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13. ABSTRACT (Maximum 200 words)
We propose to use NMR as a testbed to develop general methods for solving computational problems on EQC's, to study the fundamental physics and computer science of these machines, and to learn how to make optimal use of the trade-offs that their unique capabilities permit us to make. Specifically, we intend to explore the critical issue of decoherence in a real quantum information processor, including its nature, its simulation, and methods of controlling it. The lessons thereby learned are expected to be broadly applicable throughout the field of quantum information processing, and particularly to proposed implementations based on solid-state NMR. Liquid-state NMR is thus an invaluable if not indispensable step in the field's efforts to bootstrap its way towards scalable quantum information processing.

The results obtained during the two years covered by this report (July 1, 2001 – June 30, 2003) fall into four principal classes:

- Development of methods for obtaining precise coherent control over nuclear spin systems with a well-characterized Hamiltonian and relaxation superoperator, and for quantifying the precision of such control.
- Validation of these methods by implementing simple quantum algorithms, communications protocols, and other quantum phenomena that make essential use of entangling unitary operations and/or measurements.
- Simulation of quantum systems using the unitary and nonunitary control operations that are available in liquid-state NMR spectroscopy.
- Reviews, commentary and educational articles.

We stress that although these studies utilized liquid-state NMR spectroscopy as a testbed for the development and validation of our techniques and simulations, the results will be directly applicable to a wide range of physical systems now being studied for quantum information processing purposes, once sufficient favorable ratios of gate operation to decoherence times have been obtained; indeed, control techniques and instrumentation originally developed for NMR quantum information processing have already been used in quantum information processors based on ion traps and superconductors.

In an **Appendix**, we discuss the role and future of NMR in quantum information processing.

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ENSEMBLE QUANTUM COMPUTING BY LIQUID-STATE NMR SPECTROSCOPY

FINAL PROGRESS REPORT

TIMOTHY F. HAVEL
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OCTOBER 21, 2003

U.S. ARMY RESEARCH OFFICE
DAAD19-01-1-0678

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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Statement of the Problem Studied:

It is by now widely accepted that macroscopic or "ensemble" analogue of a quantum information processor can be implemented using nuclear magnetic resonance (NMR) spectroscopy. We have in fact already implemented a number of prototypes by putting a liquid NMR sample into a *pseudo-pure state*, the behavior of which parallels that of an isolated quantum system. We have further implemented most of the basic logic gates of quantum computing on this device, and shown how to extract the results of simple calculations from the associated NMR spectra. Finally, we have demonstrated that these calculations can be performed on a macroscopic analogue of a coherent superposition, thus obtaining a form of implicit parallelism similar to that in quantum computing.

There are nonetheless some significant differences between a true quantum computer and an NMR computer. Instead of a random eigenvalue, an NMR spectrum of a pseudo-pure state yields the expectation values of certain observables relative to the corresponding "pseudo-spinor". These measurements are nonperturbing, so that *wave function collapse does not occur*. This has some clear-cut advantages, since much of the ingenuity that has gone into devising efficient algorithms for quantum computers has had to deal with extracting a deterministic (or highly probable) result from irreproducible measurements. The high-temperature systems that are accessible to liquid-state NMR nevertheless preclude the preparation of usable pseudo-pure states in systems containing more than about 10 qubits.

We propose to use NMR as a testbed to develop general methods for solving computational problems on EQC's, to study the fundamental physics and computer science of these machines, and to learn how to make optimal use of the trade-offs that their unique capabilities permit us to make. Specifically, we intend to explore the critical issue of decoherence in a real quantum information processor, including its nature, its simulation, and methods of controlling it. The lessons thereby learned are expected to be broadly applicable throughout the field of quantum information processing, and particularly to proposed implementations based on solid-state NMR. Liquid-state NMR is thus an invaluable if not indispensable step in the field's efforts to bootstrap its way towards scalable quantum information processing.

