Spins as qubits: Quantum information processing by nuclear magnetic resonance

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Storing information in quantum mechanical degrees of freedom and processing it by unitary transformation promises a new class of computers that can efficiently solve problems for which no efficient classical algorithms are known. The most straightforward implementation of this type of information processing uses nuclear spins to store the information and nuclear magnetic resonance for processing it. We discuss the basics of quantum information processing by NMR, with an emphasis on two fields of research: the design and implementation of robust logical gate operations and the loss of quantum information, which is known as decoherence. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2838166]

I. INTRODUCTION

A. Physics of computation

Our capabilities for acquiring, storing, processing, and distributing information may be considered one of the main measures of human evolution. Originally, information existed in a number of different physical forms, and exchange of information always required a human intermediary. Since the introduction of programmable digital computers, information has become almost universally digitally encoded and exchange between different physical forms has become largely automated. Processing is mostly achieved by microprocessors built from semiconducting materials, and information processing has developed an independent status, both as a science and as an industry.

While information processing has become an independent and mature science, it is always worth remembering that the basis of information storage and processing is always a physical system.[1,2] This seemingly trivial fact has severe consequences on the possible efficiency of any computing machinery—some of them obvious, others less so. The more obvious ones depend on the physical properties of the materials used,[3] such as the mobility of charge carriers in semiconductors and the dielectric constants of insulator materials in microprocessors. The less obvious ones are valid for all types of materials but nevertheless place limitations on the computational power of devices.[4,5] Examples include the minimal amount of energy dissipated per logical operation.

Among the many versions of Moore's law,[3,6] one of the most impressive is the reduction of the amount of energy dissipated per logical operation in successive generations of computer hardware. Some numbers are represented in Fig. 1. Over the last fifty years, this number has decreased by more than ten orders of magnitude, roughly following an exponential time dependence. The reduction of energy dissipation is a requirement for a continuing improvement: if today's processors had the energy efficiency of 1950, even a single computer would require more power than a large power station can generate. As a result, it would become too hot to operate and disintegrate within a fraction of a second. Even with today's efficiency, heat dissipation is often the limiting factor for the speed of microprocessors and one of the main reasons why the clock rate has not increased significantly over the past years.

While the continued reduction of energy dissipation is thus a necessity, it will take only about ten more years until a fundamental limit is reached: Any computer working with Boolean logic (which includes all of today's digital computers) must dissipate at least an amount of $k_BT \ln 2$, since they discard information during processing.[7,8] The k_BT limit could be overcome by using reversible logical operations,[9,10] which do not discard information. Since the evolution of quantum mechanical systems can be represented as a unitary operation, it is inherently reversible and can thus, in principle, be operated dissipation-free. The principles on which information processing by quantum mechanical systems operates may thus well find applications also in electronic circuits for classical computers.

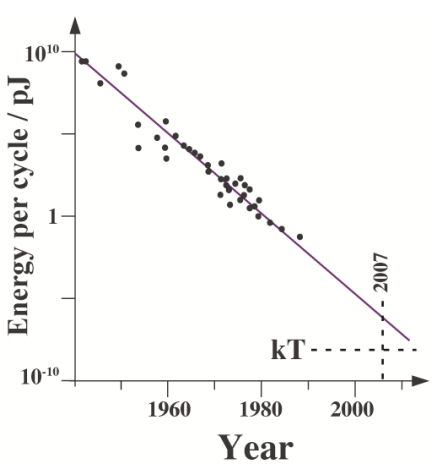

FIG. 1. (Color online) Exponential reduction of the energy dissipated per logical operation. The horizontal line labeled "kT" indicates the thermal energy per degree of freedom at room temperature.

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B. Quantum information

While the execution speed of a processor may be considered an engineering issue, which is useful but not fundamental, some other consequences of the physical nature of information affect directly the foundations of computer science. Among its most important building stones is the Church–Turing hypothesis,[11,12] which asserts that most computers are equivalent with respect to computability (not with respect to speed), allowing one to disregard the details of the information processing device for determining if a given problem can be solved on a computer. However, the strong form of the Church–Turing hypothesis, which states that any problem that can be solved *efficiently* on one computer can be solved efficiently on any other computer, appears to be wrong: some problems have been established to be solvable efficiently if the computer operates according to quantum mechanics, but not on classical computers.

This possibility is the main driving force for the research in quantum information processing (QIP), i.e., the processing of information that is represented by quantum states of physical systems and whose evolution is governed by Schrödinger's equation.[13,14] On the theoretical side, research is directed towards developing algorithms that work more efficiently on quantum computers than on classical computers. At the same time, efforts are under way to realize physical systems that can implement these quantum algorithms. These systems have to fulfill a number of conditions.[15] In particular, they must support a sufficiently large number of well-controlled quantum mechanical two-level systems, in which the information can be stored and processed and finally read out. The first[16,17] and still the most successful implementations of quantum information processing were based on nuclear spins in liquids. Since then, NMR has been used as a testbed for implementing quantum algorithms, testing new concepts and developing techniques for efficiently controlling quantum systems.

C. Historical

Quantum mechanics is, as far as we can judge today, the fundamental physical theory. In particular, we need quantum mechanics to explain, e.g., the differences between metals, insulators, and semiconductors, as well as the effect of doping on the conductivity of semiconductor materials. In this sense, quantum mechanics has always been the basis for electronic computers and, thus, for most of today's information processing. However, while quantum mechanics is necessary for understanding and designing different semiconductor materials, the engineers who build the computers from these materials need no knowledge of quantum mechanics for building ever more powerful devices.

The first suggestions that it might be possible to design computers that operate directly on the basis of quantum mechanics were put forward in 1982 by Benioff[18] and Feynman.[19] While Benioff showed that quantum systems can be used as universal computers, it was Feynman who suggested (but not proved) that they might be more powerful than classical computers. A first example of such an algorithm was provided by Deutsch in 1985 (Ref. 20) and generalized by Deutsch and Jozsa in 1992.[21]

Soon thereafter, Bernstein and Vazirani showed that quantum computers can solve "computationally hard" problems efficiently.[22] This result dramatically increased the interest in this field and thus accelerated progress: Coppersmith developed a quantum Fourier transform algorithm that is exponentially faster than the classical Fourier transform (even the fast Fourier transform that is generally used in NMR spectrometers!),[23] and Shor used this for an algorithm that can factorize large numbers efficiently.[24] Shortly thereafter, Grover showed that the database search by quantum computers can achieve a quadratic speedup over the classical computers.[25] Interestingly, it was shown later that this quadratic speedup is optimal.[26]

The increased interest in the field also resulted in efforts to experimentally implement a quantum information processor. The first proposals suggested to store the quantum information in the states of atomic ions in an electromagnetic trap,[27] but the experimental challenges associated with this proposal were not overcome until 2003.[28] Instead, the first successful realization was demonstrated by two groups in 1997, using nuclear spins in liquids.[16,17]

Nuclear spins have some obvious advantages for realizing a quantum information processing:

- Spins 1/2 are the only quantum systems whose Hilbert space is two dimensional and thus exactly realizes a qubit.
- Nuclear spins are quite well isolated from the environment, thus preserving the quantum information for a long time.
- Precise control of the evolution of nuclear spins by resonant radio-frequency fields is well established and can be implemented in commercially available spectrometers.

Of course, there is no such thing as a free lunch: the weak coupling between nuclear spins and environment also implies that it is very hard to detect individual spins. In most cases, this problem can only be overcome by working not with individual spins, but with ensembles of identically prepared spins, which together generate a signal that can be detected easily enough.

In this short review, we will highlight some of these developments, with the main emphasis on optimal control of quantum systems and the loss of information due to the inevitable coupling with the environment. The physical systems that we consider here are nuclear spins, but most of the results are applicable to a much wider range of systems.

