Precise Control of Quantum Information

by

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Abstract

Theoretical discoveries in the nascent field of quantum information processing hold
great promise, suggesting the means for increased computational power and uncon-
ditionally secure communications. To achieve these advances in practice, however,
quantum information must be stored and manipulated with high fidelity. Here, we
describe how quantum information stored in a nuclear spin system can be controlled
accurately. We describe a method creating strongly-modulating single-spin gates that
faithfully produce the desired unitary transformations. The simulated fidelity of the
best gate (under ideal conditions) reaches close to 0.99999, a value close to estimates
of the fault-tolerant threshold. In addition, we show how knowledge of experimental
errors can be used correct or compensate the gates. The experimental demonstration
of these methods yields estimated single-spin and coupling gate fidelities close to 0.99.

The methods are applicable to a variety of experimental studies in quantum in-
formation processing. We used the gates to implement strategies for combating deco-
herence, including the realization of a noiseless subsystem and the concatenation
of quantum error correction with dynamical decoupling. The gates were also used
to demonstrate the quantum Fourier transform, the disentanglement eraser, and an
entanglement swap.

Finally, we describe a nuclear magnetic resonance (NMR) implementation of a
quantum lattice gas (QLG) algorithm. Recently, it has been suggested that an array
of small quantum information processors sharing classical information can be used to
solve selected computational problems. The concrete implementation demonstrated
here solves the diffusion equation, and it provides a test example from which to
probe the strengths and limitations of this new computation paradigm. The NMR
experiment consists of encoding a mass density onto an array of 16 two-qubit quantum
information processors and then following the computation through 7 time steps of the
algorithm. The results show good agreement with the analytic solution for diffusive
dynamics.

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Dedicado a Chayito, Papi, Mima y Mi Tata
Contents

1 Introduction 19

2 Quantum Control 21
  2.1 Metrics of Control  22
  2.2 Designing Gates for Controlling Quantum Information  25
    2.2.1 NMR Spin System  25
    2.2.2 Numerical Search Method  26
    2.2.3 Gate Simulations  28
    2.2.4 Exploring Achievable Fidelities  32
  2.3 Correcting for Experimental Errors  33
    2.3.1 RF Waveform Feedback Correction  33
    2.3.2 Robustness Against RF Inhomogeneity  36
  2.4 Experimental Demonstrations  38
  2.5 Conclusion  42

3 Applications 43
  3.1 Disentanglement Eraser  43
  3.2 Quantum Fourier Transform  50
  3.3 Entanglement Swap  55
  3.4 Noiseless Subsystem  60
  3.5 Quantum Error Correction with Dynamical Decoupling  69

4 Quantum Lattice Gas Computation 77
  4.1 Lattice Gas Algorithms  78
  4.2 Solving the 1-D Diffusion Equation  79
  4.3 NMR Implementation  83
    4.3.1 Spin System and Control  83
    4.3.2 Lattice Initialization  85
    4.3.3 Collision and Swap Gates  87
    4.3.4 Measurement  89
    4.3.5 Streaming  89
  4.4 Results and Discussion  90
  4.5 Conclusion  91
List of Figures

2-1 Molecular structure and Hamiltonian parameters for alanine and crotonic acid. The chemical shift of each carbon nucleus is given in the corresponding diagonal element while the coupling strengths are given by the off-diagonal values. All values are in Hertz, and they were measured in a 300 MHz (≈7 T) magnet. ........................................ 26

2-2 Ideal RF waveform for two example pulses. The solid (dashed) line is the amplitude (phase) of the waveform. Changes in the transmitter frequency (within a single period) were implemented by a discrete linear phase ramp. The sharp discontinuities occur at the transitions between periods. Substantial filtering of these high frequency components (smoothing of the shape) has little effect on the gate fidelity. In order to experimentally implement the pulse, it is converted into a discrete series of amplitudes and phases (order 1K long) by sampling the ideal waveform at a constant rate. Details of the pulse parameters (as per Eq. (2.24)) are listed below each waveform. Due to experimental implementation issues, a 6μs period with zero RF power (i.e., $H_{ext} = 0$) is needed before and after the pulse and must be included to produce the desired propagator. ........................................ 30

2-3 Gate fidelity vs. variations in experimental parameters. The experimental parameters were varied over the range of expected errors, demonstrating that both the alanine and crotonic acid pulses are most sensitive to RF amplitude. ........................................ 30

2-4 Gate fidelity vs. spin frequency. The gate fidelities of two example pulses were calculated as a function of the resonance frequency of a test spin. The frequency was varied in the range of chemical shifts of the molecules. The solid (dashed) line is calculated with identity (desired transformation) as the theoretical transformation. The vertical dotted lines denote the actual chemical shifts for each spin. As can be seen, the gate only works when the test spin is at the appropriate resonance frequency. ........................................ 31
2-5 **Exploration of achievable fidelities.** The plot shows the maximum fidelities found for a $\pi/2^{1/2}$ alanine pulse as allowed RF power and magnetic field strengths were varied. The three lines correspond to the magnetic field strengths explored, as denoted by the legend. The dotted vertical lines mark the point of the minimum chemical shift difference at each of the three field strengths. Using ideal experimental control in a 800 MHz magnet, a single-spin gate fidelity reaching 0.99999 is potentially realizable.

2-6 **Feedback loop for correcting experimental RF waveforms.** Distorted signals arriving at the carbon coil are detected and digitized through the proton coil. The difference between the measured RF wave and the desired wave is then calculated, resulting in a fixed wave that is then retransmitted to the coil. The loop continues until the shape of the fixed wave produces the desired signal at the carbon coil.

2-7 **Improvement of errors in digitized RF waveforms.** The errors from a test sample of 25 waveforms are plotted here as a function of the feedback loop iteration number. The errors are the mean absolute differences between fits to the digitized waveform and the ideal waveform. Four to six iterations were typically sufficient to improve the RF shape.

2-8 **Distorted and corrected RF amplitude.** The dots denote the digitized values of the distorted and corrected amplitudes. The solid gray lines show the ideal pulse amplitudes. The pulse sequence shown here contains two back-to-back gates separated by a delay of 12 $\mu$s. The high frequency transients present at the transitions between periods have little effect on the overall performance of the gates.

2-9 **Simulations of normal and robust pulses as a function of RF strengths and RF distribution widths.** The dashed lines correspond to robust pulses, while the solid gray lines denote uncompensated pulses. The dotted line overlaid on the left plot shows a fit to the measured RF inhomogeneity profile. This information was utilized in the pulse parameter search to determine pulses robust against it. The left plot shows how the robust pulses maintain high fidelities even when the RF strength is scaled from the ideal value. The plot on the right simulates the same pulses as a function of the scaled width of the RF inhomogeneity profile. These results demonstrate the improved fidelity of the robust pulses for all but the narrowest RF distributions. At the small widths, the RF profile would no longer be inhomogeneous, eliminating the need for the robust gates.
2-10 Sample spectra resulting from gates. The plots show spectra resulting from different sequences of pulses applied to the thermal equilibrium density matrix \( \rho_{\text{thermal}} = I_z^1 + I_y^2 + I_z^3 \). All sequences are read from left to right. The reference spectra, resulting from a \( \frac{\pi}{2} \) pulse applied to all 3 carbons, is shown in grey. Although the chemical shift is order 1/\( \tau \), no significant phase evolution is seen. Selective coupling sequences are also demonstrated.

3-1 Logic network for the disentanglement eraser. Initially, a pseudo-pure state on spins 1, 2 and 3 is created, \( \rho_{\text{ini}} = |000\rangle\langle000| \equiv E_+^1 E_+^2 E_+^3 \). A \( \frac{\pi}{2} \) \( y \)-pulse is then applied to spin 2, followed by two controlled-not (c-NOT) gates to create the GHZ state (see text). Conditionality on the second spin being in the \( |1\rangle \) state is represented in the network by a filled circle on its time line. Finally, the two complementary measurements, \( \sigma_z^1 \) and \( \sigma_y^1 \), are applied to spin 1. State tomography was performed to fully reconstruct the density matrices at the positions indicated.