Summary of the Most Important Results:

The results obtained during the two years covered by this report (July 1, 2001 – June 30, 2003) fall into four principal classes:

I. Development of methods for obtaining precise coherent control over nuclear spin systems with a well-characterized Hamiltonian and relaxation superoperator, and for quantifying the precision of such control.

II. Validation of these methods by implementing simple quantum algorithms, communications protocols, and other quantum phenomena that make essential use of entangling unitary operations and/or measurements.

III. Simulation of quantum systems using the unitary and nonunitary control operations that are available in liquid-state NMR spectroscopy.

IV. Reviews, commentary and educational articles.

We stress that although these studies utilized liquid-state NMR spectroscopy as a testbed for the development and validation of our techniques and simulations, the results will be directly applicable to a wide range of physical systems now being studied for quantum information processing purposes, once sufficient favorable ratios of gate operation to decoherence times have been obtained; indeed, control techniques and instrumentation originally developed for NMR quantum information processing have already been used in quantum information processors based on ion traps and superconductors.

List of Publications:

We now list all the publications that we have produced in each of the above four categories during this grant, including their published abstracts:

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I. <u>Methods development</u>:

1. E. M. Fortunato, M. A. Pravia, N. Boulant, G. Teklemariam, T. F. Havel and D. G. Cory, “Design of strongly modulating pulses to implement precise effective Hamiltonians for quantum information processing,” *J. Chem. Phys.* (2002) **116:7599-606**.

> We describe a method for improving coherent control through the use of detailed knowledge of the system's Hamiltonian. Precise unitary transformations were obtained by strongly modulating the system's dynamics to average out unwanted evolution. With the aid of numerical search methods, pulsed irradiation schemes are obtained that perform accurate, arbitrary, selective gates on multi-qubit systems. Compared to low power selective pulses, which cannot average out all unwanted evolution, these pulses are substantially shorter in time, thereby reducing the effects of relaxation. Liquid-state NMR techniques on homonuclear spin systems are used to demonstrate the accuracy of these gates both in simulation and experiment. Simulations of the coherent evolution of a 3-qubit system show that the control sequences faithfully implement the unitary operations, typically yielding gate fidelities on the order of 0.999 and, for some sequences, up to 0.9997. The experimentally determined density matrices resulting from the application of different control sequences on a 3-spin system have overlaps of up to 0.99 with the expected states, confirming the quality of the experimental implementation.

2. E. M. Fortunato, L. Viola, J. Hodges, G. Teklemariam and D. G. Cory, “Implementation of universal control on a decoherence-free qubit,” *New J. Phys.* (2002) **4:5.1–20**.

> We demonstrate storage and manipulation of one qubit encoded into a decoherence-free subspace (DFS) of two nuclear spins using liquid state nuclear magnetic resonance techniques. The DFS is spanned by states that are unaffected by arbitrary collective phase noise. Encoding and decoding procedures reversibly map an arbitrary qubit state from a single data spin to the DFS and back. The implementation demonstrates the robustness of the DFS memory against engineered dephasing with arbitrary strength as well as a substantial increase in the amount of quantum information retained, relative to an un-encoded qubit, under both engineered and natural noise processes. In addition, a universal set of logical manipulations over the encoded qubit is also realized. Although intrinsic limitations prevent maintenance of full noise tolerance during quantum gates, we show how the use of dynamical control methods at the encoded level can ensure that computation is protected with finite distance. We demonstrate noise-tolerant control over a DFS qubit in the presence of engineered phase noise significantly stronger than observed from natural noise sources.

3. N. Boulant, M. A. Pravia, E. M. Fortunato, T. F. Havel and D. G. Cory, “Experimental concatentation of quantum error correction with decoupling,” *Quantum Information Processing* (2002) **1:135-44**.

> We experimentally explore the reduction of decoherence via concatenating quantum error correction (QEC) with decoupling in liquid-state NMR quantum information processing. Decoupling provides an effcient means of suppressing decoherence from noise sources with long correlation times, and then QEC can be used more profitably for the remaining noise sources.

