large sample of a known fluid, increasing the sample radius by a factor of 30 gives another factor of 10^3, and because the computation can be designed to read out on a single line, a high-Q resonantor can provide another factor of 10^3. Each factor of 10^3 provides sensitivity for 10 more qubits. Realizing these potential improvements presents a significant experimental challenge, but taken together they suggest that it might be possible to reach sizes larger than the biggest classical computers ($2^{40} \sim 10^{12}$ bits).

These refinements remain in the high-temperature limit and thus cannot be expected to scale further still. As we have noted, the underlying problem arises from the small Boltzmann factors. But Boltzmann factors of order unity are routinely observed in a number of systems, including optically pumped vapors and cryogenically cooled materials. While this work to date has focused on simple systems without the nonlinear interactions required for computation, recent experimental studies have shown that it is possible to transfer large polarizations to molecules with multiple spins (5). This is now an active research area. Given the possibility of such large Boltzmann factors, the remaining scaling limit is the decoherence time, but NMR approaches the range of the decoherence per gate required for steady-state error correction (6).

Warren concludes by stating that alternatives such as quantum dots have much more promise. This unexpected conclusion neglects the experimental reality that bulk spin resonance quantum computing is the only experimental approach to date that has implemented nontrivial quantum circuits, while quantum dots have decoherence times below nanoseconds and have yet to demonstrate a coherent quantum gate. This does not mean that NMR is the final solution; a useful quantum computer will almost surely look nothing at all like a conventional NMR spectrometer, and will draw on the best features of all of the alternative approaches. It may not necessarily even involve nuclear spins, but we are confident that it will take advantage of the desirable features, introduced by NMR, of representing quantum information in ensembles using naturally occurring nonlinear interactions and performing quantum readout by a weak ensemble measurement. Scaling beyond roughly 10 spins poses daunting experimental problems for NMR, but we have found nothing in his arguments or our experiments to dissuade us from this exciting challenge.

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REFERENCES

1. N. A. Gershenfeld and I. L. Chuang, *Science* **275**, 350 (1997).
2. I. L. Chuang, N. A. Gershenfeld, M. G. Kubinec, D. W. Leung, in preparation.
3. I. L. Chuang, in preparation.
4. S. Lloyd, *Science* **261**, 1569 (1993).
5. G. Navon *et al.*, *ibid.* **271**, 1848 (1996).
6. R. Laflamme, E. Knill, W. Zurek, Los Alamos preprint quant-ph/961011 (1997).

6 May 1997; accepted 9 June 1997