3-2 Disentanglement eraser experimental density matrices. The rows are enumerated in the standard computational basis, where for example 000 represents the state label \( |000\rangle \). Although not shown, the columns are similarly labeled with the leftmost end representing \( |000\rangle \) and the rightmost end representing \( |111\rangle \). \( \rho_{\text{ini}} \) is the three-spin pseudo-pure ground state, and \( \rho_{\text{GHZ}} \) is the pseudo-pure GHZ state. The last two plots are \( \rho_z \), which is \( \rho_{\text{GHZ}} \) after decohering spin 1 about the \( z \)-axis, and \( \rho_x \), which is after decohering it about the \( x \)-axis. (Note: \( \rho_{\text{GHZ}}, \rho_z \) and \( \rho_x \) have been magnified by a factor of two for clarity). An amount of identity, chosen to optimize the input projection, was added to all experimentally measured density matrices.

3-3 QFT input state. The plot shows the real part of the QFT input density matrix. This state, created by Hadamards on the first and second bit after the three bits were put into a pseudo-pure state, is a superposition of \( |000\rangle + |010\rangle + |100\rangle + |110\rangle \) states. Note that the input state has a periodicity of \( r = 2 \).

3-4 Output of QFT minus the swap gate. The plot shows the real part of the density matrix after implementation of the QFT without the final swap gate. The attenuated correlation is 0.78.

3-5 Output of QFT The plot shows the real part of the density matrix after the implementation of the complete QFT. Notice there is now a periodicity of \( q/r = 4 \) in the density matrix. This shows that the QFT extracted the periodicity of the input state. The attenuated correlation is 0.61.
3-6 **Logic network for the entanglement transfer experiment.** The four spins are represented by the four horizontal control lines, where each line is labeled on the left by the input state superscripted by the spin's index (where "1" indicates that the spin is depolarized and $E_+$ indicates that it was part of the pseudo-pure state). The pseudo-pure ground state on spins 2 and 3, $\rho^{23}_{pp} \leftrightarrow |00\rangle \langle 00|$, is converted by an entanglement operation on the same spins to obtain $\rho^{23}_{Ent} \leftrightarrow (|00\rangle + |11\rangle)(|00\rangle + |11\rangle)$. This state is then transferred to spins 1 and 4 by using swap gates.

3-7 **Reconstructed density matrices showing entanglement transfer.** From left to right are shown the real part of the reconstructed density matrices of the initial pseudo-pure $\rho^{23}_{pp}$, spins 2&3 entangled $\rho^{23}_{Ent}$ and spins 1&4 entangled $\rho^{41}_{Ent}$ (in normalized units). The bottom row of density matrices is obtained from the top row after having traced over the two ancilla spins. The rows and columns represent the standard computational basis in binary order, with $|0000\rangle$ starting on the leftmost column and $|1111\rangle$ being the rightmost column.

3-8 **Logical quantum network for the NS experiment.** The information is initially stored in qubit 3, while qubits 1 and 2 are initialized in the state $|0\rangle$. A unitary encoding transformation $U_{enc}$ is applied to map the initial input state space into the NS $|1\rangle$. A time delay follows, during which the qubits are stored in the NS memory. Applying the unitary transformation $U_{dec}$ returns the information to the state of carbon 2. Encoding and decoding networks are expressed in terms of controlled rotations. $U_{enc}$ is a simplified version of $U_{dec}^{-1}$ obtained by exploiting the knowledge of the initial non-data bits. For $|\psi_{in}\rangle = \alpha|0\rangle + \beta|1\rangle$ with arbitrary complex $\alpha, \beta, |\alpha|^2 + |\beta|^2 = 1$, $U_{enc}$ implements a transformation $U_{enc}(|0\rangle_1 \otimes |0\rangle_2 \otimes |\psi_{in}\rangle_3) = |\psi_{in}\rangle_1 \otimes |1/2\rangle_z$. A collective noise process $\mathcal{E}_{coll} = \{E_a\}$ only affects the Z subsystem. $U_{dec}$ decodes a generic noisy state $E_a(|\psi_{in}\rangle_L \otimes |1/2\rangle_z)$ in $\mathcal{H}_{1/2}$ to the computational basis, $U_{dec}[(\alpha|0\rangle_L + \beta|1\rangle_L) \otimes (c_a - 1/2)_z + d_a(1/2)_z)] = \alpha c_a|000\rangle + \beta c_a|010\rangle + \alpha d_a|001\rangle + \beta d_a|011\rangle$ for appropriate coefficients. This produces the intended state of qubit 2 upon discarding spins 1 and 3 i.e., $\text{Tr}_{1,3}\{U_{dec}[E_{coll}(|\psi_{in}\rangle_L \otimes |1/2\rangle_z \langle -1/2\rangle_z)]U_{dec}^\dagger\} = |\psi_{in}\rangle_2 \langle \psi_{in}|$.  

---

14
Experimentally determined entanglement fidelities for the de-coherent implementation of single-axis collective error models. We used a diffusion time $\Delta t \sim 34$ ms and gradient times $\delta \sim 5$ ms, giving a fixed $t_{ev} = 2\delta + \Delta t \sim 44$ ms. Variable-strength collective noise along either the $y$ axis (NS-encoded (squares) and un-encoded data (triangles)) or the $z$ axis (NS-encoded data only (circles)) was applied during $t_{ev}$. The decay of the un-encoded spin, $C_3$, was measured by turning off the NS-encoding and decoding sequences. Both the un-encoded and encoded data are fit to an exponential decay, with the interpolated (solid) and extrapolated (dashed) lines shown in the plot. Best estimates and uncertainties of the parameters are also given. The relatively large error bars of the data arise from a conservative estimate of the uncertainties associated with the noise strength determination.

Alanine spins as system and environment. The carbons represent the system and the protons the environment. In the array, the diagonals contain the corresponding chemical shifts, while the other terms are the coupling constants between the spins. All values are listed in Hz.

Logic network for the concatenation code. Note that the protons are included in the network but no operation is applied on them since an environment is by definition inaccessible.

Scheme for implementing the noise operator. The whole sequence is split into 3 equal parts of duration $T$. For each period, one qubit evolves with the protons under the scalar coupling term but also under the chemical shift term of the internal Hamiltonian. Each block represents a selective $\pi$ pulse about the X or Y axis while the three last pulses are individual Z rotation pulses to refocus the chemical shift evolution mentioned above.

Short time information loss. The plots show the entanglement fidelity as a function of the evolution time (from 1 up to 15ms) with and without decoupling, but with QEC in both cases. In the absence of decoupling, the coherent scalar coupling between the proton "environment" and carbon qubits introduces the observed oscillation.

Long time information loss. The plot shows the entanglement fidelity with respect to the evolution time (20 time points equally spaced from 20ms) between the carbons and the protons with the decoupling scheme, with and without QEC. For the sake of clarity, the last plot shows the two fitted curves.
4-1 **Quantum lattice gas algorithm** for solving the 1-D diffusion equation. The algorithm employs $N$ two-qubit sites to encode the discretized mass density. Each site codes for a single value of the mass density using the quantum state of the two qubits. The encoded information is subjected to a series of local transformations that evolve the system. The collision operator $C$ is the only entangling operation in the algorithm, and it creates quantum coherences limited to each two-qubit system. The streaming is executed by classical communication, and it moves the occupation numbers up and down the lattice as denoted by the arrows. The sectioned cylinder depicts the position of the sites in the NMR sample. Each site is physically realized as an addressable slice of isotopically-labeled Chloroform solution.

4-2 **NMR methodology for QLG algorithm.** The NMR implementation consists of four main sections, each corresponding to the prescribed QLG algorithm step. The top two lines in the diagram correspond to RF pulses applied to the proton and carbon qubits, respectively. The third line shows the application of magnetic field gradients. In the encoding section, the initial carbon magnetization is recorded on the protons before being transferred to the carbons. The starting magnetization is specified by using a RF pulse shaped as the Fourier transform of the desired magnetization. The shaped pulses are applied in the presence of gradients so that each site can be addressed. A carbon decoupling sequence prevents the scalar coupling from interfering with the low power shaped pulses. The $\pi/2$ at the end of the encoding move the information form the $x$-axis to the $z$-axis, as required by the QLG algorithm. The collision operator follows the encoding, and it is implemented without gradients to ensure that all of the sites in the sample feel the same transformation. The results are observed in two experiments, each time using the more sensitive proton channel. A swap gate is added when measuring the carbon magnetization. Finally, the streaming operation is applied by shifting the frequencies of the carbon and proton shapes in opposite directions.