4. T. F. Havel, "The real density matrix," *Quantum Information Processing* (2002) **1:511-38**.

We introduce a nonsymmetric real matrix which contains all the information that the usual Hermitian density matrix does, and which has exactly the same tensor product structure. The properties of this matrix are analyzed in detail in the case of multi-qubit (e.g.~spin $= 1/2$) systems, where the transformation between the real and Hermitian density matrices is given explicitly as an operator sum, and used to convert the essential equations of the density matrix formalism into the real domain.

5. T. F. Havel, "Procedures for converting among Kraus, Lindblad and matrix representations of quantum dynamical semigroups," *J. Math. Phys.* (2003) **44:534-57**.

Given a quantum dynamical semigroup expressed as an exponential superoperator acting on a space of *N*-dimensional density operators, eigenvalue methods are presented by which canonical Kraus and Lindblad operator sum representations can be computed. These methods provide a mathematical basis on which to develop novel algorithms for quantum process tomography --- the statistical estimation of superoperators and their generators --- from a wide variety of experimental data. Theoretical arguments and numerical simulations are presented which imply that these algorithms will be quite robust in the presence of random errors in the data.

6. N. Boulant, T. F. Havel, M. A. Pravia and D. G. Cory, "A robust method for estimating the Lindblad operators of a dissipative quantum process from measurements of the density operator at multiple time points" *Phys. Rev. A* (2003) **67:042322**.

We present a robust method for quantum process tomography, which yields a set of Lindblad operators that optimally fit the density operators measured at a sequence of time points. The benefits of this method are illustrated using a set of liquid-state nuclear magnetic resonance measurements on a molecule containing two coupled hydrogen nuclei, which are sufficient to fully determine its relaxation superoperator. It was found that the complete positivity constraint, which is necessary for the existence of the Lindblad operators, was also essential for obtaining a *robust* fit to the measurements. The general approach taken here promises to be broadly useful in studying dissipative quantum processes in many of the diverse experimental systems currently being developed for quantum information processing purposes.

7. M. A. Pravia, N. Boulant, J. Emerson, E. M. Fortunato, T. F. Havel, D. G. Cory and A. Farid, "Robust unitary control in the presence of incoherent processes" *J. Chem. Phys.* (2003) **119**, in press.

Errors in the control of quantum systems may be classified as unitary, decoherent and incoherent. Unitary errors are systematic, and result in a density matrix that differs from the desired one by a unitary operation. Decoherent errors correspond to general completely positive superoperators, and can only be corrected using methods such as quantum error correction. Incoherent errors can also be described, on average, by completely positive superoperators, but can nevertheless be corrected by the application of a locally unitary operation that "refocuses" them. They are due to reproducible spatial or temporal variations in the system's Hamiltonian, so that information on the variations is encoded in the system's spatiotemporal state and can be used to correct them. In this paper liquid-state nuclear magnetic resonance (NMR) is used to demonstrate that such refocusing effects can be built directly into the control fields, where the incoherence arises from spatial inhomogeneities in the quantizing static magnetic field as well as the radio-frequency control fields themselves. Using perturbation theory, it is further shown that the eigenvalue spectrum of the completely positive superoperator exhibits a characteristic spread that contains information on the Hamiltonians' underlying distribution.

II. Methods validation:

1. G. Teklemariam, E. M. Fortunato, M. A. Pravia, T. F. Havel and D. G. Cory, "An NMR analog of the quantum disentanglement eraser," *Phys. Rev. Lett.* (2001) **86:5845–9**.

We report the implementation of a 3-spin quantum disentanglement eraser on a liquid-state NMR quantum information processor. A key feature of this experiment was its use of pulsed magnetic field gradients to mimic projective measurements. This ability is an important step towards the development of an experimentally controllable system which can simulate any quantum dynamics, both coherent and decoherent.

2. G. Teklemariam, E. M. Fortunato, M. A. Pravia, Y. Sharf, T. F. Havel, D. G. Cory, A. Bhattaharyya and J. Hou, "Quantum erasers and probing classifications of entanglement via NMR," *Phys. Rev. A* (2002) **66:012309**.

