NMR Quantum Computing

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Nuclear magnetic resonance (NMR) is one of the most important methods for the identification of molecules and for the determination of their structure and dynamics. However, during the last few years, there has been a series of stimulating publications,[1, 2] in which the methods of NMR spectroscopy were applied to very simple and well known compounds. The goal of these projects was not to refine existing models of the structure or dynamics of these compounds but to realize experimentally the until then, purely theoretical concept of quantum computing. The idea to construct computers based on quantum-mechanical principles was first suggested in 1982 by the physicist Richard Feynman.[3]

In order to understand why quantum computers are of interest, it is helpful to compare the ways information is stored in classical and in quantum computers, respectively. In a classical computer, the smallest unit of information, a bit, can take values represented by either 0 or 1. In a quantum computer, the smallest unit of information is a quantum bit (qubit), which corresponds to a quantum-mechanical two-level system with basis states $|0\rangle$ and $|1\rangle$. For example, such a qubit can be represented by a ½-spin particle, in which the states $|0\rangle$ and $|1\rangle$ correspond to a parallel or an antiparallel alignment of the spins relative to an external magnetic field (Figure 1 a). However, in contrast to its classical analogue, a

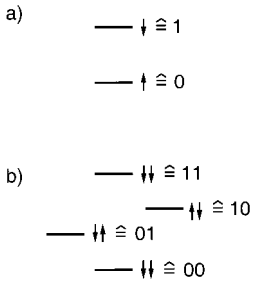

Figure 1. a) A ½-spin nuclei in an external magnetic field with basis states "spin up" and "spin down" is an example of a quantum-mechanical two-level system, which corresponds to a qubit with states 0 and 1, respectively. b) Two ½-spins in an external magnetic field form a four-level system. The basis states and the corresponding values of the two qubits are shown schematically. In contrast to classical bits, the quantum-mechanical system can also exist in a superposition of the basis states shown.

qubit can also exist in a quantum-mechanical superposition of $|0\rangle$ and $|1\rangle$ and is hence characterized by two complex numbers c_1 and c_2, the probability amplitudes of the two basis states. The state function is $|\psi\rangle = c_1|0\rangle + c_2|1\rangle$ with the normalization condition $|c_1|^2 + |c_2|^2 = 1$. For example, in NMR the superposition states $|\psi\rangle_x = 2^{-1/2}(|0\rangle + |1\rangle)$ and $|\psi\rangle_y = 2^{-1/2}(|0\rangle + \mathrm{i}|1\rangle)$ correspond to transverse x and y magnetization, respectively. With every additional qubit (such as a ½-spin particle), the number of base states of the quantum-mechanical system doubles (Figure 1 b). Hence, the complete characterization of a register consisting of N qubits (such as N coupled ½-spins) requires 2^N complex numbers (probability amplitudes), whereas a register of N classical bits is, by definition, completely characterized by N integers (0 or 1). The superposition principle and the exponential growth of the size of the quantum-mechanical state space makes it possible to perform a large number of quantum computations simultaneously, that is, in parallel. However, this requires the development of appropriate computational procedures (quantum algorithms) that make the best use of the laws of quantum mechanics.[4–6]

A quantum algorithm for prime factorization, developed by Peter Shor, is of particular interest.[5] One of the most important methods for cryptography is based on the difficulty of prime factorization (the RSA method)[7] because, for classical algorithms, the time required for the factorization of a given number increases exponentially with the number of digits. In contrast, the time required by Shor's quantum algorithm grows at a significantly slower rate (only as a polynomial function of the number of digits). Hence, this quantum algorithm could be a potential threat for encrypted messages if a sufficiently large quantum computer (with hundreds or thousands of qubits) could be realized. However, as stated 1998, "Many years will pass until a computer with the necessary number of qubits will crack private keys on this planet—a quantum computer with more than four qubits in this millennium would already be a sensation".[8]

Current experimental approaches for the realization of quantum computers are ion traps,[9] quantum dots,[10] Josephson contacts, [11] and NMR spectroscopy;[1] the latter is, so far, most advanced in the practical implementation of quantum algorithms. NMR spectroscopy provides elegant methods for the controlled manipulation of nuclear spins, which are particularly well suited to act as qubits because of their isolation from the environment. However, a liquid NMR sample contains an ensemble of many identical spin systems and it is not possible to manipulate or to detect individual spin systems. Hence, at the beginning of a computation, NMR quantum computers are commonly prepared in a "pseudo-pure" state rather than in a pure state and, furthermore, ensemble-averaged expectation values are detected rather than the observables of individual spin systems.[1] The basic computational steps of quantum algorithms can be realized with the help of radio-frequency pulses and can be broken down to spin-selective pulses and CNOT (conditional NOT) gates (Figure 2) between pairs of spins. The number of qubits is mainly restricted by the availability of compounds with suitable spin systems.