4-3 **QLG algorithm experimental results.** The experimental mass densities are plotted in the figure, together with plots of the analytical solution and the numerical simulation of the NMR experiment. Seven steps of the algorithm were implemented on 16 two-qubit sites. The simulations were performed using the actual RF mutation rates and times of the experimental setup. The calculations closely match the data, suggesting that the deviation between the analytical results and the data can be attributed imperfections in the methodology. As a result, the simulations promise to be useful in exploring the errors from alternate methods.
List of Tables

2.1 Summary of relevant characteristics for an example set of transformations. The three columns list the pulse duration (in $\mu$s), maximum power (in kHz), and the gate fidelity of the simulated pulse. While the maximum power is relatively large, all powers are experimentally feasible. The pulses designed for the crotonic acid sample require longer times and yield lower fidelities due to the decreased chemical separation and increase of coupling strengths. .......................... 29

2.2 Summary of experimental results. The variables $P$, $A$, and $C$, refer to the projection, attenuation, and attenuated correlation, as defined in section 2.1. The subscripts specify whether the pulses employed were made robust against RF inhomogeneity. The attenuated correlations for all the robust gates were appreciably higher than the corresponding values for the normal pulses. .......................... 42

2.3 Results of single-pulse rotation experiments. The ability to include robustness against RF inhomogeneity into the pulse design yields measurable improvements in the attenuated correlation. .......................... 42

3.1 Three-spin pseudopure state creation sequence. The table shows the transformations used to obtain the initial state $|000\rangle$ from the thermal state, $\rho_{eq}$. ....................................................... 45

3.2 Summary of experimental data for the incoherent implementation of various collective error models. The first column lists the one-bit quantum processes realized in the experiment. Gradient fields with maximum strength $\sim 0.5$ T/m were applied during a fraction $\delta \sim 0.5$ ms of the evolution period, $t_{ev} \sim 3, 6, 9$ ms for single-, double-, and triple-axes error models, respectively. In addition to the applied error model, $\mathcal{E}_x, \mathcal{E}_y, \mathcal{E}_z, \mathcal{E}_{xz}, \mathcal{E}_{zy}, \mathcal{E}_{yz}$, the channel label specifies whether (ns) or not (un) encoding and decoding procedures were implemented. The processes $Q_{0,ns}, Q_{00,ns}, Q_{000,ns}$ differ in the length of the evolution period over which they apply the trivial error model (i.e., the identity evolution). For each process, the input-output fidelities $F_{\psi_{in}}$ involved in the process tomography as well as the resulting entanglement fidelities $F_e$ are listed. Statistical uncertainties are $\sim 2\%$, arising from errors in the tomographic density matrix reconstruction. .... 67
Chapter 1

Introduction

Computers have revolutionized many aspects of daily life, bringing to the home desktop machines with the computational power of the supercomputers of a decade ago. The explosion in computing speed has followed Moore's Law, a rule of thumb stating that the computing power of the latest processors doubles roughly every 18 months. Amazingly, the computing industry has followed this law since the development of the first computers in 1946. Such an exponential and rapid acceleration in computing ability is impressive. However, the basic technologies that have enabled Moore's Law are reaching fundamental physical limits. The miniaturization of processor components, which has taken transistor sizes from one centimeter in 1965 to 0.1 microns today, will hit the atomic limit in about 15 years. Current technologies cannot possibly continue miniaturization beyond the scale of atoms. In addition to the size barrier, atomic-scale objects behave under the rules of quantum mechanics. Present technologies do not fully exploit quantum effects, and in many cases quantum effects interfere with the proper performance of electronic devices. Quantum effects, however, due to their profoundly different nature, may someday help overcome current limitations.

In the past decade, the new field of quantum information processing (QIP) has quickly developed, and with it the promise of using quantum computers to solve problems that will forever be intractable to classical computers. Factoring large numbers [2] and simulating many-body quantum systems [3, 4, 5, 6] are two specific problems that are difficult for classical computers to solve but are in theory exponentially easier for a quantum computer to solve. The task of building a quantum computer, however, requires both precise control of a quantum system and isolation from the noisy effects of the environment. These conflicting requirements are two of the main obstacles in the quest for a working quantum computer.

In this thesis, we present experimental results that show how quantum information stored in nuclear spins can be controlled and protected. In the next chapter, we discuss a method for creating strongly-modulating radiofrequency (RF) gates that dominate the internal Hamiltonian of a spin system to implement precise unitary transformations. Using the strong modulation, robustness against common errors can be included in the gate design. The gates are used in a variety of demonstrations of quantum information processing (Chapter 3). The applications include studies of
entanglement and quantum error correction, two topics that will play central roles in any future quantum computer. In the last chapter, we describe a methodology for running quantum lattice gas (QLG) algorithms on a classically parallel array of NMR quantum information processors. The implementation examines the experimental challenges involved with the QLG method. As a whole, the results represent a first step in the development of the experimental methods to control quantum information.
Chapter 2

Quantum Control

The past decade has seen a substantial interest in improving coherent quantum control. Coherent control had origins in both nuclear magnetic resonance (NMR) [7, 8] and optical spectroscopy [9, 10]. For an overview of advances in both fields, the reader is referred to [11]. Since coherent control’s inception, many different techniques have been used both to improve selectivity and to reduce the duration of control pulses. For spin systems, the Fourier transform has been used to approximate the excitation profile in the limit of low power and no spin-spin couplings [12] and more complete analytic solutions have been developed to aid in general pulse design and analysis [13, 14, 15, 16, 17, 18]. Alternatively, very sophisticated shaped pulses have been designed using a variety of computer-aided methods [19, 20] or feedback from system observables [21]. Equivalent analytic theories [22, 23], computer-aided methods [24] and feedback techniques [25, 26] have also been developed by the optics community. Similar techniques are also used in other fields such as the control of trapped ions [27, 28].

The development of liquid-state NMR systems as prototype quantum information processors [29, 30] has enabled experimental demonstration of quantum algorithms [31, 32, 33], quantum error correction [34, 35], and quantum simulations [36]. These experiments built upon well-established spectroscopic techniques developed over the past four decades, such as using low-power (soft) shaped radio-frequency (RF) pulses to obtain selective operations. However, the selective pulses employed to date have the disadvantage that low power implies long duration. This not only introduces errors due to relaxation, or decoherence, but also allows significant evolution under the action of the internal Hamiltonian. In the past, this evolution was rarely of concern because there was little importance placed on implementing a particular operation. For example, in spectroscopy there are entire classes of propagators that selectively excite a single spin from its equilibrium state, but for applications such as quantum computing the transformation must act as expected for all input states.

A second problem with soft-pulse techniques is that selective pulses simultaneously applied to different spins interfere with each other, thus causing significant deviation from the desired action [37]. To address some of these problems, several groups pre-calculate these errors and incorporate corrections into their analysis and pulse design [38, 39]. However, not all errors can be corrected using these techniques\(^2\), and it would be preferable to average out unwanted evolution by the use of strong control fields, so that no additional corrections are required.

In this chapter, we present a procedure for finding high-power pulses that strongly modulate the system’s dynamics to produce precisely a desired spin-selective unitary propagator. These operations, or gates, allow arbitrary rotations of each spin around independent single-spin axes, while refocusing the internal evolution. They are “self-contained,” in the sense that they can be placed back to back in longer sequences without requiring additional computational resources or post-experiment corrections. By using high-power, pulse durations are decreased by almost an order of magnitude, thereby significantly reducing the effects of relaxation. The simulated gate fidelities of the pulses are high, reaching past 0.9999 on the three-spin system \(^{13}\text{C}\)-alanine placed in a 800 MHz magnet. Finally, the use of strong modulation also allows the incorporation of robustness against slowly varying or time independent incoherent errors such as those caused by RF inhomogeneities [40, 41, 42]. Our control methods are the first to combine all of these features.