We report the implementation of two- and three-spin quantum erasers using nuclear magnetic resonance (NMR). Quantum erasers provide a means of manipulating quantum entanglement, an important resource for quantum information processing. Here, we first use a two-spin system to illustrate the essential features of quantum erasers. The extension to a three-spin ''disentanglement eraser'' shows that entanglement in a subensemble can be recovered if a proper measurement of the ancillary system is carried out. Finally, we use the same pair of orthogonal decoherent operations used in quantum erasers to probe the two classes of entanglement in tripartite quantum systems: the Greenberger-Horne-Zeilinger state and the W state. A detailed presentation is given of the experimental decoherent control methods that emulate the loss of phase information in strong measurements, and the use of NMR decoupling techniques to implement partial trace operations.

3. L. Viola, E. M. Fortunato, M. A. Pravia, E. Knill, R. Laflamme and D. G. Cory, "Experimental realization of noiseless subsystems for quantum information processing," *Science* (2001) **293:2059–63**.

We demonstrate storage and manipulation of one qubit encoded into a decoherence-free subspace (DFS) of two nuclear spins using liquid state nuclear magnetic resonance techniques. The DFS is spanned by states that are unaffected by arbitrary collective phase noise. Encoding and decoding procedures reversibly map an arbitrary qubit state from a single data spin to the DFS and back. The implementation demonstrates the robustness of the DFS memory against engineered dephasing with arbitrary strength as well as a substantial increase in the amount of quantum information retained, relative to an un-encoded qubit, under both engineered and natural noise processes. In addition, a universal set of logical manipulations over the encoded qubit is also realized. Although intrinsic limitations prevent maintenance of full noise tolerance during quantum gates, we show how the use of dynamical control methods at the encoded level can ensure that computation is protected with finite distance. We demonstrate noise-tolerant control over a DFS qubit in the presence of engineered phase noise significantly stronger than observed from natural noise sources.

4. E. M. Fortunato, L. Viola, M. A. Pravia, E. Knill, R. Laflamme, T. F. Havel and D. G. Cory, "Exploring noiseless subsystems via nuclear magnetic resonance," *Phys. Rev. A* (2003) **67:062303**.

> Noiseless subsystems offer a general and efficient method for protecting quantum information in the presence of noise that has symmetry properties. A paradigmatic class of error models displaying nontrivial symmetries emerges under collective noise behavior, which implies a permutationally invariant interaction between the system and the environment. We expand our previous investigation of the noiseless subsystem idea by reporting and analyzing NMR experiments that demonstrate the preservation of a qubit encoded in a three-qubit noiseless subsystem for general collective noise. A complete set of input states is used to determine the superoperator for the implemented one-qubit process and to confirm that the fidelity of entanglement is improved for a large, noncommutative set of engineered errors. To date, this is the largest set of error operators that has been successfully corrected for by any quantum code.

5. N. Boulant, E. M. Fortunato, M. A. Pravia, G. Teklemariam, D. G. Cory and T. F. Havel, "Entanglement transfer experiment in NMR quantum information processing," *Phys. Rev. A* (2002) **65:024302**.

> We report the implementation of an entanglement transfer on a four-qubit liquid-state NMR quantum information processor. This consists of creating an ~pseudopure! entangled state among two directly coupled spins, and then transferring this two-spin state to another pair of spins whose direct interactions are negligible. Such transfers are expected to be an essential operation in scalable quantum computer architectures, and provide a useful benchmark for the coherent control available in specific implementations.

6. N. Boulant, K. Edmonds, J. Yang, M. A. Pravia and D. G. Cory, "Experimental demonstration of an entanglement swapping operation and improved control in NMR quantum information processing" *Phys. Rev. A* (2003) **68:032305**.

> We demonstrate the implementation of an entanglement swapping operation on a four-qubit liquid-state nuclear-magnetic-resonance ~NMR! quantum-information processor. We use this experiment as a benchmark to illustrate the progress made in the field of quantum control using strongly modulating pulses and a correction scheme for removing distortions introduced by the nonlinearities in the transmitter and probe circuits. The advances include compensating for incoherent errors caused by the spatial variation of the system Hamiltonian in the NMR sample. The goal of these control sequences is to cause the collapse of the Kraus operator-sum representation of the superoperator into one unitary operator so that the ensemble appears to evolve as one coherent whole.