II. BASICS OF QUANTUM INFORMATION PROCESSING

A. Bits and qubits

All information that we consider in this context is represented in binary digital form. The smallest units of information are thus bits, i.e., memory cells that can assume two

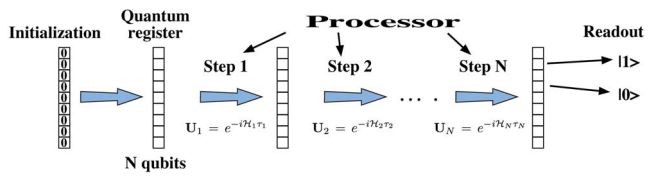

FIG. 2. (Color online) Principle of operation of a quantum computer.

distinct values, which are usually labeled as 0 and 1. Information processing corresponds to the manipulation of strings of bits, applying rules or algorithms that take one string as input, perform logical operations on it, and finally output a modified string. Each bit can be in one of two distinguishable states of a device, which differ, e.g., by the amount of charge on a capacitor or the direction of the magnetization of a magnetic domain.

In the case of quantum information processing,[13,14,29] the information is also represented in digital form. However, in this case, the individual bits are stored in quantum systems that have two orthogonal states that are labeled $|0\rangle$ and $|1\rangle$. Each such two-level system is described by a two-dimensional Hilbert space. To distinguish these from the classical bits, one usually refers to them as quantum bits or qubits. Since any quantum mechanical two-level system is equivalent to a spin-1/2 system, we will discuss here only spins 1/2.

The main difference between the classical and the quantum computer, which results in the qualitatively higher capabilities of the quantum computer is that the quantum information can not only be in the computational basis states $000\cdots0$, $000\cdots1$,…, $111\cdots1$, but equally well in arbitrary superpositions of these states. This is a direct consequence of the superposition principle of quantum mechanics. In the context of quantum information processing, it implies that whenever an algorithm works on two different states, it also works on any superposition of these states. Applied to a single qubit, it implies that if the states $|\uparrow\rangle$ and $|\downarrow\rangle$ are legal inputs to a quantum algorithm, the spin can be oriented in any direction and the algorithm will produce a well-defined and admissible result.

If the quantum register (= the string of qubits that contain the information that the current quantum algorithm processes) consists of N qubits, 2^N complex coefficients are required to identify the state at each point of the operation. A quantum information processor that operates on such a superposition state may be considered a highly parallel computer: a suitable input represents the superposition of 2^N orthogonal input states, and the final state the superposition of 2^N calculations performed on all these input states. This is a direct consequence of the linearity of the Schrödinger equation, and has no correspondence in classical computers, where superpositions of two input states, e.g., $(-1/\sqrt{2})(0+1)$, are not even allowed states.

B. Processing

Quantum information processing implies three types of operations that must be executed on the quantum register, as represented in Fig. 2:

- The bits of the quantum register must be initialized into a well-defined state.
- Logical operations are performed on the quantum register, according to the algorithm being implemented. Each operation can be represented as a unitary transformation acting on the qubits.
- The result of the processing is read out, i.e., the final state is converted into classical information.

The different logical operations U_i required by the quantum algorithms must be driven by suitable Hamiltonians,

$$U_i = e^{-i\mathcal{H}_i\tau_i},$$

where the index i labels the computational step, $\mathcal{H}_i$ the Hamiltonian driving the operation, and τ_i the duration of this step. The experimental apparatus controlling the quantum information processor must be capable of generating these Hamiltonians by suitable control fields; in the case of an NMR quantum information processor that we consider here, these control fields are static and radio-frequency magnetic fields (in addition to the spin-spin couplings, which are always acting between the qubits). In most cases, it is not possible to generate the Hamiltonian $\mathcal{H}_i$ directly, but it is always possible to decompose it into a sequence of operations that can be generated by suitable sequences of radio-frequency pulses applied to the spins.

The initialization and readout operations are fundamentally different from the processing: both operations are intrinsically irreversible and thus nonunitary. In the case of the initialization, the contents of every qubit must be erased and replaced by the starting value (in most cases the starting value is 0). In most quantum algorithms, the readout process must act like an ideal quantum measurement, where the state collapses onto an eigenstate of the observable. Typically, these states correspond to the computational basis states $|0\rangle$ and $|1\rangle$, but for some quantum algorithms, the readout projects onto superposition states, such as $(1/\sqrt{2})(|0\rangle+|1\rangle)$.

The conditions that must be fulfilled by a physical implementation of a quantum information processor have been laid out by DiVincenzo.[30] The exact means of control and the type of interqubit interactions can vary and are specific to various proposed architectures for quantum computing.[14,31]

III. QIP BY NMR

A. Nuclear spins as qubits

1. Why nuclear spins?

Spins with an angular momentum of $I=\hbar/2$ are the only physical systems whose Hilbert space corresponds exactly to that of a qubit, i.e., it is spanned by two orthogonal states. In the case of nuclear spins, the spin degree of freedom is also very well isolated from all other degrees of freedom, making them almost ideal qubits. Nevertheless, nuclear spins were not the first candidates for qubits, mostly because it was considered necessary to measure the state of individual particles to determine the outcome of a quantum computation.

Since the interaction of nuclear spins with their environment is quite weak, it is very hard to detect individual nuclear spins.

The usual solution to this problem is to use an ensemble of nuclear spins whose members are all prepared identically, evolve under the same Hamiltonian, and therefore contribute identical contributions to the signal. The most difficult part in this respect is the identical preparation: NMR usually prepares the spin system by letting it equilibrate with its environment. The resulting state corresponds to the equilibrium density operator

$$\rho_{\mathrm{eq}} = e^{-i\mathcal{H}_z/k_BT}, \tag{1}$$

where $\mathcal{H}_z$ is the Zeeman Hamiltonian of the system and k_BT the thermal energy. Since this is not a pure state, it was thought to be impossible to use NMR for executing quantum algorithms that require pure states as input. All of the early quantum algorithms explicitly require pure states to encode the information.

A possible solution to this problem was found by Cory *et al.*[17] and by Gershenfeld and Chuang:[16] they added different signals in such a way that the total signal obtained was identical to what would be obtained from a single experiment with a pure initial state. We will refer to this approach as using pseudopure states (PPS) and discuss it in more detail in Sec. III B 3.

While the use of ensembles was mostly considered a problem that needs to be overcome, it was also shown that it can also be seen as an opportunity that provides additional possibilities. Brüschweiler showed[32] that an ensemble quantum computer can execute quantum algorithms at a speed that is exponentially faster than that of single issue quantum computers. This proposal was realized and implemented by Yang *et al.*,[33] and Stadelhofer *et al.* demonstrated a similar scheme for oracle-based quantum algorithms.[34]

2. NMR quantum registers

Single quantum bits are not useful for information processing; instead, a quantum register is required, consisting of as many quantum bits as possible. There must be some type of interaction between the individual qubits, in order to be able to implement multiqubit (i.e., conditional) logical operations. Ideally, these interactions can be turned on and off.

In NMR, these interactions are provided by nuclear spin couplings, which in most systems are static (i.e., "always on"). In liquid-state NMR, the isotropic J couplings are the relevant interactions, since dipolar couplings are averaged out. Since these couplings are active only within a molecule, the quantum register is naturally confined to individual molecules. Implementing quantum algorithms by NMR consists mainly of choosing the appropriate molecular system and "compiling" the quantum algorithms into appropriate sequences of radio-frequency pulses, using mostly established procedures from NMR spectroscopy.[35,36]

Figure 3 shows how the size of NMR quantum registers has increased over the last decade. The initial experiments were all done using isotropic liquids, with the quantum register size increasing up to 12 qubits.[37] Obtaining larger qubit-system using liquid state NMR is challenging, mainly because the J couplings are weak interactions, of the order of 10–100 Hz for nearest neighbors, and <1 Hz for nuclei separated by more than four to five chemical bonds. Smaller couplings mean longer durations for nonlocal gate operations[38,39] and therefore bigger problems with relaxation.