The pulses presented here have been applied in recent Quantum Information Processing (QIP) experiments to demonstrate algorithms [33], study notions of measurement [43], and test new methods for noise control [44]. They promise to be increasingly useful in future NMR QIP experiments, where larger numbers of qubits will necessitate increasing the number of homonuclear spins. In addition, these methods can be adapted to develop improved pulses for selective spectroscopy [45] and imaging [46]. Finally, although presented within the context of NMR, these methods are applicable to any system where the total Hamiltonian is well known and the external degrees of freedom allow for universal control, both requirements of any quantum information processor.

### 2.1 Metrics of Control

In designing gates for controlling quantum information, a metric is required to judge how well a specific implementation compares to the ideal, desired transformation. A metric of a gate’s performance should describe the quality of a general transformation, including the possibility of non-unitary evolution. Unfortunately, such information is not directly accessible by experiment, so we choose a metric comprised only of sets of state measurements. For an input state, \(\rho_n\), the ideal transformation maps the

\(^2\)For instance, not all errors can be represented as a composition of phase shifts, \(\sigma_z\sigma_z\) couplings and ideal \(\pi/2\) or \(\pi\) pulses.
system to a theoretical output state, \( \rho_{th} \), i.e.,

\[
\rho_{in} \xrightarrow{U_{th}} \rho_{th}.
\]  

(2.1)

On the other hand, a simulated or experimentally implemented control sequence will produce a different output state, \( \rho_{out} \), i.e.,

\[
\rho_{in} \rightarrow \rho_{out}.
\]

(2.2)

Noting that \( \rho \) is Hermitian, the projection between these two states, defined as

\[
P(\rho_{th}, \rho_{out}) = \frac{\text{trace}(\rho_{th} \rho_{out})}{\sqrt{\text{trace}(\rho_{th}^2)\text{trace}(\rho_{out}^2)}},
\]

(2.3)

quantifies how similar in 'direction' the two states are. This metric is analogous to the dot product between two vectors, varying from \(-1\) for anti-parallel states to \(1\) for identical states. A value of zero indicates orthogonal density matrices. In order to account for non-unitary evolution, a second term multiplies the projection yielding the attenuated correlation, namely,

\[
C(\rho_{th}, \rho_{out}) = P(\rho_{th}, \rho_{out}) \sqrt{\frac{\text{trace}(\rho_{out}^2)}{\text{trace}(\rho_{in}^2)}}
\]

(2.4)

\[
= \frac{\text{trace}(\rho_{th} \rho_{out})}{\sqrt{\text{trace}(\rho_{th}^2)\text{trace}(\rho_{in}^2)}}.
\]

(2.5)

The projection and the attenuated correlation serve as metrics for state fidelity.

The gate fidelity, \( F \), of a transformation is defined as

\[
F = \overline{C}(\rho_{th}, \rho_{out}),
\]

(2.6)

where \( \overline{C} \) represents the average attenuated correlation over an orthonormal set of input density operators (i.e., \( \text{Trace}[\rho_j \rho_k] = \delta_{jk} \)) that span the Hilbert space. It should be noted that \( F \) is maximized (with a value of one) when the implemented and ideal transformations are the same, and is insensitive to differences in the global phase between the ideal and implemented transformation.

We can derive a useful alternate form for the gate fidelity in terms of the actual and theoretical transformations instead of the input-output state relations. This form is both easier to compute and has intuitive appeal in that knowledge of the transformation can be directly translated to gate fidelities. First we assume that our ideal transformation is unitary, and the implemented transformation is a completely positive, trace-preserving linear map [47]. In other words, the implemented transformation takes normalized density operators to normalized density operators and if the system starts as subsystem of an entangled system, then the full system's density operator also maps in a reasonable way. Under these assumptions, Eqs. (2.1) and
(2.2) are explicitly given by
\[ \rho_{th} = U_{th}\rho_{in}U_{th}^\dagger, \tag{2.7} \]
and
\[ \rho_{out} = \sum_{\mu} A_\mu\rho_{in}A_\mu^\dagger, \tag{2.8} \]
where the \( A_\mu \) satisfy
\[ \sum_{\mu} A_\mu^\dagger A_\mu = 1. \tag{2.9} \]
We now show that the gate fidelity reduces to
\[ F = \sum_{\mu} |\text{Trace}(U_{th}^\dagger A_\mu)/N|^2, \tag{2.10} \]
where \( N \) is the dimension of the Hilbert space. Using the normalized Pauli basis, \( \sigma_j \), as the orthonormal input density operators and the cyclic properties of the trace, Eq. (2.6) becomes
\[ F = \sum_{j=1}^{N^2} \text{Tr}[(U_{th}\sigma_j U_{th}^\dagger)(\sum_{\mu} A_\mu\sigma_j A_\mu^\dagger)]/N^2 \tag{2.11} \]
\[ = \sum_{j=1}^{N^2} \text{Tr}[\sigma_j \sum_{\mu} U_{th}^\dagger A_\mu\sigma_j A_\mu^\dagger U_{th}]/N^2. \tag{2.12} \]
Expanding the product of \( U_{th}^\dagger A_\mu \) in terms of the orthonormal Pauli basis \( (U_{th}^\dagger A_\mu = \sum_k B_{\mu k}^k \sigma_k) \), yields
\[ = \sum_{j\mu} \text{Tr}[\sigma_j (\sum_k B_{\mu k}^k \sigma_k)\sigma_j (\sum_m B_{\mu m}^m \sigma_m)]/N^2 \tag{2.13} \]
\[ = \sum_{j\mu k m} B_{\mu k}^k B_{\mu m}^m \text{Tr}[\sigma_j \sigma_k \sigma_j \sigma_m]/N^2. \tag{2.14} \]
Because the \( \sigma \) basis is orthogonal, only terms where \( k = m \) contribute. Therefore, Eq. (2.14) reduces to
\[ F = \sum_{j\mu k} |B_{\mu k}^k|^2 \text{Tr}[\sigma_j \sigma_k \sigma_j \sigma_k]/N^2. \tag{2.15} \]
If \( \sigma_k \) is not proportional to identity, it will anti-commute with exactly half the \( \sigma_j \) terms in the sum, while commuting with the other half. Therefore, two sets of terms cancel and have no contribution to \( F \). Defining \( \sigma_1 \) to be the element that is proportional to identity, Eq. (2.15) further reduces to
\[ F = \sum_{j\mu} |B_{\mu j}^1|^2 \text{Tr}[\sigma_j \sigma_j]/N^3 \tag{2.16} \]
\[ = \sum_{j\mu} |B_{\mu j}^1|^2 / N^3 = \sum_{\mu} |B_{\mu}^1|^2 / N. \tag{2.17} \]
This is clearly equal to Eq. 2.10. Thus, the gate fidelity corresponds to how well the
actual transformation reverses the action of $U_{th}$. In this form it is obvious that the gate Fidelity is independent of which orthonormal basis of input states are used as $\rho_{in}$.

2.2 Designing Gates for Controlling Quantum Information

In the standard model of quantum computing, an algorithm can be expressed as a series of unitary operations that maps a set of input states to a particular set of output states. The physical implementation of an algorithm requires the use of a quantum system with a Hamiltonian that contains a sufficient set of externally controlled parameters to allow for the generation of a universal set of gates [48]. The task of control is to find a time-dependent sequence of values for these control parameters that modulates the system’s dynamics in order to generate a particular gate to the required precision.

Given a control sequence, solving for the effective Hamiltonian is straightforward. Unfortunately, going the other way is much more difficult. That is, finding a RF waveform that produces a propagator with desired properties is an inverse problem. Traditionally, analytic techniques, such as average Hamiltonian theory [8], have been used to determine an appropriate control sequence. With modern computer resources, numerical methods provide a more efficient and accurate solution to this problem.