7. Y. Weinstein, S. Lloyd, J. Emerson and D. G. Cory, "Experimental implementation of the quantum baker's map," *Phys. Rev. Lett* (2002) **89:157902**.

> This Letter reports on the experimental implementation of the quantum baker's map via a three bit nuclear magnetic resonance quantum information processor. The experiments tested the sensitivity of the quantum chaotic map to perturbations. In the first experiment, the map was iterated forward and then backward to provide benchmarks for intrinsic errors and decoherence. In the second set of experiments, the least significant qubit was perturbed in between the iterations to test the sensitivity of the quantum chaotic map to controlled perturbations. These experiments can be used to investigate existing theoretical predictions for quantum chaotic dynamics.

III. <u>Simulation protcols</u>:

1. T. F. Havel, Y. Sharf, L. Viola and D. G. Cory, “Hadamard products of product operators and the design of gradient-diffusion experiments for simulating decohrence by NMR spectroscopy,” *Phys. Lett. A* (2001) **280:282–8**.

An extension of the product operator formalism of NMR is introduced, which uses the Hadamard matrix product to describe many simple spin 1/2 relaxation processes. The utility of this formalism is illustrated by deriving NMR gradient-diffusion experiments to simulate several decoherence models of interest in quantum information processing, along with their Lindblad and Kraus representations.

2. G. Teklemariam, E. M. Fortunato, M. A. Pravia, T. F. Havel and D. G. Cory, “Experimental investigations of decoherence on a quantum information processor”, *Chaos, Solitons and Fractals* (2002) **16:457–65**.

The process of quantum decoherence has two distinct steps. Initially, the system of interest gets entangled to a quantum apparatus. In the second stage of this process, the interference (or coherence) term of this joint state of the system and apparatus decays to zero with time. The state of the system is now in a classical, statistical mixture of possible outcomes. Here we investigate these aspects of the decoherence program through the study of discrete decoherence maps. An example of a system that undergoes a discrete decoherent evolution is one where a system S, prepared in a superposition state, gets entangled to a measuring apparatus M, by a CNOT interaction. Subsequently, the system density matrix can be recovered by a partial trace over the measuring apparatus M, resulting in a mixed state for the system S. Thus, the system will have undergone non-unitary dynamics. With this example in mind, we experimentally investigate the following questions:

(1) How does the system S behave under measurements and partial traces of the apparatus M?

(2) Under different entangling interactions, how much of its quantum nature does the system S retain following measurements, or partial traces of the apparatus M?

Our focus is the practical considerations of physically realizable decoherence maps to understand the stability of quantum information in realistic settings.

3. G. Teklemariam, E. M. Fortunato, C. C. Lòpez, J. Emerson, J.-P. Paz, T. F. Havel and D. G. Cory, “Method for modeling decoherence on a quantum information processor”, *Phys. Rev. A* (2003) **67:062316**.

We develop and implement a method for modeling decoherence processes on an N-dimensional quantum system that requires only an N2-dimensional quantum environment and random classical fields. This model offers the advantage that it may be implemented on small quantum-information processors in order to explore the intermediate regime between semiclassical and fully quantum models. We consider in particular sz sz system-environment couplings which induce coherence ~phase! damping, although the model is directly extendable to other coupling Hamiltonians. Effective, irreversible phase damping of the system is obtained by applying an additional stochastic Hamiltonian on the environment alone, periodically redressing it and thereby irreversibliy randomizing the system phase information that has leaked into the environment as a result of the coupling. This model is exactly solvable in the case of phase damping, and we use this solution to describe the model’s behavior in some limiting cases. In the limit of small stochastic phase kicks the system’s coherence decays exponentially at a rate that increases linearly with the kick frequency. In the case of strong kicks we observe an effective decoupling of the system from the environment. We present a detailed implementation of the method on a nuclear magnetic resonance quantum-information processor.