For the efficient implementation of an NMR quantum computer with N qubits, a molecule with N coupled ½-spins is

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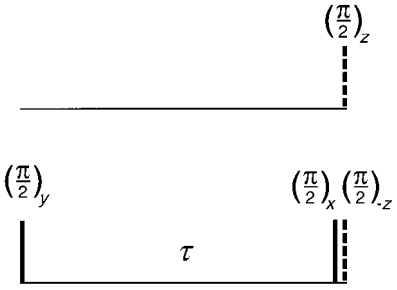


Figure 2. Schematic representation of an NMR pulse sequence to realize the logic CNOT(I,S) gate for a heteronuclear I,S spin system with coupling constant $J_{I,S}$.[14] I- and S-spin selective radio-frequency pulses and z rotations are shown schematically on the upper and lower line, respectively. The period τ corresponds to $1/(2J_{I,S})$.

required. In order to be able to perform many basic computational steps (logic quantum gates), the time required for each quantum gate must be considerably smaller than the relaxation time of the nuclear spins. As the basic computational steps rely on the selective manipulation of individual spins, the frequency differences of nuclear spins should be as large as possible. In this respect, heteronuclear spin systems and spins with a large range of chemical shifts are advantageous. In addition, large couplings should exist between the nuclear spins because the time required for the implementation of direct logical combination of two qubits is inversely proportional to the size of the coupling between the corresponding nuclear spins. However, it is not required that all spins are mutually coupled (Figure 3a): It is sufficient if the spins form a contiguous coupling network (Figure 3b).[12]

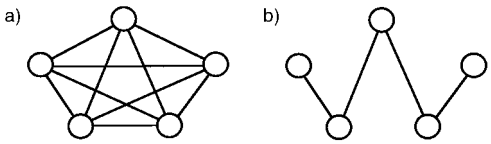
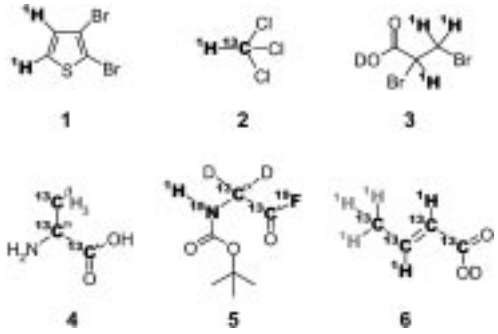


Figure 3. a) Schematic representation of a system consisting of $N=5$ pairwise-coupled spins (qubits). b) A linear coupling network is sufficient to realize all possible logic operations between arbitrary spins (qubits) in an N-spin system.[12]

For the first NMR quantum computers with up to three qubits, readily available compounds were used, such as 2,3-dibromothiophene **1**,[1a, 2f] [^{13}C]chloroform **2**,[2a] 2,3-dibromopropanoic acid **3**,[2e, 12] and [$^{13}C_3$]alanine **4**.[13] In Scheme 1, atoms whose nuclear spins represent the individual qubits are printed in boldface. For the realization of the first NMR quantum computer with more than four qubits, compound **5** was synthesized.[14] If the deuterium spins are decoupled, the nuclear spins of $^1H^N$, ^{15}N, $^{13}C^{\alpha}$, $^{13}C'$ (=CO), and ^{19}F form a coupled spin system consisting of five ½-spins. The ^1J coupling constants range between 13.5 Hz ($^1J_{N,C^{\alpha}}$) and 366 Hz ($^1J_{C',F}$) and, for a magnetic field of 9.4 T, the frequency differences vary between 12 kHz ($\nu_{C'}-\nu_{C^{\alpha}}$) and 360 MHz ($\nu_H-\nu_N$). Recently, [$^{13}C_4$]crotonic acid **6** was proposed[15] as a compound that may be suited for quantum computing with seven qubits. In a magnetic field of 9.4 T, the ^{13}C resonances are well separated with a minimal frequency difference of 2.5 kHz but the smallest frequency difference of the ^{1}H spins is only



Scheme 1. Compounds suitable to form the molecular basis of NMR quantum computers with up to seven qubits. The atoms of the nuclear spins, which act as qubits, are printed with boldface. In **6**, the (gray) protons of the methyl group represent just one qubit if only the ½-spin part of total spin of the methyl group is exploited.[15]

500 Hz.[15] The design and synthesis of molecules with suitable spin systems for 10–20 qubits is not a trivial challenge.

If the compound serving as a quantum computer is dissolved in a liquid crystal, not only scalar J couplings but also large dipolar couplings can be exploited to reduce the time required for quantum gates.[16] Another possible approach for the realization of a molecular architecture with more than ten coupled spins is the synthesis of polymers with a repetitive unit consisting of three or more spins.[17]

With an increasing number of qubits, not only the synthetic requirements grow but also the demands with respect to NMR instruments and pulse-sequence design, in order to keep the effects of experimental imperfections (such as the inhomogeneity of the radio-frequency fields) under control. In addition, the preparation of a pseudopure state (a prerequisite for most quantum algorithms) becomes very inefficient as the number of qubits increases.[18] This results in a dramatic sensitivity loss of the experiments. Possible solutions could be the use of the laser-polarized ^{3}He or ^{129}Xe nuclei[19] or the spin order of *para*-hydrogen[20] or of electron spins.[21] It is very unlikely that it will be possible to realize an NMR-based quantum computer that is large and powerful enough to surpass classical computers. However, the methods of NMR spectroscopy are almost ideally suited to experimentally realize and test theoretical quantum algorithms for small spin systems. The investigation of the limits of this approach is an exciting subject of current research.

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