2.2.1 NMR Spin System

As an example, liquid-state NMR is used to demonstrate how to find control sequences to implement particular gates. In NMR, spins in a large static magnetic field (in our case, $\sim 7$ T) are controlled via external RF pulses. The internal spin Hamiltonian is composed of both Zeeman interactions with the applied field modified by electron screening (chemical shift) and scalar couplings with other spins. Together these provide the QIP requirements of addressability and conditional logic respectively. In terms of spin operators, the internal Hamiltonian is

$$H_{int} = \sum_{k=1}^{n} \omega_k I_z^k + 2\pi \sum_{j>k}^{n} \sum_{k=1}^{n} J_{kj} I^k_+ I^j_-, \quad (2.18)$$

where $\omega_k$ represent the chemical shifts of the spins, $J_{kj}$ the coupling constant between spins $k$ and $j$, and $n$ is the number of spins. The test molecules used throughout this document are shown in Fig. 2-1, along with the relevant internal Hamiltonian values.

The external Hamiltonian describing the coupling between the spins and an oscillating RF field generated by a single transmitter is

$$H_{ext}(\omega_{RF}, \phi, \omega, t) = \sum_{k=1}^{n} e^{-i(\omega_{RF}t+\phi)} I_z^k (-\omega I^k_+) e^{i(\omega_{RF}t+\phi)} I_z^k, \quad (2.19)$$
where \( \omega_{RF} \) is the transmitter’s angular frequency, \( \phi \) the initial phase, and \( \omega \) the power\(^3\). Of course, additional species can be added by including appropriate terms in \( H_{int} \) and an additional \( H_{ext} \) for each additional RF field.

### 2.2.2 Numerical Search Method

Using this knowledge of the internal Hamiltonian and the form of the external Hamiltonian, the parameter values that generate the desired gate must be determined. Here, a quality factor \( Q = 1 - \sqrt{F} \) is minimized by searching through the mathematical parameter space using the Nelder-Mead Simplex algorithm [49]. While this function has many local minima, the Simplex algorithm often succeeds in finding satisfactory solutions. Our goal is to show that sufficient, implementable control sequences can be found. Finding the optimal solution is much more challenging and based on our system and control parameter values, is not expected to improve pulse performance significantly. We have parameterized the control sequence as a cascade of RF pulses with fixed power, transmitter frequency, initial phase, and pulse duration (\( \tau \)). As will be seen, this is a particularly convenient and completely general parameterization, but we make no claims that it is the only, nor necessarily the best choice. If the RF power is constant over the duration of a pulse, \( i.e. \), the pulse’s amplitude is square, the total Hamiltonian \( H_{tot} = H_{int} + H_{ext} \) can be made time independent by transforming into the frame that rotates at the frequency of the transmitter. This allows the Liouville-von Neumann equation of motion to be solved by a single diagonalization.

---

\(^3\)Actually, \( \omega \) equals a spin’s nutation rate caused by an RF field. Because this parameter is experimentally controlled by attenuating the RF power, it is commonly referred to as the pulse power.
Initially, the starting density matrix is the same in both frames ($\tilde{\rho}(0) = \rho(0)$), so that at the end of the pulse, the density matrix in the new frame is given by

$$\tilde{\rho}(\tau) = e^{-iH_{eff}\tau}\rho(0)e^{iH_{eff}\tau},$$

(2.20)

where $H_{eff}$ is the effective Hamiltonian in the new frame [50]. Transforming this density matrix back to the original rotating frame gives

$$\rho = U_z(\tau)^{-1}e^{-iH_{eff}\tau}\rho(0)e^{iH_{eff}\tau}U_z(\tau),$$

(2.21)

where

$$U_z(\tau) = (e^{i\omega RF\sum_{k=1}^{n}l_k^z\tau}).$$

(2.22)

Therefore, in the original rotating frame, the transformation is given by

$$U_{\text{period}}(\tau) = U_z^{-1}(\tau)e^{-iH_{eff}\tau}.$$

(2.23)

Because the evolution under the whole sequence is given in the original rotating frame, no additional resources are required to concatenate pulses, nor is any mathematical correction required at the end of an experiment.

Cascading these periods yields the net transformation

$$U_{\text{net}} = \prod_{m=1}^{N} U_z^{-1}(\tau_m)e^{-iH^m_{eff}(\omega^m RF, \phi^m)\tau_m}$$

(2.24)

where the index $m$ refers to the $m^{th}$ period, i.e., to the $m^{th}$ square pulse, with a corresponding set of 4 parameters. In other words, $N$ constant amplitude pulse periods, each with a different transmitter frequency and initial phase, are applied in series. Clearly, a single period is not sufficient to generate an arbitrary transformation; therefore the number of periods is increased until a suitable net transformation is found. Using desktop computing resources, this yields convergence times for three- and four-spin systems that are typically seconds to minutes.

In addition to the desired propagator, $U_{\text{ideal}}$, an initial set of starting parameters for the pulse shape is required. While this initial guess must be reasonable (i.e., in the vicinity of the solution), many different starting points typically converge to equally deep minima. We have observed that the number of acceptable solutions for this parameterization is very large, allowing experimental implementation issues to be considered. For example, experimental limitations do not allow arbitrarily high powers or frequencies to be implemented. To keep the algorithm from returning infeasible solutions, a penalty function that increases as the parameter value moves towards infeasible solutions is added to the quality factor. Penalty functions are also used to guide the algorithm towards more favorable pulse solutions. In our case, penalties are placed on high powers, large frequencies, and negative- or long-time periods.
2.2.3 Gate Simulations

The methods described above were used to obtain a set of pulses that implement each of a set of important single-spin gates. To study the performance of these gates, propagators for each of the pulses were simulated under different conditions. In the first set of simulations, the pulse performance was calculated for ideal implementations using current experimental conditions. Second, the gate fidelity was simulated as a function of systematic distortions of the pulse parameters. From these results, the relative importance of implementation precision is determined. A final set of calculations showed how a pulse can generate quite different evolutions as the resonant frequency of a test spin is varied over a range of chemical shifts.

Ideal Pulse Simulations

Pulses were created for three- ($^{13}$C-labeled alanine) and four- ($^{13}$C-labeled crotonic acid) spin homonuclear systems. The chemical shifts and scalar coupling constants for each of these systems are listed in Fig. 2.1. As a representative set, each of the single spin $\pi/2$, and nearest-neighbor paired $\pi$ pulses were simulated with the relevant characteristics summarized in Table 2.1 and example waveforms shown in Fig. 2.2. The duration of the pulses are on the order of 200$\mu$s for the three-spin system and 420$\mu$s for the four-spin system, both significantly shorter than those that could be obtained using low-power pulses. The average fidelities for each system are 0.9995 and 0.995, demonstrating that, at least under ideal conditions, control sequences that implement the desired transformation with high fidelity can be found.

The ultimate goal of control in quantum computing is to attain fault-tolerant computation. While it has been proven that perfect control is not required [51], estimates of the precision needed vary from 0.9999 to 0.999999 depending on the assumptions used. These simulations predict an achievable level of control that approaches the most optimistic estimates for fault tolerant computation. As expected, the pulse duration decreases with increasing chemical shifts dispersion (selectivity condition) and, for the case that $J_{jk} << |\omega_k - \omega_j|$, the fidelity of the sequence decreases with increasing ratio of the couplings (bilinear terms) to chemical shift.

