

# Nuclear Magnetic Resonance Approaches to Quantum Information Processing and Quantum Computing

## A Quantum Information Science and Technology Roadmap

### Part 1: Quantum Computation

#### Section 6.1

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## List of Acronyms and Abbreviations

DFS	decoherence-free subspace	QIP	quantum information processing
GHZ	Greenberger, Horne, and Zeilinger	QIS	quantum information science
Hz	hertz	QFT	quantum Fourier transform
kHz	kilohertz	rf	radio frequency
NMR	nuclear magnetic resonance	TEP	Technology Experts Panel
QC	quantum computation/computing		



## 1.0 Groups Pursuing This Approach

Note: This document constitutes the most recent draft of the Nuclear Magnetic Resonance (NMR) detailed summary in the process of developing a roadmap for achieving quantum computation (QC). Please submit any revisions to this detailed summary to Todd Heinrichs ([tdh@lanl.gov](mailto:tdh@lanl.gov)) who will forward them to the relevant Technology Experts Panel (TEP) member. With your input can we improve this roadmap as a guidance tool for the continued development of QC research.

**Table 1-1**  
**Nuclear Magnetic Resonance QC Research**

Research Leader(s)	Research Location
Cory & Havel	MIT Nuclear Engineering
Gershenfeld & Chuang	MIT Media Lab
Glaser	Munich
Jones	Oxford
Kim	Korea
Kumar	Bangalore, India
Knill	Los Alamos
Laflamme	Waterloo
Zeng	China

## 2.0 Background and Perspective

More than 50 years ago Bloch, Purcell, and coworkers demonstrated the coherent control and detection of nuclear spins via NMR. Shortly thereafter, pulse techniques were developed (e.g., by Ramsey, Torrey, Hahn, and Waugh) to extend coherent control to multispin systems, and to permit the measurement of decoherence and dissipation rates. Since then, NMR technologies have advanced to permit applications ranging from medical imaging, materials science, molecular structure determination, and reaction kinetics (see the texts by Abragam [1], Slichter [2] and Ernst [3] for example).

The NMR approach to quantum information processing (QIP) capitalizes on the successes of this well-proven technology, in order to engineer a processor that fulfills the five requirements for a quantum computer as outlined by David DiVincenzo. Electron and nuclear spins turn out to be nearly ideal qubits which can be manipulated through well-developed radio-frequency (rf) irradiation. The natural interactions (chemical screening, dipolar, indirect, and hyperfine) provide the quantum communication links between these qubits and have been well characterized. The amplitude of noise and imperfections are small and understood enough to realize proof-of-principle demonstrations of this technology for applications to quantum information science (QIS).

By now, many algorithms and other benchmarks have been implemented on liquid-state NMR QIPs, bringing theoretical ideas into the laboratory and enabling the quantitative evaluation of lacks in precision and imperfections of methods for achieving quantum control. In addition, manufacturers have begun work on improving commercially available spectrometers so as to facilitate these and future implementations of QIP.

While liquid-state NMR is expected to remain the most convenient experimental testbed for theoretical QIP advances for some time to come, its limitations (low polarization, limited numbers of resolvable qubits) have been thoroughly documented [4,5,6,7,8]. Its success has, however, also suggested several complementary new routes toward scalable devices, and contributed greatly to the drawing of this roadmap. Most of the new routes lead immediately into the realm of solid-state magnetic resonance, bringing NMR into closer contact with many of the other approaches to QIP now being pursued.

In solid-state NMR, the manipulation of large numbers of spins has already been amply demonstrated [9,10], e.g., by creating correlated states involving 100 or more spins, and with sufficiently precise control to follow their dynamics. This has enabled the first quantitative studies of decoherence as a function of the Hamming weight of the coherence. Solid-state NMR further permits the engineering of larger QIP devices [11] than is possible in the liquid state, because

1. polarizations of order unity have been achieved,
2. the interactions are stronger and hence two-qubit gates are faster,
3. the decoherence times are much longer, and
4. it is possible to implement resettable registers.