IV. Reviews, commentary and educational articles:

1. T. F. Havel, C. J. L. Doran, "Interaction and entanglement in the multiparticle spacetime algebra," in Applications of Geometric Algebra in Computer Science and Engineering, (L. Dorst, C. J. L. Doran and J. Lasenby, eds.), Birkhauser (2001).

The multiparticle spacetime algebra (MSTA) is an extension of Dirac theory to a multiparticle setting, which was first studied by Doran, Gull and Lasenby. The geometric interpretation of this algebra, which it inherits from its one-particle factors, possesses a number of physically compelling features, including simple derivations of the Pauli exclusion principle and other nonlocal effects in quantum physics. Of particular importance here is the fact that all the operations needed in the quantum (statistical) mechanics of spin 1/2 particles can be carried out in the "even subalgebra" of the MSTA. This enables us to "lift" existing results in quantum information theory regarding entanglement, decoherence and the quantum / classical transition to space-time. The full power of the MSTA and its geometric interpretation can then be used to obtain new insights into these foundational issues in quantum theory. A system of spin 1/2 particles located at fixed positions in space, and interacting with an external magnetic field and/or with one another via their intrinsic magnetic dipoles, provides a simple paradigm for the study of these issues. This paradigm can further be easily realized and studied in the laboratory by nuclear magnetic resonance spectroscopy.

2. T. F. Havel, D. G. Cory, S. Lloyd, N. Boulant, E. M. Fortunato, M. A. Pravia, G. Teklemariam, Y. S. Weinstein, A. Bhattacharyya and J. Hou, "Quantum information processing by nuclear magnetic resonance spectroscopy," *Am. J. Phys.* (2002) **70:345–61**.

Nuclear magnetic resonance (NMR) is a direct macroscopic manifestation of the quantum mechanics of the intrinsic angular momentum of atomic nuclei. It is best known for its extraordinary range of applications, which include molecular structure determination, medical imaging, and measurements of flow and diffusion rates. Most recently, liquid-state NMR spectroscopy has been found to provide a powerful experimental tool for the development and evaluation of the coherent control techniques needed for quantum information processing. This burgeoning new interdisciplinary field has the potential to achieve cryptographic, communications and computational feats far beyond what is possible with known classical physics. Indeed, NMR has made the demonstration of many of these feats sufficiently simple to be carried out by high school summer interns working in our laboratory (see last two authors). In this paper the basic principles of quantum information processing by NMR spectroscopy are described, along with several illustrative experiments suitable for incorporation into an undergraduate physics curriculum. These experiments are spin-spin interferometry, an implementation of the quantum Fourier transform, and the quantum simulation of a harmonic oscillator.

3. R. Laflamme, D. Cory, C. Negrevergne and L. Viola, "NMR quantum information processing and entanglement", *Quantum Inform. Processing and Comput.* (2002) **2:166–76**.

In this essay we discuss the issue of quantum information and recent nuclear magnetic resonance (NMR) experiments. We explain why these experiments should be regarded as quantum information processing (QIP) despite the fact that, in present liquid state NMR experiments, no entanglement is found. We comment on how these experiments contribute to the future of QIP and include a brief discussion on the origin of the power of quantum computers.

Reportable Inventions: NONE

Participating Scientific Personell (and Degrees Earned on this Project):

- David G. Cory, Principal Investigator (Nuclear Engineering, MIT)
- Timothy F. Havel, co-Principle Investigator (Nuclear Engineering, MIT)
- Seth Lloyd, collaborator (Mechanical Engineering, MIT)
- Lorenza Viola, Los Alamos Postodoctoral Fellow (now at Dartmouth University)
- Juan-Pablo Paz, Los Alamos Visiting Scientist (University of Buenos Aires)
- Emanuel Knill, Los Alamos Staff Scientist (now at NIST, Boulder)
- Raymond Laflamme, Los Alamos Staff Scientist (now at the Perimeter Institute, CANADA)
- Joseph Emerson, Postdoctoral Fellow (now at the Perimeter Institute, CANADA)
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APPENDIX: The Role and Future of NMR in Quantum Information Processing

NMR has without a doubt carried out the most diverse set of experiments in the largest Hilbert spaces and with precision unequalled in the exploration of QIP. It is also the implementation where we know best the internal Hamiltonian and how to control it. We even know most of the sources of errors and of decoherence, and we can simulate the dynamics in small Hilbert spaces precisely. NMR is broadly seen as the most useful testbed of QIP today.