Variations in the External Hamiltonian

The external RF parameters are determined by a minimization procedure, suggesting that small variations of the external parameters should have little effect on the quality of the pulses. To check this assumption, the gate fidelity was calculated as each of the six pairs of the four control parameters were varied over a range of errors typical of an experimental implementation. As a sample set, one pulse for each of the two systems is presented here. The results shown in Fig. 2.3 demonstrate the natural robustness against typical variations in the initial phase, frequency, and duration of each period. Clearly, the sequence is most sensitive to power variations. For the pulses listed in Table 2.1, if the power’s amplitude is changed by 5% the average fidelity falls to 0.96 $\pm$ 0.01 for alanine pulses and 0.94 $\pm$ 0.04 for crotonic acid pulses. For the 25 pulses used in [44] the average fidelity at 5% amplitude deviation is 0.97 $\pm$ 0.02.
<table>
<thead>
<tr>
<th>Pulse</th>
<th>Time ($\mu$s)</th>
<th>Max. Power (kHz)</th>
<th>Fidelity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\pi/2\left</td>
<td>_{1}^{1}\right.$</td>
<td>202</td>
<td>7.9</td>
</tr>
<tr>
<td>$\pi/2\left</td>
<td>_{2}^{1}\right.$</td>
<td>221</td>
<td>9.3</td>
</tr>
<tr>
<td>$\pi/2\left</td>
<td>_{3}^{1}\right.$</td>
<td>212</td>
<td>9.0</td>
</tr>
<tr>
<td>$\pi/2\left</td>
<td>_{12}^{1}\right.$</td>
<td>194</td>
<td>8.5</td>
</tr>
<tr>
<td>$\pi/2\left</td>
<td>_{23}^{1}\right.$</td>
<td>179</td>
<td>9.2</td>
</tr>
<tr>
<td>$\pi/2\left</td>
<td>_{123}^{1}\right.$</td>
<td>163</td>
<td>10.3</td>
</tr>
<tr>
<td>$\pi\left</td>
<td>_{12}^{2}\right.$</td>
<td>252</td>
<td>8.0</td>
</tr>
<tr>
<td>$\pi\left</td>
<td>_{13}^{2}\right.$</td>
<td>129</td>
<td>10.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Pulse</th>
<th>Time ($\mu$s)</th>
<th>Max. Power (kHz)</th>
<th>Fidelity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\pi/2\left</td>
<td>_{1}^{4}\right.$</td>
<td>389</td>
<td>8.5</td>
</tr>
<tr>
<td>$\pi/2\left</td>
<td>_{2}^{4}\right.$</td>
<td>610</td>
<td>4.8</td>
</tr>
<tr>
<td>$\pi/2\left</td>
<td>_{3}^{4}\right.$</td>
<td>392</td>
<td>6.3</td>
</tr>
<tr>
<td>$\pi/2\left</td>
<td>_{4}^{4}\right.$</td>
<td>559</td>
<td>7.6</td>
</tr>
<tr>
<td>$\pi\left</td>
<td>_{12}^{4}\right.$</td>
<td>326</td>
<td>9.0</td>
</tr>
<tr>
<td>$\pi\left</td>
<td>_{13}^{4}\right.$</td>
<td>315</td>
<td>11.3</td>
</tr>
<tr>
<td>$\pi\left</td>
<td>_{123}^{4}\right.$</td>
<td>345</td>
<td>8.4</td>
</tr>
</tbody>
</table>

Table 2.1: **Summary of relevant characteristics for an example set of transformations.** The three columns list the pulse duration (in $\mu$s), maximum power (in kHz), and the gate fidelity of the simulated pulse. While the maximum power is relatively large, all powers are experimentally feasible. The pulses designed for the crotonic acid sample require longer times and yield lower fidelities due to the decreased chemical separation and increase of coupling strengths.
Figure 2-2: **Ideal RF waveform for two example pulses.** The solid (dashed) line is the amplitude (phase) of the waveform. Changes in the transmitter frequency (within a single period) were implemented by a discrete linear phase ramp. The sharp discontinuities occur at the transitions between periods. Substantial filtering of these high frequency components (smoothing of the shape) has little effect on the gate fidelity. In order to experimentally implement the pulse, it is converted into a discrete series of amplitudes and phases (order 1K long) by sampling the ideal waveform at a constant rate. Details of the pulse parameters (as per Eq. (2.24)) are listed below each waveform. Due to experimental implementation issues, a 6μs period with zero RF power (i.e., $H_{\text{ext}} = 0$) is needed before and after the pulse and must be included to produce the desired propagator.

Figure 2-3: **Gate fidelity vs. variations in experimental parameters.** The experimental parameters were varied over the range of expected errors, demonstrating that both the alanine and crotonic acid pulses are most sensitive to RF amplitude.
Figure 2-4: Gate fidelity vs. spin frequency. The gate fidelities of two example pulses were calculated as a function of the resonance frequency of a test spin. The frequency was varied in the range of chemical shifts of the molecules. The solid (dashed) line is calculated with identity (desired transformation) as the theoretical transformation. The vertical dotted lines denote the actual chemical shifts for each spin. As can be seen, the gate only works when the test spin is at the appropriate resonance frequency.

For 10% deviation, the gate fidelity drops to 0.86 ± 0.03 for the alanine pulses and 0.81 ± 0.12 for the crotonic acid pulses. This pulse sensitivity to RF amplitude suggests that RF inhomogeneity may be a leading cause of experimental errors. While techniques to select homogeneous regions are available [39, 52], the loss in signal to noise is significant, especially if multiple coils are used. Instead, because these errors are incoherent in nature, it is possible to design pulse sequences that refocus such inhomogeneities (see section 2.3.2).

Variations in the Internal Hamiltonian

For NMR spectroscopy, the goal is to excite selectively spins in a band of frequencies leaving all other possible spins (with unknown precession frequencies) along the z axis. This requires that the propagator for spins at any other frequency be, at most a phase change. With detailed knowledge of the internal Hamiltonian, the effect of the applied RF field needs only be considered at the resonance frequencies of the chemical species present in the given molecule. By relaxing the requirement that the effective Hamiltonian be zero for all chemical shifts other than those in the band of excitation, a RF shape can be found that more efficiently implements the desired gate for the frequencies of concern yielding high-power yet selective pulses. To demonstrate this idea more clearly, the gate fidelities of the two sample pulses considered in the subsection B were calculated as a function of a test spin's resonant frequency. As can be seen in Fig. 2-4, the fidelity is close to unity only near the resonance frequency.
Figure 2-5: Exploration of achievable fidelities. The plot shows the maximum fidelities found for a $\pi/2|z$ alanine pulse as allowed RF power and magnetic field strength were varied. The three lines correspond to the magnetic field strengths explored, as denoted by the legend. The dotted vertical lines mark the point of the minimum chemical shift difference at each of the three field strengths. Using ideal experimental control in a 800 MHz magnet, a single-spin gate fidelity reaching 0.99999 is potentially realizable.

for which the pulse was designed to work. This stresses the necessity of having accurate knowledge of the system's Hamiltonian. On the other hand, looking at the region immediately around the resonance we see the fidelity falls off quite slowly. This implies that small variations in the chemical shift do not significantly affect the fidelity of the pulses. For example, in the experiments presented below, the unwanted scalar couplings to the hydrogen atoms, which are equivalent to errors in the resonance frequency, were automatically refocused by the control pulse. It should be noted that no constraint was used to require this robustness, but that it results from the use of strongly modulating pulses. If this natural robustness is not sufficient, additional constraints can be added. Of course, this robustness also implies that selective pulses will be harder to design for spin systems where the spectrum is dense.

2.2.4 Exploring Achievable Fidelities

One of the most important results in QIP is the discovery that indefinite, fault-tolerant computation is possible when the gates used to correct for experimental errors have a fidelity below a certain level [51]. The simulated single-spin gate fidelities of the alanine pulses in Table 2.1 reach the lower end of the threshold, but it is important to explore further what fidelities are achievable (with the present method) in situations with extended experimental capabilities. For this purpose, we extensively explored the parameter space of a $\pi/2|z$ alanine pulse by running hundreds of Simplex searches, each time varying the initial guess, the penalty function for the maximum allowable RF, or the magnetic field strength. Fig. 2-5 summarizes the findings.

The three curves represent the results for each of three magnetic field strengths tested. The stronger fields allow pulse solutions with higher fidelities because of the
increased chemical shift dispersion. The stronger fields cause the spin frequencies to widen, allowing more spectral room for addressability and control. Fidelities also tended to increase with the maximum RF power for values between \( \sim 1 \) Hz and \( \sim 10^4 \) Hz. At low powers, the RF control is insufficient to average out the internal Hamiltonian, resulting in low fidelities. At high RF control power, the strength of the RF dominates the internal Hamiltonian, resulting in the desired control. The three vertical dotted lines (one for each field) indicate where the smallest chemical shift frequency differences fall relative to the RF power strength. As expected, the sharp increase in the fidelities occurs when the RF power is able to dominate the chemical shift terms in the internal Hamiltonian. The maximum gate fidelity in the plot is close to 0.99999, suggesting that, for the single-spin gate examined, the fault-tolerant limit is potentially achievable.