In the longer term, investigations will be undertaken to achieve single-spin detection, using force detection, algorithmic amplification and / or optical hyperfine interactions. By integrating the control learned in the liquid state with the polarization and longer decoherence times of the solid state, along with the detection efficiency provided by optics, a firm foundation on which to design engineered, spin-based, and scalable QIP devices can be built. It is anticipated that this experience will be combined with the engineering developments of the spintronic and solid-state proposals, as well as the knowledge on pure-state dynamics from optics and ion traps to provide a complete solution to building a quantum computer. Preliminary proposals for scalable implementations based on solid-state NMR have been suggested and are starting to be explored experimentally [12,13].

### 3.0 Summary of NMR QC: The DiVincenzo Criteria

**Note:** For the five DiVincenzo QC criteria and the two DiVincenzo QC networkability criteria (numbers six and seven in this section), the symbols used have the following meanings:

- a)  = a potentially viable approach has achieved sufficient proof of principle;
- b)  = a potentially viable approach has been proposed, but there has not been sufficient proof of principle; and
- c)  = no viable approach is known.

1. A scalable physical system with well-characterized qubits  (overall)
  - 1.1 Chemically distinct nuclear spins in liquid state; chemically, spatially, or crystallographically distinct nuclear spins in the solid state.   
(internal spin-dependent Hamiltonian is very well known)
  - 1.2 Scalability: liquid state is limited by chemistry and by low polarization. 
  - 1.3 Solid-state approaches based on spatially distributed spin ensembles as qubits have been proposed to be scalable. In the solid-state polarization near one is achievable via dynamic nuclear polarization. 
2. The ability to initialize the state of the qubits to a simple fiducial state 
  - 2.1 Pseudopure states in liquids
  - 2.2 Dynamic nuclear polarization in solids
  - 2.3 Optical nuclear polarization in solids
3. Long (relative) decoherence times, much longer than the gate-operation time 
  - 3.1 Liquid state:  $T_1 \gg 1 \text{ sec}$ ,  $T_2 \approx 1 \text{ sec}$ ,  $J \approx 10\text{--}200 \text{ Hz}$ ;
    - 3.1.1 For spin-1/2 nuclei, noise generators and their approximate spectral distributions are known.
  - 3.2 Solid state:  $T_1 \gg 1 \text{ min}$ ,  $T_2 \gg 1 \text{ sec}$ ,  $J \approx 100 \text{ Hz--}20 \text{ kHz}$ ;
    - 3.2.1  $T_1$  is typically limited by unpaired electrons in lattice defects
    - 3.2.2  $T_2$  is limited by all spin inhomogeneities (after refocussing of dephasing via dipolar couplings to like spins).
  - 3.3 The following means of controlling decoherence have been investigated:
    - 3.3.1 Quantum error correction;
    - 3.3.2 Decoherence-free subspaces (DFSs);
    - 3.3.3 Noiseless subsystems; and
    - 3.3.4 Geometric phase.
  - 3.4 Full-relaxation superoperators have been measured in a few cases.
4. A universal set of quantum gates 
  - 4.1 Single-qubit rotations depend on differences in chemical shifts.
  - 4.2 Multiple-qubit rotations rely on the bilinear coupling of spins (scalar or dipolar).
  - 4.3 Strongly modulated control sequences for up to four qubits have achieved experimental single-qubit gate fidelities  $F > 0.98$ .
  - 4.4 Full superoperator of complex control sequences have been measured in a few cases (including QFT [quantum Fourier transform] on three qubits).
  - 4.5 There are proposals for achieving fast gates through control of the hyperfine interaction modulated via optical cycling transitions (preliminary results have been obtained).
  - 4.6 Two encoded qubits have been created and controlled (for a simple collective noise model).

5. A qubit-specific measurement capability 
  - 5.1 Ensemble weak measurement, normally requiring  $>10^{14}$  spins at room temperatures.
  - 5.2 Ensemble measurement permits controlled decoherence to attenuate off diagonal terms in a preferred basis.
  - 5.3 Optically detected NMR has demonstrated the detection of the presence of single spins and there are proposals for detecting the state of single spins (none yet realized).

Presently there are no schemes for using NMR as part of a communication protocol.

6. The ability to interconvert stationary and flying qubits: **none** 
7. The ability to faithfully transmit flying qubits between specified locations: **none** 

## 4.0 What Has Been Accomplished

The accomplishments described in this section will be presented as a direct listing of the major highlights and against the benchmarking outline used in the other roadmap documents.