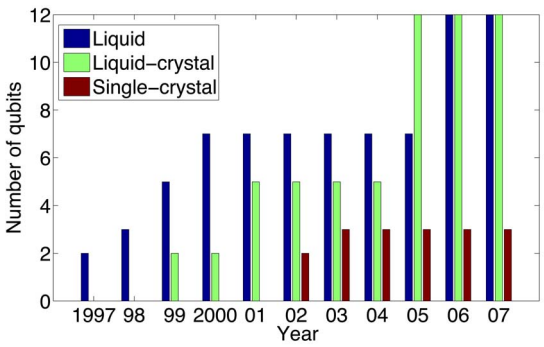

FIG. 3. (Color online) Size of nuclear-spin quantum registers vs year.

While most of the work has been carried out using spin 1/2 nuclei, QIP with spins $>1/2$ have also been demonstrated. There are two ways of doing this. The first is to choose nuclei having 2^n energy levels, in which case each nucleus can be thought of an n-qubit system.[40–43] For example, a spin 3/2 nucleus has four energy levels and can be considered as a two-qubit system;[44] a spin 7/2 nucleus has eight energy levels and can be considered as a three-qubit system.[45,46]

Instead of two-state qubit system and binary logic, one can also think of using an $(n \neq 2)$-state quantum system as the unit of quantum information. For example, the three eigenstates of a spin-1 nucleus can be thought as a single qutrit. Experiments on such a system have been demonstrated by Das *et al.*[47]

3. Dipolar coupled systems

Some of the difficulties of liquid-state NMR can be overcome by using solid materials. If isotopically labeled molecules are embedded in a single crystal, it is possible to use similar techniques as in liquid-state NMR.[48] In addition, the strength of the couplings between nuclear spin qubits can be tuned by orienting them in a single crystal.[38,49,50] This can be used, e.g., to create low-dimensional spin networks by using a special orientation of the crystal with respect to the static magnetic field.[51] Alternatively, the couplings between them could be mediated by electrons,[52–54] similar to the J-couplings familiar from liquid-state NMR, but with much bigger strengths (of the order of megahertz), and, in a suitable architecture, tunable by external gates.[52]

To initialize the nuclear spins into a pure state, it may be possible to transfer polarization from electron spins, which can be fully polarized in thermal equilibrium at low temperature and high magnetic fields. The transfer could use dynamic nuclear polarization[38,49] or coherent evolution under a resolved hyperfine coupling.[55]

Addressing individual qubits in solids can be achieved by using different spin species and chemical shift differences, in close analogy to liquid-state NMR. In addition, it is

possible to apply magnetic field gradients to distinguish spins whose environment is otherwise identical.[49,53]

Since dipolar couplings can be stronger than chemical shift differences, the usual computational basis states $|\uparrow\rangle$ and $|\downarrow\rangle$ are no longer eigenstates of the Hamiltonian in a solid. It is then often advantageous to choose a different basis, by labeling the eigenstates of the Hamiltonian with the logical basis states $|000\cdots0\rangle,\ldots,|111\cdots1\rangle$. The gate operations have then to be adapted to this set of basis states. Another difficulty that is often encountered in solids is caused by long range couplings and crystal defects, impurities, etc., which broaden the resonance lines and contribute to the loss of quantum information.

A clear advantage for solid-based NMR quantum information processors may turn up for the readout process: measuring the state of individual nuclear spins may be possible either optically,[56,57] or by transferring the information to electron spins and reading out their state via single electron transistors.[52]

While dipolar couplings promise significantly larger coupling strengths than indirect (J) couplings, the use of solid state systems also implies that dipolar couplings to distant spins outside of the quantum register contribute to the decoherence process. This problem can be avoided by going to an intermediate system: if the molecule that forms the quantum register is dissolved in a liquid crystal, the dipolar couplings between the qubit spins are retained, while the intermolecular couplings are averaged out.[42,58,59] Lee and Khitrin have demonstrated initialization and preparation of a cat state[172] for a 12 spin system oriented in a liquid crystal.[60,61]

B. Initialization

Before a quantum algorithm can be executed, the quantum register must be initialized into a well-defined state.[13,14,62] Many quantum algorithms require this initial state to be a pure state, i.e., it should be possible to write it as a single ket $|i\rangle$ or the density operator should satisfy $\rho^2=\rho$.

Unfortunately, nuclear spin systems in thermal equilibrium are never in a pure state, but highly mixed. The high-temperature expansion of the equilibrium density operator (1) is

$$\rho_{\mathrm{eq}} = \frac{1}{2^n} I + \epsilon \sum_{j=1}^{n} I_{jz}, \tag{2}$$

where I is the unity operator and $\hbar I_z^j$ is the z component of the angular momentum operator of jth spin. The traceless part $\epsilon \Sigma I_z^j = \rho_{\mathrm{dev}}$ is called the *deviation* density matrix. The coefficient is $\epsilon = \gamma\hbar H_0 / k_B T \sim 10^{-5}$, with γ, H_0, and $k_B T$ corresponding to the gyromagnetic ratio, magnetic field strength, and thermal energy at room temperature, respectively. Unrealistic magnetic field strengths and/or extremely low sample temperatures are required for a thermal equilibrium state that would be close enough to a pure state. However, some clever alternatives have been suggested and Fig. 4 summarizes various schemes that tackle the challenge of initialization in NMR-QIP.

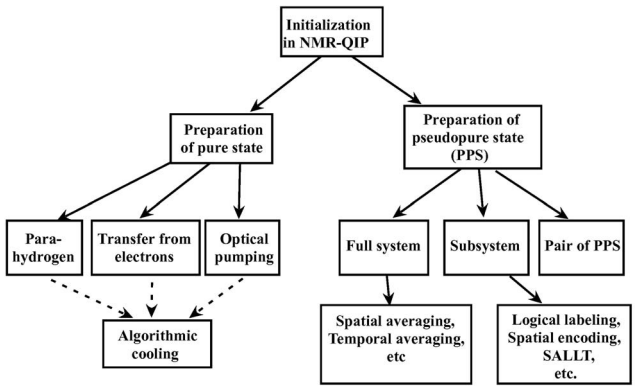

FIG. 4. Various schemes developed for state initialization in the context of NMR-QIP.

1. Highly polarized spins

Several techniques exist for increasing the polarization of nuclear spins by several orders of magnitude above the thermal polarization. The most important ones are optical pumping,[63,64] dynamic nuclear polarization,[65,66] and the use of parahydrogen.[67–69] Only the last one is applicable to liquid-state NMR. It uses the fact that the two nuclear spins of molecular hydrogen (in its electronic ground state) must be in a spin-singlet state, while the triplet states occur only in the rotationally excited state. At low temperature, molecular hydrogen is thus almost completely in the singlet state, i.e., the *relative* spin polarization of the two ^{1}H nuclei is almost complete.

Of course, a spin-singlet state does not produce an observable signal in NMR, but as soon as the symmetry is broken, e.g., by chemically fixing the two hydrogen atoms to a molecule, the evolution under the new, asymmetric chemical shift Hamiltonian can generate antiphase magnetization with a large amplitude. This approach has been used to generate highly spin-polarized molecules.[68,69] By controlling the timing of the chemical reaction with laser pulses, the resulting spin polarization can be increased to $\epsilon \approx 0.92$.[70,71] The corresponding spin state is truly entangled, i.e., it cannot be described by local hidden variable models.

2. Algorithmic cooling

While these techniques can increase the nuclear spin polarization by several orders of magnitude compared to thermal states, the limiting polarization is always <1. While it is not possible to eliminate the remaining disorder, there are possible ways to move it to a part of Hilbert space that is not used for quantum information processing, thus increasing the polarization of the quantum register.