It is important to emphasize that the maximum achievable fidelities of Fig. 2-5 represent the best gates achieved using the current pulse parameterization and available search method and resources. The results do not preclude other methods and pulse strategies from yielding higher fidelities.

### 2.3 Correcting for Experimental Errors

The above results demonstrate how knowledge of the internal and the control Hamiltonians can be used to design custom sequences for generating unitary transformations. Although simulations of the pulses demonstrate that the gates are robust against small deviations in some of the control parameters, a substantial loss of fidelity occurs when the RF amplitudes deviate from the prescribed values. In this section, we describe a feedback procedure that detects and corrects experimental deviations from the ideal RF shapes. In addition, we demonstrate how the gates can be made robust against uncorrectable errors due to RF inhomogeneity. The methods allow for knowledge of experimental errors to be used for both correcting and compensating imperfections, creating improved gates in practice.

#### 2.3.1 RF Waveform Feedback Correction

The experiments discussed in section 2.4 were performed on a Bruker Avance 300 MHz spectrometer. In this spectrometer, a digital waveform generator creates the desired shape. The signal is then amplified and routed to a coil in the probe that is tuned to the carbon resonance frequency (\( \sim 75 \) MHz). The sample is inserted in the coil, where it is exposed to the RF irradiation that generates the desired gates. Because of nonlinearities in the transmitter and probe circuits, the waveforms observed by the spins are distorted from the intended shapes. For a set of 25 sample waveforms, the mean absolute deviation between the observed RF amplitudes and the intended amplitudes was about 150 Hz, while the mean phase deviations were comparatively smaller, at about 0.7 degrees. Using Fig. 2-3 as a reference, one can expect that the phase errors cause negligible loss in fidelity. In contrast, the amplitude errors cause the RF nutation rate in each period to vary up to 4 percent for typical alanine pulses,
Figure 2-6: Feedback loop for correcting experimental RF waveforms. Distorted signals arriving at the carbon coil are detected and digitized through the proton coil. The difference between the measured RF wave and the desired wave is then calculated, resulting in a fixed wave that is then retransmitted to the coil. The loop continues until the shape of the fixed wave produces the desired signal at the carbon coil.

resulting in a significant drop in fidelity. Simulations of alanine gates having errors of this magnitude have fidelities about 0.01 smaller than the fidelities of the ideal transformations, suggesting a need for improved RF shaping.

To correct the amplitude and phase errors, we used an iterative feedback procedure to determine the prewarped RF waveforms that, when distorted through the transmitter chain, would create a RF shape close to the intended shape. The feedback was accomplished by using the hydrogen coil as a spy pick-up antenna to observe the final RF wave transmitted to the sample. The hydrogen resonant circuit was tuned to 300 MHz, and, as a result, it attenuated the 75 MHz carbon signals by about 30 dB. In addition, its response at the low carbon frequencies was expected to be nearly flat for a 1 MHz band around the carbon resonance frequency[4] . Both the attenuation factor and the flat response made the hydrogen coil a useful observation tool for the carbon waveforms. The signals collected from the hydrogen coil were directed to a mixer and finally to a digitizer for measurement.

[4]The probe response of a 400 MHz coil was measured at 100 MHz, and it was found to be very flat. We expected a similar result in the 300 MHz system.
Figure 2-7: Improvement of errors in digitized RF waveforms. The errors from a test sample of 25 waveforms are plotted here as a function of the feedback loop iteration number. The errors are the mean absolute differences between fits to the digitized waveform and the ideal waveform. Four to six iterations were typically sufficient to improve the RF shape.

The digitizer scale was calibrated by measuring the waveforms of pulses with known spin responses. In separate experiments, we applied a series of on-resonance, square pulses with varying power settings. For each pulse, we determined the time necessary to generate a \(4\pi\) rotation on the middle carbon. We then digitized each pulse using time steps \(\Delta t = 1 \mu s\). Because each pulse generated a \(4\pi\) rotation, a properly calibrated digitizer scale would result in the total integral of the magnitude of each waveform to equal \(4\pi\). We made use of this fact to determine the scaling constant \(C_N\) that converted the arbitrary digitizer units into units of angular frequency. Given in terms of the digitized values \(d_n\), the time step \(\Delta t\), and the chosen rotation angle \(4\pi\), the scaling constant is

\[
C_N = \frac{4\pi}{\sum d_n \Delta t}
\]  \hspace{1cm} (2.25)

and, when multiplied against each digitizer bin value \(d_n\), converts it to the mutation rate \(w_n = C_N d_n\). In practice, the scaling constant used for the tested waveforms was the average of the individual constants obtained for a range of calibration power settings. The constants \(C_N\) obtained from pulses with different power settings varied less than 0.2 percent from pulse to pulse. This calibration was carried out each time a new feedback procedure was begun.

The properly normalized scale was then used to analyze all of subsequent digitized waveforms. The feedback loop for a given pulse began by digitizing the RF shape \(\omega_{\text{dig}}(k)\) generated at the sample from the input waveform \(\omega_{\text{input}}(k)\) specified to the waveform generator. The variable \(k\) denotes the iteration number. For the first iteration, the input waveform used was the ideal shape. The magnitude and phase
of each period in $\omega_{\text{dig}}(k)$ were then fit using low order polynomials, yielding the corresponding fitted waveform $\omega_{\text{fit}}(k)$. For the magnitude, the order of the polynomial was 2 or 3, depending on the length of the period, while the phases were fit with a line. The new fixed waveform $\omega_{\text{fix}}(k)$ was constructed by subtracting from the input waveform the difference between the ideal waveform $\omega_{\text{ideal}}$ and the fitted signal $\omega_{\text{fit}}$, as shown in

$$\omega_{\text{fix}}(k) = \omega_{\text{input}}(k) - \alpha (\omega_{\text{ideal}} - \omega_{\text{fit}}(k))$$ (2.26)

The variable $\alpha$ denotes the fraction of the deviation to subtract into the fixed shape, and it controls the rate of convergence of the feedback loop. We typically employed values ranging from 1/1.5 to 1/1.3. The fixed signal $\omega_{\text{fix}}$ was then sent to the waveform generator and the transmitter chain, resulting in the digitized shape for the next loop.

Using the above mentioned values of $\alpha$, the iterative scheme typically converged the digitized pulses $\omega_{\text{dig}}(k)$ to the ideal shapes $\omega_{\text{ideal}}$ in four to six steps, as shown in Fig. 2-7. The average difference between the final digitized amplitude and the ideal amplitude was reduced to about 20 Hz, while the average phase difference was reduced to 0.08 degrees. The signal to noise in the digitized signal was the limiting factor. Fig. 2-8 shows the digitized amplitudes of two back-to-back pulses, both before and after the feedback procedure. The amplitude of the corrected pulse matches very well with the ideal pulse.

### 2.3.2 Robustness Against RF Inhomogeneity

As discussed above, RF wave distortions cause gate fidelities to drop by about 0.01. The dominant error in experimental implementations, however, is due to RF inhomogeneity. RF inhomogeneity occurs when different parts of the NMR sample feel unequal RF fields. The result is a dephasing of the spins that attenuates the signal and introduces errors in the rotations of the spins. RF inhomogeneity is essentially the imperfect field distribution generated by the RF coils in the probe, and to correct it would require smaller samples (and less signal) or new coil hardware. An alternative, however, is to take advantage of the strong modulation to create gates that are robust against the known errors.

The RF inhomogeneity was measured using a spin nutation experiment in which the transverse magnetization of the spin system was measured after on-resonance pulses of increasing duration. In the case of perfect homogeneity, this experiment would cause all of the spins in the sample to oscillate at the same frequency. When RF inhomogeneity is present, however, the signal decays as a function of time. The various strengths of RF that compose the inhomogeneity are extracted by measuring the frequencies present in the decaying signal. This is trivially accomplished by taking a Fourier transform of the results of the nutation experiment. The results can then be adjusted to account for the fact that the detection is also carried out with the same coil, further attenuating or enhancing the signal based on its nutation frequency (this step was skipped in the results presented here). The dotted line in Fig. 2-9a is a fit to the measured RF inhomogeneity in the carbon coil of the 300 MHz magnet.
Figure 2-8: **Distorted and corrected RF amplitude.** The dots denote the digitized values of the distorted and corrected amplitudes. The solid gray lines show the ideal pulse amplitudes. The pulse sequence shown here contains two back-to-back gates separated by a delay of 12 μs. The high frequency transients present at the transitions between periods have little effect on the overall performance of the gates.
Robust pulses were created by including the RF distribution in the numerical parameter search. The inhomogeneity was incorporated into the analysis by calculating its Krauss form

\[ A_k = \sqrt{p_k} U_k \]  

(2.27)

and evaluating the gate fidelity using Eq. (2.10). In the above equation for the Krauss operators, the index \( k \) refers to a spin sub-ensemble feeling a unitary transformation \( U_k \) generated by the corresponding scaled RF. The variable \( p_k \) denotes the fraction of spins in the \( k \)th sub-ensemble, and \( \sum_k p_k = 1 \).