### 4.1 Highlights of the accomplishments of the NMR approach

1. Precise coherent and decoherent control
  - 1.1 Geometric phase gates
  - 1.2 Strongly modulating pulses
  - 1.3 Gradient-diffusion-induced decoherence
  - 1.4 Precise control methods in the presence of incoherent interactions
2. Control of decoherence
  - 2.1 DFSs
  - 2.2 Noiseless subsystems
  - 2.3 Quantum error correction (independent errors)
  - 2.4 Quantum error correction (correlated errors)
  - 2.5 Active control (decoupling)
  - 2.6 Concatenation of quantum error correction and active control
  - 2.7 Quantum simulation with decoherence
3. Benchmarking
  - 3.1 Entanglement dynamics (Bell; Greenberger, Horne, & Zeilinger [GHZ]; and extensions to seven qubits)
  - 3.2 Quantum teleportation and entanglement transfer
  - 3.3 Quantum eraser and disentanglement eraser
  - 3.4 Quantum simulation (harmonic oscillator/ driven harmonic oscillator)
  - 3.5 QFT and baker's map
  - 3.6 State, process, and decoherence tomography

4. Algorithms
  - 4.1 Deutsch-Joza
  - 4.2 Grover's algorithm
  - 4.3 Shor's algorithm and quantum counting
  - 4.4 Approximate quantum cloning
  - 4.5 Hogg's algorithm
  - 4.6 Teleportation

## 4.2 A long-term view

**Note:** For the status of the metrics of QC described in this section, the symbols used have the following meanings:

- a)  = sufficient experimental demonstration;
- b)  = preliminary experimental demonstration, but further experimental work is required; and
- c)  = no experimental demonstration.

1. Creation of a qubit
  - 1.1 Demonstrate preparation and readout of both qubit states. 
    - 1.1.1 Observation of both states, predates QIP (see Abragam [1]).
    - 1.1.2 Pseudo-pure state preparation.
      - gradient-based spatial average [14] ( $F \sim 0.99$  in reference [15])
      - temporal average [16] (no fidelities given in this paper)
      - effective [17], aka logically labeled [18] ( $F \sim 0.95$ ), aka conditional
      - conditional spatial average [19,20] ( $F \sim 0.95$ )
2. Single-qubit operations
  - 2.1 Demonstrate Rabi flops of a qubit. 
    - predates QIP (see Abragam [1])
  - 2.2 Demonstrate decoherence times much longer than Rabi oscillation period. 
    - predates QIP (see Abragam [1])
  - 2.3 Demonstrate control of both degrees of freedom on the Bloch sphere. 
    - predates QIP (see Ernst [3])
  - 2.4 Demonstrate precise qubit selective rotations. 
    - strong modulation methods [21] ( $F > 0.98$  for one-qubit gates)
    - selective transition methods [22] (numbers given in this paper imply  $F > 0.85$ )
  - 2.5 Demonstrate control robust to variations in the system Hamiltonian. 
    - composite pulses [23,24] (no fidelities given in these papers)
    - strong modulation [25] (one-qubit:  $F > 0.995$ ; two-qubit  $F > 0.986$ )
  - 2.6 Demonstrate control based on geometric phase [26] ( $F \sim 0.98$ ). 