The technique was inspired by Peres' recursive algorithm[72] of von Neumann's extraction of fair coin flips from a sequence of biased ones. Schulman and Vazirani[73] developed a strategy that is generally referred to as purification. They described a quantum mechanical heat engine that operates in a similar way as a classical Carnot engine to separate hot and cold regions. However, the Shannon bound on the entropy-preserving purification ability of reversible data compression results in purifying only a small fraction of

bits, meaning that thousands of bits are required in order to obtain one or a few purified bits (with a reasonable probability of success).

Boykin *et al.* presented an *algorithmic cooling* scheme that goes beyond the Shannon bound, because it does not preserve entropy of the system but removes entropy into a spin-polarization heat bath.[74] To pump entropy into this bath, algorithmic cooling uses computational bits having very long relaxation times and bits that rapidly reach thermal relaxation (RRTR bits). The algorithm involves a reversible compression (via permutation) performed on the computational bits, purifying (cooling) some while concentrating the entropy (heat) of the others. Then the hotter bits, whose temperature is above the bath temperature, are brought in contact with the RRTR bits, resulting in an overall cooling of the system. Repeating the process many times via a recursive algorithm can, in principle, be achieved.

The algorithmic cooling scheme was improved by Fernandez *et al.*[75] and more recently by Schulman *et al.*,[76] who proposed a partner pairing algorithm (PPA). Laflamme and co-workers have carried out an experimental demonstration of the PPA algorithm on a Malonic acid single crystal having an ensemble of 5 qubits in which three ^{13}C spins act as computational bits and two methylene ^{1}H spins act as RRTR bits.[77,78] Fernandez *et al.* have also investigated the ratio of the thermalization times of computational qubits (carbons) and a reset qubit (hydrogen).[79]

3. Pseudopure states

The most common scheme for NMR quantum computation is based on the observation that the intensity of the NMR signal depends only on the difference between the populations in various states and not on the absolute populations. Since the identity part does not evolve under the Hamiltonian and commutes with the detection operator, it has no effect on the NMR observables. Only the deviation density matrix evolves under the Hamiltonian and leads to a detectable signal. Converting this deviation part of the full density operator into an operator that is directly proportional to the density operator of a pure state is relatively straightforward. The state evolves in exactly the same way as a true pure state and generates the same signal (up to a proportionality constant). This type of states is therefore referred to as PPS.

The density operator ρ_{pps} of a PPS is isomorphic to that of a pure state $\rho_{\mathrm{pure}}=|\psi\rangle\langle\psi|$,

$$\rho_{\mathrm{pps}} = (1-p)\cdot\frac{1}{2^n}I + p\cdot|\psi\rangle\langle\psi|, \tag{3}$$

where $p\sim n\epsilon/2^{n-1}$ (see Appendix A of Ref. 74). The exponential drop in the coefficient reflects the exponential reduction in signal as the number of qubits in the pseudopure state is increased. This is one of the big obstacles that make scaling of NMR quantum information processors to large numbers of qubits so difficult.[80]

Preparing an n-qubit pseudopure state over an n-qubit system is a nonunitary process and requires averaging of certain magnetization modes. The averaging can be performed in different ways, e.g., in space, in time, or in Hilbert space. A number of techniques have been developed for preparing pseudopure states and a brief description of them is presented in the following.

Let us consider a homonuclear two spin system in thermal equilibrium. In the *spatial averaging* method,[17] the PPS corresponding to the $|00\rangle$ state is prepared by using three rf pulses, two pulsed field gradients, and a $1/2J$ delay for evolution under the coupling between the two spins,

$$I_z^1 + I_z^2 \xrightarrow{\left(\frac{\pi}{3}\right)_x^2, G_z, \left(\frac{\pi}{4}\right)_x^1, \frac{1}{2J}, \left(\frac{\pi}{4}\right)_{-y}^1, G_z'} \frac{1}{2}[I_z^1 + I_z^2 + 2I_z^1 I_z^2]. \tag{4}$$

Here, the superscripts of the pulses denote the spin indices, the subscripts denote the phases, and G_z, G_z' denote pulsed field gradients. The resulting state is isomorphic to the $|\uparrow\uparrow\rangle$ state, which is usually taken as the computational basis state $|00\rangle$. More complex sequences are required for larger spin systems, in particular, if they consist of heteronuclear spins having different gyromagnetic ratios.

In the *temporal averaging* method,[81] the PPS is prepared by adding experiments with different initial states obtained by permuting all the states except one. Permutations can be carried out by transition selective π pulses. For example, in the case of a two spin system, one needs to take the average of the thermal state and two states in which the populations of the thermal state were permuted to prepare a $|00\rangle\langle 00|$ pseudopure state,

$$\frac{1}{3}\begin{bmatrix} (1+4\varepsilon)/4 & & & \\ & \frac{1}{4} & & \\ & & \frac{1}{4} & \\ & & & (1-4\varepsilon)/4 \end{bmatrix} + \frac{1}{3}\begin{bmatrix} (1+4\varepsilon)/4 & & & \\ & (1-4\varepsilon)/4 & & \\ & & \frac{1}{4} & \\ & & & \frac{1}{4} \end{bmatrix} + \frac{1}{3}\begin{bmatrix} (1+4\varepsilon)/4 & & & \\ & \frac{1}{4} & & \\ & & (1-4\varepsilon)/4 & \\ & & & \frac{1}{4} \end{bmatrix}$$
$$= \frac{1-p}{4}I + p\begin{bmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & 0 \end{bmatrix},$$

where $p=3\epsilon/4$.

Often a *subsystem* PPS is prepared by sacrificing one or more qubits. For example, in the *logical labeling* method one obtains two subsystems of 2 qubits each, whose PPS depends on the state of the labeling qubit.[16,82,83] Combinations of spatial averaging and logical labeling into hybrid schemes such as *spatial encoding*[84] and *spatially averaged logical labeling technique*[85] (SALLT) have also been used.

Fung has proposed a simple method for preparing a *pair of pseudopure states*.[86] It involves inverting a transition using a selective π pulse and subtracting the resulting signal from that obtained from an identical experiment performed on the thermal equilibrium initial state.[87]

An algorithmic approach to preparing a subsystem pseudopure state has also been developed.[88] It involves creating multiple quantum coherence by an *encoding* sequence, selecting the highest quantum coherence ($\approx$ a cat state) by using gradients, followed by *decoding* it to a subsystem diagonal state.

IV. COHERENT CONTROL

A. Robust gate operations

The ability to perform a general quantum gate is one of the five important criteria (DiVincenzo criteria[30]) for the physical realization of QIP. A quantum gate can be described as a target unitary operator U_T, which has to be constructed using the control parameters available for the specific system. In general, the gate should be independent of the input state, which may not be known.

Any experimental implementation of such a unitary transformation suffers from imperfections in the control fields, which can only be generated with a finite precision. As a result, the actual gate operation U_{exp} differs from the target operation U_T. As a measure of the deviation, one usually uses the fidelity

$$F = |\text{Tr}\{U_T^\dagger U_{\text{exp}}\}/N|^2, \tag{5}$$

where N is the dimension of the operators: if the experimental operation is identical to the target operation, the operator product becomes the unity operator and the fidelity reaches the limiting value of 1.

In any single experiment, one initializes the system in a specific input state $|\psi_{\text{in}}\rangle$ and applies the control sequence, which converts the system to the final state $|\psi_{\text{exp}}\rangle$, which typically differs from the ideal output state $|\psi_T\rangle$ (see Fig. 5). The difference between the two states can be measured and represents a measure of the quality of the operation; however, for quantum information processing, the operation must perform well for all possible input states. The fidelity measure (5), which does not depend on a state, is therefore more appropriate. To measure the fidelity, it is necessary to eliminate the dependence on the specific input state by averaging the deviation over all possible input states. This is achieved by "process tomography."[44,89]

Since the fidelity of individual quantum logical gate operations has to be very high (of the order of >0.999), it is important to design them in such a way that the fidelity remains close to unity even if the experimental parameters deviate from the ideal values. This type of gate operations are called robust and their design is the field of coherent control. Although here we discuss coherent control in terms of NMR parameters, the strategies are applicable to all subfields of quantum control.