There is however great confusion over the future role of NMR in both QIP and QC. Here we would like to clear up some of these misconceptions.

First let us define NMR, nuclear magnetic resonance. NMR concerns the observation and dynamics of nuclear spins in high magnetic fields, in which detection is via a resonant coupling of the detection apparatus to the magnetic field of the nuclear spin(s). Thus NMR is carried out in all phases (gas, liquid and solid), involves both the observation of individual spins and ensembles of spins, and includes inductive, capacitive, optical and mechanical couplings of the detector to the spin. So in addition to the commonly known approaches to NMR, mechanical force detection and optically detected NMR are also included in the field. However, non-resonant detection is generally not included.

Nuclear spins evolve under the laws of quantum mechanics. It is strange to have to defend this since systems with finite numbers of energy levels are one of the archetype quantum systems. The confusion arose from an incorrect reading of the publications from Carl Caves group (see the following description on entanglement). There are no known classical theories that correctly predict the dynamics of nuclear spins in full generality, or even in liquid-state NMR experiments.

One can not uniquely prove entanglement in a highly mixed system. This is a common problem in QIP, that a mixed density matrix permits multiple microscopic interpretations and there is no unbiased reason to select a particular one. Thus when the purity of the system is below a threshold there will exist microscopic interpretations that do not involve entanglement (regardless of the form of the traceless part of the density matrix). Below this threshold (given in Caves work) we do not know how to use ensemble average measurements to prove things like Bell's inequality. That entanglement can not be proven to exist in a highly mixed system says nothing about the underlying dynamics. It is merely a statement about the statistic of measurements on a single state and has no direct bearing on how one computes through a sequence of states.

The density matrix of liquid state NMR is highly mixed. Liquid state NMR is necessarily carried out at high temperatures relative to the Zeeman energy splitting of nuclear spins in realistic magnetic fields ($\leq$ 20T). At 20T and for 1H's the ratio of $DE/kT = 1$ at $T \sim 20$ mK, and at room temperature $DE/kT \sim 10^{-5}$. While there are means of increasing the polarization of the nuclear spins in liquids beyond that at thermal equilibrium, significant purity ($> 10^{-3}$) has never been achieved.

For selected systems in gas and solid state high purity (~ 1) nuclear spin ensembles are relatively easy to achieve and have been robustly observed by many laboratories. In the gas phase optical pumping is possible and in the solid state at low temperatures electron spin polarization can be transferred to nuclear spins.

Using well controlled non-unitary dynamics we can extract a portion of a mixed ensemble that is isomorphic to a pure state, which we have named a pseudo-pure state. The use of pseudo-pure states is a convenience in investigating the quantum dynamics of pure states using mixed systems. The use of pseudo-pure states does not scale, since for a system of constant polarization the amplitude of the pseudo-pure state decreases exponentially with the number of qubits.

The question of scalability does not depend on purity. As shown by Schulman and Vazirani, any finite, constant purity, ensemble of quantum processors can be made pure if there are sufficient (but polynomial) numbers of qubits in each quantum processor, and if the control of the processors is at the fault tolerant limit. The reason that liquid-state NMR is not scalable is that we do not know how to add sufficient numbers of qubits while retaining a high fidelity of coherent control.

There are proposals for scalable spin-based implementations of a QC in the solid state. These are based on defects in simple solids or using an ensemble of dipolarly coupled spins as a qubit. Experimental studies of these ideas is just starting and the proposals have yet to show that there is a proven, viable approach to QC. However, given the long history of coherent control over nuclear spins these are attractive options.