3. Two-qubit operations
  - 3.1 Implement coherent two-qubit quantum logic operations. 
    - early example showing spinor behavior [27] (no fidelities given)
    - C-NOT and swap gates [28,29,30] (no fidelities given in these papers)
    - conditional Berry's phase [26] (other numbers in this paper imply  $F \sim 0.98$ )
  - 3.2 Produce and characterize Bell states. 
    - pseudo-pure to Bell state [31 & papers in #3.4 below] (no fidelities given in [31])  
**Note:** *While the pseudo-pure to Bell operation has high fidelity, the final state remains highly mixed.*
    - electron/nuclear spin Bell state [32] ( $F \sim 0.99$ )
    - in the solid state there is potential for creating nearly pure Bell states
  - 3.3 Demonstrate decoherence times much longer than two-qubit gate times. 
    - predates QIP (see references [2,3])
    - use of dipolar couplings in a liquid crystal phase to increase gate speed [33]
  - 3.4 Two-qubit examples of algorithms. 
    - quantum counting [34] (no fidelities given)
    - Deutsch-Josza [35,36] (no fidelities given), [37] ( $F \sim 0.99$ )
    - Grover [38] (no fidelities given)
    - Hogg [39] (other numbers in this paper imply  $F \sim 0.95$ )
  - 3.5 Demonstration of 1 logical qubit DFS [40] ( $F > 0.93$ ). 
  - 3.6 Demonstration of quantum error detection [41] (detailed error analysis but no clear overall fidelity given). 
4. Operations on 3–10 physical qubits
  - 4.1 Produce a GHZ-state of three physical qubits. 
    - pseudo-pure GHZ state [42,43] ( $F \cong 0.95$ ); note this  $F$  only tracks the deviation part of the density mat—the system remains highly mixed
  - 4.2 Produce maximally entangled states of four and more physical qubits. 
    - 7-spin cat state [44] ( $F \cong 0.73$ ); note this  $F$  only tracks the deviation part of the density matrix—the system remains highly mixed
  - 4.3 Quantum state and process tomography. 
    - state tomography [most papers cited herein] (errors estimated at 2%–5%)
    - quantum process tomography [45,46] (no rigorous error analysis available)
  - 4.4 Demonstrate decoherence-free subspace/system. 
    - one logical qubit subsystem for collective isotropic noise from three physical qubits [47] ( $F \cong 0.70$  for encoding, application of noise, & decoding)
  - 4.5 Demonstrate the transfer of quantum information (e.g. teleportation, entanglement swapping, multiple SWAP operations, etc.) between physical qubits. 

- teleportation [48] ( $F \sim 0.50$ )
  - entanglement swap [49] ( $F \approx 0.90$ )
  - quantum erasers [50] ( $F \sim 0.90$ ), [51] ( $F \sim 0.75$ )
- 4.6 Demonstrate quantum error correcting codes. 
- three-qubit code [52] ( $F \sim 0.80$ ), [53] ( $F \sim 0.98$ ), [15] ( $F \approx 0.99$ )
  - five-qubit code [54] ( $F \approx 0.75$ )
- 4.7 Demonstrate simple quantum algorithms (e.g., Deutsch-Josza) on three or more qubits. 
- quantum Fourier transform [55] ( $F \approx 0.80$  w/o swap, 0.52 with)
  - Shor's algorithm [56] (no fidelities reported)
  - quantum baker's map [57] ( $F \approx 0.76$  forward, 0.56 forward & back)
  - adiabatic quantum optimization algorithm [58] (fidelity not applicable)
- 4.8 Demonstrate quantum logic operations with fault-tolerant precision 
5. Operations on one logical qubit
- 5.1 Create a single logical qubit and "keep it alive" using repetitive error correction. 
- 5.2 Demonstrate fault-tolerant quantum control of a single logical qubit. 
6. Operations on two logical qubits
- 6.1 Implement two-logical-qubit operations [59]. 
- 6.2 Produce two-logical-qubit Bell states. 
- 6.3 Demonstrate fault-tolerant two-logical-qubit operations. 
- 6.4 Demonstrate simple quantum algorithms with two logical qubits. 
7. Operations on 3–10 logical qubits
- 7.1 Produce a GHZ-state of three logical qubits. 
- 7.2 Produce maximally entangled states of four and more logical qubits. 
- 7.3 Demonstrate the transfer of quantum information between logical qubits. 
- 7.4 Demonstrate simple quantum algorithms (e.g., Deutsch-Josza) with 3 or more logical qubits. 
- 7.5 Demonstrate fault-tolerant implementation of simple quantum algorithms with logical qubits. 

## 5.0 Considerations

1. Strengths
- 1.1 Very well characterized experimental system with proven ability to achieve arbitrary unitary dynamics in Hilbert spaces of at least seven qubits.
  - 1.2 Stable and precise instrumentation, most of which is commercially available.
  - 1.3 Convenient means of implementing a wide variety of decoherence models.
  - 1.4 Solid-state implementations have demonstrated coherent control over larger Hilbert spaces (of order 100 spins), but so far without a convenient mapping to qubits.