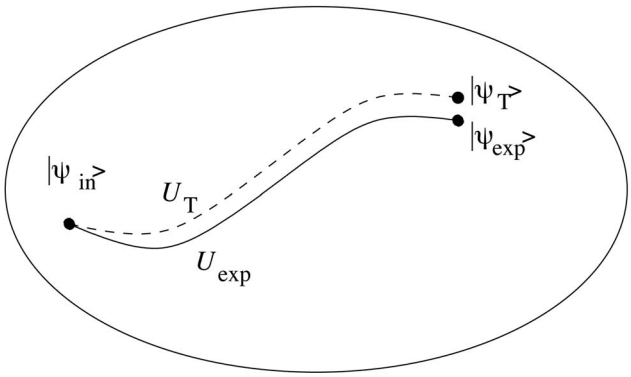

FIG. 5. Dynamics in the Hilbert space corresponding to a desired target operation U_T and the experimentally realized operation U_{exp}.

Control over spin dynamics is the main part of any NMR experiment. For this purpose numerous rf techniques have been developed over the last fifty years,[35,36] including composite pulses, adiabatic pulses, shaped pulses, amplitude and/or frequency modulated pulses, etc. However, not all of these techniques are directly applicable to quantum information processing. In particular, QIP requires (in most cases) gate operations that do not depend on the initial condition, but effectively realize the target unitary operation (type A pulses in Ref. 90).

B. Strongly modulating pulses

In the context of quantum information processing, it has turned out to be useful to implement unitary transformations by suitable sequences of rf pulses, whose amplitude, frequency, and phase are made time-dependent in such a way that the overall transformation of the system effected by the rf pulse sequence in combination with the internal Hamiltonian realizes the target operation in such a way that small deviations of the experimental parameters do not cause a large deviation. In this context, they are often called "strongly modulating pulses" (SMPs).[91]

A number of techniques have been developed to find suitable SMPs for a given target operation. They mostly rely on numerical optimization of the overall transformation by searching the available parameter space. We discuss here two techniques that have shown their usefulness for this search. Fortunato *et al.*[91] described the construction of SMPs using stochastic search methods, while Khaneja *et al.* suggested the gradient ascent pulse engineering (GRAPE) technique.[92]

Consider a rf pulse of duration (τ), amplitude (ω_q), angular frequency (Ω_q), and phase (ϕ_q) applied to a nuclear species q with gyromagnetic ratio γ_q. The rotating frame Hamiltonian is then[36]

$$\mathcal{H}_E^{(\mathrm{rf})} = \mathcal{H}_{\mathrm{int}} + \sum_{q=1}^{m} [\lceil \gamma_q \rfloor \omega_q \{h_x^q \cos(\phi_q) + h_y^q \sin(\phi_q)\} - \Omega_q h_z^q], \quad (6)$$

where $\mathcal{H}_{\mathrm{int}}$ is the internal Hamiltonian of the system, $\lceil \gamma_q \rfloor$ denotes the sign of γ_q, and $h_\alpha^q = \Sigma_{j=1}^{n_q} I_\alpha^{qj}$, is the collective spin operator for each nuclear species q. The corresponding propagator in the rotating frames of the rf channels for the system evolution over a duration τ is $\exp(-i\mathcal{H}_{\mathrm{E}}^{(\mathrm{rf})}\tau)$. The propagator in the common reference frame (wherein chemical shifts and rf frequencies are measured) for the kth rf pulse is[91]

$$U_k(\tau_k, \omega_{qk}, \phi_{qk}, \Omega_{qk}) = \exp\left(-i\sum_{q=1}^{m} \Omega_{qk} h_z^q \tau_k\right) \cdot \exp(-i\mathcal{H}_{Ek}^{(\mathrm{rf})}\tau_k). \quad (7)$$

While it is, in principle, possible to choose any time dependence for the phase, frequency, and amplitude of the rf field, it is in practice convenient to choose piecewise constant functions. It is then possible to decompose the Hamiltonian of the SMP into a sequence of S piecewise constant segments, each consisting of a rf pulse of duration τ_k followed by a delay δ_k. Without loss of generality, we will assume that duration and delay of each segment are the same for all the channels but the amplitudes, phases, and frequencies can differ between channels. In addition, the sequence may start with an initial delay of duration δ_0. The propagator for the entire SMP can be written as

$$U_{\mathrm{SMP}} = \left[\prod_{k=\mathrm{S}}^{1} \Delta_k(\delta_k) \cdot U_k(\tau_k, \omega_{qk}, \phi_{qk}, \Omega_{qk})\right] \cdot \Delta_0, \quad (8)$$

where $\Delta_k = \exp(-i\delta_k\mathcal{H}_{\mathrm{int}})$ is the delay propagator, and $\Delta_0 = \exp(-i\delta_0\mathcal{H}_{\mathrm{int}})$ is the initial delay propagator.

Designing an SMP for a given target operator U_T thus reduces to a numerical search problem to determine the set of control parameters $\{\tau_k, \omega_{qk}, \phi_{qk}, \Omega_{qk}, \delta_k\}$ that maximize the fidelity,

$$F = |\langle U_{\mathrm{SMP}}|U_T\rangle|^2 = |\mathrm{Tr}\{U_{\mathrm{SMP}}^\dagger U_T\}|^2. \quad (9)$$

Since most search algorithms are designed to minimize a function, it is often easier to minimize the deviation $Q = |1 - \sqrt{F}|$. To limit the control parameters to an experimentally well accessible range, a penalty function P is added so that the quality factor becomes

$$Q = |1 - \sqrt{F}| + P(\{\tau_k, \omega_{jk}, \Omega_{jk}, \delta_k\}). \quad (10)$$

The penalty function is designed such that whenever a parameter gets beyond the experimental limit (e.g., too long rf pulses, too large rf power, etc.), it acquires a large value so as to lift the quality factor above the minimum. The total number of segments in a SMP depends on the complexity of the internal Hamiltonian, the target operator, the proximity of the initial guess to the target operator, and the desired fidelity.

This method has been successfully applied to a number of experiments.[37,50,59,93–97] Boulant *et al.*[93,95] have used SMPs for efficient entanglement transfer on a four-qubit system. Teklemariam *et al.*[94] have used SMPs to obtain high precision quantum eraser scheme applied to various types of entangled states. Weinstein *et al.*[96] have used SMPs for implementing quantum process tomography of the quantum fourier transform on a three-qubit system. Boulant *et al.*[97] have also used SMPs to demonstrate a concatenated quantum error-correcting code. Other SMPs have also been used to control a 12-qubit system, the largest qubit system to date, by implementing the cat-state benchmark experiment.[37] In a single crystal environment, SMPs were used to control two-qubit and three-qubit systems.[50] More recently, a single SMP implementing an entire algorithm has been demonstrated on a strongly dipolar coupled four-qubit system partially oriented in a liquid crystal.[59]

C. Gradient ascent pulse engineering

The numerical search method to find the appropriate sequence for a given target operation can be chosen from the usual minimization algorithms, such as the Nelder–Mead simplex algorithm.[98,99] Another technique is based on a standard protocol in optimal control theory for steering an initial state to a target state. It is useful when gradients of the fidelity with respect to its control parameters can be calculated.[100] The control parameters are incremented in the direction of the fidelity ascent leading to a fast convergence towards a local maximum. If the converged minimum does not have the desired fidelity, the algorithm can be repeated with different initial guesses or a larger number of segments until the desired fidelity is reached.

In the model suggested by Khaneja *et al.*[92] an SMP consists of a set of N equal duration (Δt) segments. The Hamiltonian $\mathcal{H}_k$ of the kth segment is expanded in terms of the internal Hamiltonian $\mathcal{H}_0$ and a set of M available control Hamiltonians $\mathcal{H}_{k,m}$,

$$\mathcal{H}_k = \mathcal{H}_0 + \sum_{m=1}^{M} u_{k,m}\mathcal{H}_{k,m}, \quad (11)$$

where $u_{k,m}$ are the scalar quantities of the corresponding control parameters. In NMR, the relevant control rf parameters are x amplitude $\omega_{k,x}$, y amplitude $\omega_{k,y}$, and frequency $\omega_{k,rf}$ (the rf phase can be calculated from the x and y amplitudes). For an SMP with N segments with propagators $\{U_1, \cdots, U_N\}$, the fidelity to be maximized can be written as[92]

$$F = |\langle U_T|U_N \cdots U_1\rangle|^2 = \langle P_k|X_k\rangle\langle X_k|P_k\rangle,$$

(using cyclic permutations within the trace operation), where $P_k = U_{k+1}^\dagger \cdots U_N^\dagger U_T$ and $X_k = U_k \cdots U_1$. The gradients of the fidelity F with respect to the mth control parameter $u_{k,m}$ of the kth segment can be calculated as[92]

$$\frac{\delta F}{\delta u_{k,m}} = -2\,\mathrm{Re}\{\langle P_k|i\Delta t\mathcal{H}_{k,m}X_k\rangle\langle X_k|P_k\rangle\}. \quad (12)$$

The fidelity of the SMP can be increased by incrementing each control parameter of each segment in the direction of its gradient $u_{k,m} \rightarrow u_{k,m} + \epsilon(\delta F/\delta u_{k,m})$, where ϵ is a small step size. The process of finding the gradients and incrementing the control parameters can be repeated until the maximum is reached. The duration and number of segments can be cho-

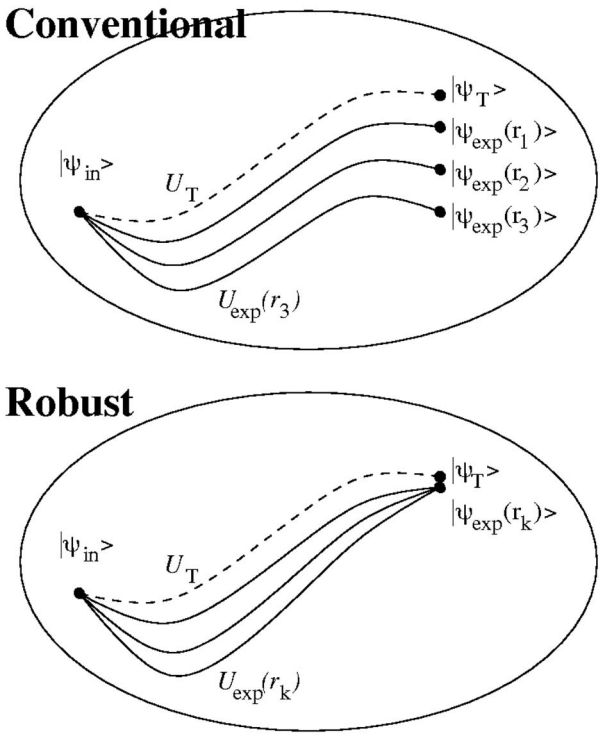

FIG. 6. Upper part: Evolution of a quantum state under an inhomogeneous Hamiltonian. Subsystems in different parts of the sample reach different final states. The dashed line represents the ideal evolution. Lower part: A robust SMP refocuses the effects of the inhomogeneities and the spinsystems in all parts of the sample end up close to the target state.

sen carefully to obtain "time-optimal" solutions. Penalty factors can be subtracted from the gradients to ensure that the control parameters are limited to a desired range.

A possible generalization of this scheme is to use, instead of equal duration pulses, segments with variable durations. This approach may lead to SMPs with smaller numbers of segments and better performance. The gradient of the fidelity F with respect to the duration τ_k of the kth segment is

$$\frac{\partial F}{\partial \tau_k} = -2\,\mathrm{Re}\{\langle P_k|i\mathcal{H}_k X_k\rangle\langle X_k|P_k\rangle\}. \tag{13}$$

It is also possible to introduce delays in the GRAPE method. For their duration, the gradient is

$$\frac{\partial F}{\partial \delta_k} = -2\,\mathrm{Re}\{\langle P_k|i\mathcal{H}_{\mathrm{int}} X_k\rangle\langle X_k|P_k\rangle\}. \tag{14}$$

D. Inhomogeneities and decoherence

The static field inhomogeneity (SFI) of the magnet and the rf field inhomogeneity (RFI) of the probe create spatial dependencies of the chemical shifts $\nu(\mathbf{r})$ and the local rf amplitudes $\omega(\mathbf{r})$. As a result, even though the local evolutions are unitary, the coherence of the ensemble decays, as spins in different parts of the sample undergo slightly different evolutions and reach different final states (see Fig. 6).

For a given system, the SFI and RFI can be determined from the spectral line shapes and the decay of nutating magnetization.[101] An SMP robust against RFI and SFI is constructed by maximizing the average fidelity $F_{\mathrm{av}}=\Sigma_i p_i F_i$. The individual terms F_i represent the fidelity for an ensemble in an area with a fixed rf and static magnetic field and p_i the corresponding probability.[50,102] Errors in rf amplitudes can also occur due to nonlinearities in the spectrometer components. Such errors can be compensated iteratively by fitting the nonlinearity to a suitable (e.g., polynomial) function and applying the inverse of the function to the SMPs.[95]

For the physical realization of QIP, it is also necessary to contain decoherence, i.e., irreversible loss of information due to the interaction between the quantum system and its environment. There are several ways of controlling decoherence which will be described in detail in Sec. V. Encoding qubits into subspaces called decoherence free subspaces (DFS) is one way of protecting the quantum information against certain kinds of noises. Another approach is dynamical decoupling by which one attempts to decouple the system from the environment by modulating the dynamics of the system faster than the system-environment interaction. Capellaro *et al.* have set down the principles for achieving coherent control on DFS encoded qubits (logicqubits).[103] Using this coherent control of logic qubits has been demonstrated by implementing conditional gates that are necessary to create entanglement between logic qubits.[104] An optimal control approach has also been applied to obtain relaxation optimized pulse sequences.[105]

E. Other control methods

A number of alternative approaches has been developed. Chuang and co-workers have used analytical methods to calculate accurate composite pulses.[106,107] While the analytical solutions can give more insight into the spin dynamics, the technique becomes tedious for large spin systems. Systematic methods for designing refocusing schemes for multiqubit systems have been developed based on Hadamard matrices.[108,109]

Several groups, including Kumar and co-workers have suggested using transition selective shaped pulses for implementing unitary operations.[110–112] The main advantage of this approach is that it leads to relatively simple pulse sequences and they are applicable to a wide variety of systems such as spin systems with equivalent spins,[113] quadrupolar coupled systems,[43] and strongly coupled systems.[114] However, transition selective shaped pulses have long durations and are not applicable for arbitrary initial states.