2. Unknowns, weaknesses
  - 2.1 Unknowns
    - 2.1.1 Spectral densities of noise generators (liquid state); ultimate causes of decoherence (solid state).
    - 2.1.2 Limitations on the number of qubits tied to frequency addressing of qubits based on the internal Hamiltonian.
    - 2.1.3 Single-spin detection.
  - 2.2 Weaknesses
    - 2.2.1 Use of the internal Hamiltonian (chemistry) to define qubits is not scalable (presumed limits are about 10 qubits in liquids and somewhat larger in the solid state).
    - 2.2.2 Clock speed, when using the internal Hamiltonian for gates, is extremely slow ( $< 1$  kHz in liquid state and somewhat larger in solids).
    - 2.2.3 Liquid-state polarization is very low ( $\sim 10^{-5}$ ), meaning all states are highly mixed and thus do not have unique microscopic interpretation.
    - 2.2.4 In the solid state, polarization  $> 0.9$  has been achieved, which is sufficient for Schumacher compression—if sufficient control is available.
    - 2.2.5 Single-spin detection and/or control has not been achieved (at least  $\sim 10^6$  nuclear spins are needed).
    - 2.2.6 There are a variety of single-spin proposals for the solid state, although this is an old problem that has been attacked for many years. I am not aware of any proposals for detecting single spins in the liquid state.
3. Goals 2002–2007
  - 3.1 Process tomography for gates, algorithms, and decoherence.
  - 3.2 Metrics for control, especially in large Hilbert spaces.
  - 3.3 Approach fault-tolerant threshold for single-gate errors.
  - 3.4 Demonstrate fault-tolerant gates on encoded qubits and decoherence-free subsystems.
  - 3.5 Obtain high polarization in the solid state for a system that can be conveniently mapped to qubits.
  - 3.6 Perform simple computations and prove attainment of quantum entanglement at high polarizations in the solid state.
  - 3.7 Combine quantum error correction with subsystem encoding.
  - 3.8 Explore quantum error-correction codes to second order.
  - 3.9 Prepare Bell states of two logical qubits.
4. Goals 2007–2012
  - 4.1 Transfer knowledge and experience for the liquid-state control techniques to solid-state and further improve the precision.
  - 4.2 Achieve single-nuclear-spin detection, measurement, and control (or know why it cannot be achieved).

- 4.3 Implement and control  $>10$  qubits in the solid state.
- 4.4 Create a GHZ state of three logical qubits.
- 4.5 Quantify the fidelity of entanglement transfer between logical qubits.
- 4.7 Develop optical means of coherently controlling the hyperfine interaction.
- 4.8 Explore spintronics (i.e., interfaces to electronic degrees of freedom).
5. Necessary achievements
  - 5.1 Learn to spatially address single spins (cf. 4.2), or
  - 5.2 Learn to create coherences among polarized spin ensembles.
6. Trophies
  - 6.1 Shor's algorithm [56]
  - 6.2 Bell's inequality violation in a true pure state
7. Connections to other technologies
  - 7.1 Methods and metrics of control developed for NMR will transfer to many other technologies.
  - 7.2 Understanding decoherence and the control of decoherence is fundamental to the entire field of QIP.
8. Subsidiary developments
  - 8.1
9. Role of theory
  - 9.1 Allows simulation of experiments on small systems (Hamiltonians are known with high precision).
  - 9.2 Complex theoretical models may be needed to describe real decoherence mechanisms.
  - 9.3 Achieving and benchmarking control in Hilbert spaces too large to simulate classically; it will require new theoretical techniques.
  - 9.4 Methods of control (trajectory planning, holonomic control, error correction, and decoherence-free subsystems) require sophisticated mathematics.
  - 9.5 New concepts are needed to understand complex dynamics.

## 6.0 Timeline



Figure 6-1. Nuclear magnetic resonance QC developmental timeline

## 7.0 Glossary

### Correlation

Cosine of the angle between two states.

### Fidelity

Magnitude of the projection of one state on another.

### Physical qubit

A system that has observables that behave as the Pauli matrices.

### Logical qubit

A combination of physical qubits that is more robust against a specific set of noise generators.

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