For cases where qubit-selective pulses can be used, Freeman and co-workers have developed several useful control techniques. The trick is to divide a coupled multispin system into a small subset of "active" spins which undergo the gate operation and a larger subset of "spectator" spins, which are returned to their initial states using refocusing techniques.[115,116] They used this technique to demonstrate a universal SWAP gate.[117]

Geometric phases have also been used to achieve controlled phase shift gates.[118–120] The geometric phases are independent of the path traversed and are therefore robust against errors in control fields.[118,119] Multifrequency pulses have also been used to obtain selective rotations at desired frequency ranges.[41,121]

Khaneja *et al.* have also proposed a geometric optimal control approach.[122] They have shown that the problem of finding the shortest time for implementing a unitary propagator can be reduced to finding the shortest paths on certain coset spaces.[122] Using such techniques, they have also demonstrated that optimized pulse sequences can reduce the duration of CNOT gates by up to 38%, SWAP gates by about 25%,[123] and indirect SWAP gates by about 42.3%.[124] The geometric optimal control approach has also been applied to several problems in conventional NMR, such as coherence transfer,[125–127] designing broadband excitation pulses,[124,128–131] inversion pulses,[132] universal rotations,[133] homonuclear recoupling,[134] and for polarization transfer experiments.[135]

F. Scaling issues

The numerical search for a specific SMP involves the simulation of the dynamics of a quantum system and is therefore a computationally hard problem. Nevertheless, it is possible to find suitable SMPs even for relatively large systems within certain approximations. For a local gate (or a nonlocal gate within a subsystem) in a weakly coupled system, finding an approximate solution can be speeded up by decomposing the system into subsystems: $U_T \approx U_{T1} \otimes \cdots \otimes U_{Tn}$, where n is the total number of subsystems. An SMP that maximizes simultaneously the fidelities F_n for all the subsystems also optimizes the product of fidelities $F = \Pi_{i=1}^{n} |\langle U_{\mathrm{SMP}i} | U_{Ti} \rangle|^2$. Here, $U_{\mathrm{SMP}i}$ is the net propagator for the ith subsystem. Once a good guess is obtained, the full system fidelity is calculated by turning on all the couplings. If the fidelity is less than the desired value, then this guess can be optimized further to obtain a full system SMP.

The ultimate goal of coherent control is to achieve fault-tolerant computation. While perfect control is not necessary,[136] the threshold gate fidelity for fault-tolerant computation has yet to be reached. The best control approaches for future applications depend on the kind of architecture that promises a scalable quantum information processor. There might be a hybrid method using optimal control theory, average Hamiltonian theory, and numerical methods such as genetic and evolutionary algorithms. As long as classical computers are used to calculate control fields for quantum computers, the scaling of the computational cost with increasing number of qubits is an important issue.

V. DECOHERENCE

A. The problem

Possibly the biggest obstacle for the construction of large quantum information processors is the loss of quantum information before the end of the computation. While loss of information must be avoided also in classical computers, it turns out to be much more difficult to preserve quantum information than it is to preserve classical information. The additional difficulty present in quantum mechanics can be tracked to two closely related fundamental properties of quantum mechanics.

The first is Heisenberg's uncertainty principle: a quantum mechanical measurement cannot be performed without perturbing the variable that is conjugate to the measurement variable. It is therefore not possible to perform measurements on the quantum register while a computation is ongoing. This makes it difficult to detect errors and correct them.

The second problem is the impossibility of exactly duplicating quantum systems, which is known as the no-cloning theorem.[137,138] In classical computers, the simplest error detection schemes duplicate some information and detect differences between the multiple copies. Since exact duplication is not possible in quantum systems, this procedure is not directly applicable.

The loss of information can be traced to two different mechanisms:

- The quantum register is never completely isolated from its environment. Couplings to the environment dissipate quantum information. In NMR this effect is known as relaxation, while in quantum information processing it is usually referred to as decoherence.
- Experimental imperfections of gate operations and fluctuations in the control fields cause the system evolution to differ from the intended evolution.

As we have shown in the section on coherent control, optimizing the control operations can go a long way towards improving the quality of he gate operations. However, even if fidelities of individual gate operations can reach values of >0.999, this will not be sufficient for completing many potentially useful calculations, which may involve thousands of gate operations acting on hundreds or thousands of qubits. It will therefore be necessary to develop techniques that detect and correct errors also in quantum mechanical systems.

B. Scaling of decoherence

In NMR, we are used to quantify relaxation by the two time constants T_1 and T_2. These time constants correspond to the time that it takes for the average magnetization to approach its equilibrium value. One has to be careful, however, when one takes these time constants as a measure of the decoherence time of quantum information: Magnetization corresponds to population differences or superpositions of the states of individual spins. Relaxation of magnetization is therefore governed by the interaction of individual spins with their environment (the "lattice"). Quantum information, however, is stored not in the state of any individual spin, but in the state of the complete system, which may consist of a very large number of spins (or other qubits).

It has been realized for a long time, that quantum mechanical systems with many degrees of freedom tend to decay more rapidly than simple systems with a small number of degrees of freedom. Probably the most famous discussion of this issue was put forward by Schrödinger[139] with the drastic example of the superposition state between a living and a dead cat. The generally accepted resolution of the question why such states have not been observed (and probably never will) is that in such complex systems, coherence decays more rapidly than it can be created. Nevertheless, the limiting size of quantum systems where superpositions and interference effects can be observed has increased dramati-

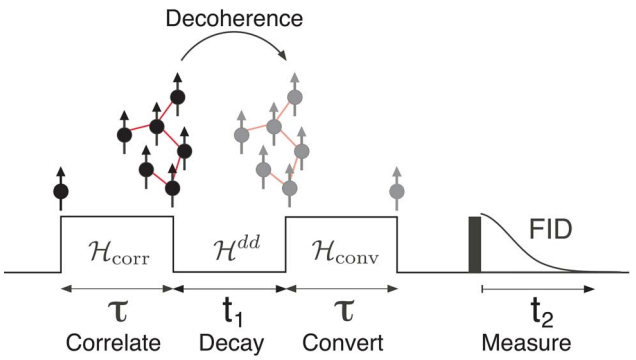

FIG. 7. (Color online) Measurement of the excitation and decay of high-order multiple quantum coherence. The (effective) Hamiltonian $\mathcal{H}_{\rm corr}$ correlates the spin qubits. The resulting highly correlated states decay during t_1. The Hamiltonian $\mathcal{H}_{\rm conv}$ converts the remaining order into measurable magnetization, which is then detected as the amplitude of the free induction decay.

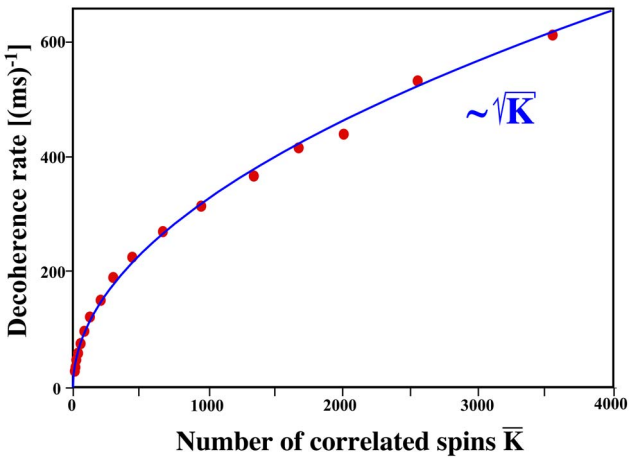

FIG. 8. (Color online) Scaling of the decoherence rate with the size of the quantum register. The solid curve shows a $\sqrt{K}$ function fitted to the experimental data points.

cally over the last decades, from individual spins and atoms to molecules with >100 atoms.[140] In the context of quantum information processing, it is important to not only observe the superposition states and their decay,[141] but also quantify the decay rates and its dependence on the number of degrees of freedom.

Nuclear spin systems are well suited for this purpose, since they can be manipulated in a precise manner and it is possible to create states that involve thousands of spins and measure the decay of these states.

Figure 7 shows a possible approach: The nuclear spins in a solid are correlated by letting them evolve under the Hamiltonian

$$\mathcal{H}_{\rm corr} = -\sum_{i,j} \frac{d_{ij}}{4}[I_+^i I_+^j + I_-^i I_-^j], \tag{15}$$

which can be generated by different multiple pulse sequences.[142,143] When this sequence is applied to nuclear spins in thermal equilibrium, it generates clusters of correlated spins, which can be used as models of quantum registers.

The size of these clusters grows with the time during which the Hamiltonian is applied to the system. The average size can be measured by comparing the amplitudes of different multiple quantum components:[143] if all possible transitions contribute equally to the signal, the signal amplitude decreases $\propto e^{-M^2/K^2}$, where M is the multiple quantum order and K is proportional to the cluster size.

The decay of these multiple quantum signals can be measured by letting them decay and then converting them to observable magnetization by inverting the evolution that created them.[144] Figure 8 shows the decoherence rates measured in adamantane as a function of the number of correlated spins.[145,146] The experimental data points can be well approximated by a function $r \propto M^{1/2}$. This scaling behavior is considerably more benign than a simple model would predict that assumes that the coupling of the spins to the environment is independent of each other. This is not completely unexpected, however the decoherence process is driven by magnetic dipole-dipole interactions between the qubit spins and their environment, and since the distances between the spins that are part of the quantum register and those spins that form the environment are comparable, the couplings of different spins with the environment must be correlated. In such a case, the contributions of the different processes to the total relaxation rate can add or subtract, depending on the signs of the coupling constants.[147–149]

C. Fighting decoherence

In NMR, it was realized early on that some effects of relaxation can be reversed by applying radio-frequency pulses to the spin system in such a way that they effectively invert the time evolution of the system.[150–152] In quantum information processing, it was suggested to use similar approaches[153] to suppress decoherence. The pulse sequences to suppress decoherence must be designed to modulate the interaction that causes the decoherence in such a way that its average is minimized.[154]

In the example of nuclear spins in solids, the main contribution to the relaxation is from dipolar couplings to neighboring spins. Pulse sequences that eliminate dipolar broadening have been designed in the context of high-resolution NMR in solids.[151,154–158] These sequences were originally designed to extend the coherence time of transverse magnetization; their effect corresponds to a modification of the effective Hamiltonian. Most of them are independent of the state of the system and can therefore be used also to extend the lifetime of highly correlated states involving hundreds or thousands of spins.[159]

Figure 9 shows the decoherence rates of high-order multiple quantum coherences as a function of the number of correlated spins. The experimental data points near the upper curve were measured[159] when the system was allowed to evolve freely under the dipolar coupling between the nuclear spins. The experimental data points were fitted to a power function, $r \propto K^n$, where the exponent was found to be $n \sim 0.48$. When the couplings were modulated by the multiple pulse sequence, the decay rates were reduced by a factor $r_{\rm free}/r_{\rm dec} \sim 50$, for all cluster sizes. As shown in the figure, the decay rates measured with decoupling can be fitted with

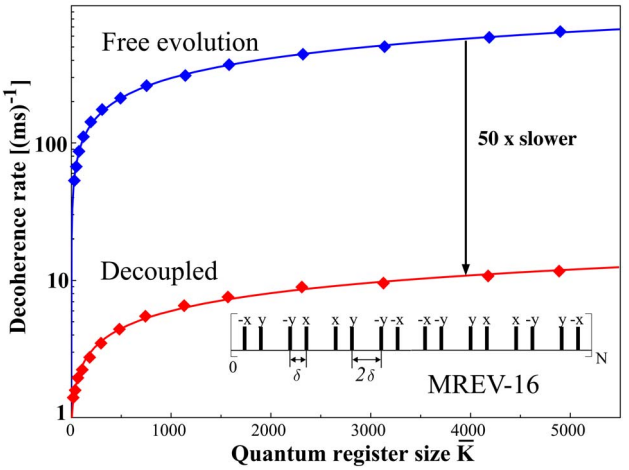

FIG. 9. (Color online) Comparison of the decay times of highly correlated nuclear spin states during free evolution under the dipolar Hamiltonian (upper half) and with modulation of the dipolar coupling by a MREV-16 pulse sequence (lower half).

the same function as the rates measured with free evolution. The observed exponent is even slightly lower, $n_{\mathrm{dec}} \sim 0.43$, indicating that the effect of the decoupling works even slightly better for the larger clusters.

VI. CONCLUSIONS AND OUTLOOK

Using quantum mechanical systems for processing information promises a new generation of computers that could be qualitatively more powerful than today's already very powerful machinery. This potential has created a lot of interest for very diverse reasons. Probably the most publicized potential of quantum computers is that for factoring large numbers and searching large databases. While these may be the applications with the largest commercial potential, there are others that appear more attractive from the point of view of a physicist: Quantum computers may be the only possible way for exactly calculating the dynamics of mesoscopic quantum systems. Possibly the most straightforward application consists in the calculation of eigenvalues and eigenvectors of Hamiltonians, which appears to be one of the cases where quantum computers provide exponential speedup over classical computers.[160]

Quantum simulations were the first proposed applications of quantum computers.[19] Interestingly, it may also turn out to be the field where quantum computers first successfully challenge classical computers. While algorithms such as Shor's factoring algorithm[24] require quantum computers with at least a few thousand qubits, it may be possible to perform useful quantum simulations with quantum computers that incorporate as few as 20–50 qubits. According to the projection by the Advanced Research and Development Activity (ARDA),[161] quantum computers operating some 50 qubits should be available by 2012. Even if this turns out to be an optimistic projection, it might be possible to combine quantum and classical parallelism.[34] Such a hybrid machine would couple many small quantum information processors either by classical or quantum communication in such a way that they together form a powerful "quantum computing cluster." Some physics problems are particularly well suited to such an approach; examples include molecular dynamics[162] and lattice QCD models.[163]

As another possibility, it has been shown that, for some physical simulation problems, not all of the DiVincenzo criteria have to be met. In particular, it is sometimes possible to build quantum simulators where it is not possible to address individual qubits to simulate the dynamics of many-body systems.[164] Examples of such processors include atoms trapped in optical lattices, which have been shown to be well suited for simulating phenomena from condensed matter physics.[165]

For this type of quantum simulations, development of more powerful processors still has to go a considerable distance. On the other hand, even today's quantum computer can be used to simulate or demonstrate fundamental physical relations, which are usually considered to be mere theoretical constructs. As an example, consider the concept of complementarity, which was introduced by Bohr[166] to describe the fact that quantum systems do not behave either as classical particles or classical waves. Instead, they possess both types of properties, which are classically incompatible. The concept became one of the foundations of quantum mechanics and was applied to a large variety of phenomena and quantitative relations were derived from it.[167] NMR quantum simulators turned out to be an excellent system for demonstrating and verifying several (in-)equalities that quantify complementarity.[168]

Similarly, it has been shown that it is not possible to measure the complete quantum state of a system with a single measurement.[169] However, if the system whose state is to be measured is first coupled to a second system in a suitable way, it becomes possible to perform a single measurement on the combined system and infer the complete quantum state of the original system from this measurement.[170] Again, NMR quantum computers turned out to be an excellent tool to demonstrate this possibility.[171]

So far, liquid-state NMR has been by far the most successful technique for demonstrating quantum information processing. While this may well change in the future, as more powerful solid-state systems will become available, it is more than likely that these systems will have to use the concepts and techniques developed in NMR to implement control fields in such a way that the system reliably performs the quantum gate operations for which it has been designed. We therefore expect that NMR will remain a testbed for this development for the foreseeable future.

ACKNOWLEDGMENTS

While we have tried to give an overview over the field of quantum information processing, we have emphasized the fields with which we are most familiar. Most of our own work was performed at the University of Dortmund. Here, we have drawn profit from collaborations with various members of the group E3 and the "Gradulertenkolleg" 726 on quantum information processing. Funding came from different sources, with the most important contributions from the DFG, the Alexander von Humboldt foundation, and the EU.

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