The search results for 11 test gates are shown in Fig. 2-9. Fig. 2-9a shows the gate fidelities as a function of the RF scaling. The robust pulses are noticeably less sensitive to changes in the RF. The uncompensated pulses, however, have the overall highest fidelities when the RF is ideal. The second figure graphs the fidelities as a function of RF distributions with increasing width. The results show the net fidelity in the more realistic situation where multiple RF frequencies are present simultaneously. The distributions used were stretched and narrowed versions of the measured RF profile. As a result, the simulated fidelities corresponding to the experimental setup employed are those where the RF width is 1. The simulations of the robust pulses suggest that a fidelity improvement of 2 to 3 percent can be achieved experimentally.

### 2.4 Experimental Demonstrations

In this section we experimentally demonstrate the efficacy of a representative set of pulses via both spectra and reconstructed density matrices. The experimental tests were carried out on the three carbons of \(^{13}\text{C}\)-labeled alanine (see Fig. 2-1 for internal Hamiltonian parameters) using a 300 MHz Bruker Avance spectrometer.

First, a series of selective single-spin pulses were applied to the thermal state to demonstrate that these selective rotations fully refocus the internal Hamiltonian and so can be concatenated arbitrarily. Fig. 2-10 shows sample sequences and the resulting spectra. In addition, because the internal Hamiltonian is fully refocused, applying selective transformations on different spins sequentially has an effect equivalent to applying all the appropriate transformations to each of the spins simultaneously (neglecting relaxation). With simultaneous, fully self-refocused \( \pi \) pulses, selective couplings can be efficiently implemented using previously published techniques [50, 53], and they are also demonstrated in Fig. 2-10.

While spectra contain information about the observables of the current state of the system (single-spin transitions in the case of NMR), a single spectrum does not contain enough information to reconstruct the entire state of the system. The full state, or density matrix, can be obtained by using state tomography [54], a procedure that employs "read-out" pulses to rotate unobservable elements of the state into the single-spin transitions. In the case of three spins, seven or eight repetitions of the experiment, each with a different readout pulse, are sufficient to reconstruct the density matrix\(^5\)

---

\(^5\)Eight readout transformations suffice for the density matrix reconstruction: identity, \( \pi/2 \),
Figure 2-9: Simulations of normal and robust pulses as a function of RF strengths and RF distribution widths. The dashed lines correspond to robust pulses, while the solid gray lines denote uncompensated pulses. The dotted line overlaid on the left plot shows a fit to the measured RF inhomogeneity profile. This information was utilized in the pulse parameter search to determine pulses robust against it. The left plot shows how the robust pulses maintain high fidelities even when the RF strength is scaled from the ideal value. The plot on the right simulates the same pulses as a function of the scaled width of the RF inhomogeneity profile. These results demonstrate the improved fidelity of the robust pulses for all but the narrowest RF distributions. At the small widths, the RF profile would no longer be inhomogeneous, eliminating the need for the robust gates.
Figure 2.10: **Sample spectra resulting from gates.** The plots show spectra resulting from different sequences of pulses applied to the thermal equilibrium density matrix $\rho_{\text{thermal}} = I^1_z + I^2_z + I^3_z$. All sequences are read from left to right. The reference spectra, resulting from a $\frac{\pi}{2}$ pulse applied to all 3 carbons, is shown in grey. Although the chemical shift is order $1/\tau$, no significant phase evolution is seen. Selective coupling sequences are also demonstrated.
To determine the actual experimental gate performed, however, one requires knowledge about the action of the transformation on a full set of orthogonal input states (process tomography)\cite{55, 56}. To carry out a process tomography for a single alanine gate requires the state tomography of the input and output density matrices for the 64 possible inputs. In other words, the process tomography for one gate demands $2 \times 64 \times 8 = 1024$ separate experiments. While this is certainly doable, we chose instead to limit the number of total experiments for one gate by performing state tomographies on three input states and the corresponding output states. The results do not fully characterize the experimental transformations, but they provide a valuable estimate of the quality of the gates.

The experiments tested robust and normal versions of seven individual pulses and the two selective scalar couplings $J_{12}$ and $J_{23}$. The scalar coupling sequences employed four $\pi$ pulses spaced between four delay periods. The total delay time was chosen to be $1/(2J)$ in each case. The waveforms of all the pulses were corrected using the RF feedback correction procedure described in section 2.3.1. The transformations were applied on the three input states

$$\rho_m = I^1_j + I^2_j + I^3_j,$$  

(2.28)

where $j = x, y, z$. The input states were created using robust or normal pulses, depending on the type of gate tested. The input and output density matrices were measured using state tomography, and they were used in Eq. (2.4) to evaluate the projection, attenuation, and attenuated correlation (see section 2.1). In all cases, the state tomography for the thermal state $I^1_z + I^2_z + I^3_z$ was used as the reference for for attenuation ($\rho_m$ in Eq. (2.4)). For each transformation, the average over the three input states was calculated, and the results are shown in Tables 2.2 and 2.3. The first table shows results of input states, the selective couplings, and an average over all the single pulse experiments. The second table shows the specific results for each single pulse experiment.

The most notable difference between the results of robust and normal gates is in the severe attenuation caused by RF inhomogeneity on the non-robust gates. The value $A_{\text{robust}}$ is more than 0.03 higher than the corresponding value for normal pulses. In addition, $A_{\text{robust}}$ for the $J_{23}$ coupling is 0.06 higher than $A_{\text{normal}}$, although $A_{\text{robust}}$ for $J_{12}$ is only slightly higher than $A_{\text{normal}}$ for the $J_{12}$ coupling. The projections for the robust gates averaged 0.991, slightly but consistently below an average of 0.995 for the normal gates. The attenuated correlations for the robust gates were higher, mostly due to the sharp differences in the attenuations. The results confirm how incorporating RF inhomogeneity into the pulse design can yield better and more robust gates. While the goal of fault tolerance clearly has not been met, these results indicate that the experimental implementation is nearing ideal simulation results.

$\pi/2|_{y}^{12}, \pi/2|_{z}^{23}, \pi/2|_{y}^{13}, \pi/2|_{z}^{31}, \pi/2|_{z}^{1,2,3}, \pi/2|_{y}^{1,2,3}$. All of the density matrices dicussed in this section were acquired using the eight readouts, with the exception of the input states, which used the last seven. The last seven readouts alone are also sufficient, but we included the identity because of its particularly simple implementation.
Table 2.2: Summary of experimental results. The variables $P$, $A$, and $C$, refer to the projection, attenuation, and attenuated correlation, as defined in section 2.1. The subscripts specify whether the pulses employed were made robust against RF inhomogeneity. The attenuated correlations for all the robust gates were appreciably higher than the corresponding values for the normal pulses.

<table>
<thead>
<tr>
<th></th>
<th>$J_{12}$</th>
<th>$J_{23}$</th>
<th>$J_{13}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{robust}$</td>
<td>0.993</td>
<td>0.991</td>
<td>0.986</td>
</tr>
<tr>
<td>$P_{normal}$</td>
<td>0.995</td>
<td>0.955</td>
<td>0.975</td>
</tr>
<tr>
<td>$A_{robust}$</td>
<td>0.998</td>
<td>0.987</td>
<td>0.954</td>
</tr>
<tr>
<td>$A_{normal}$</td>
<td>0.970</td>
<td>0.949</td>
<td>0.951</td>
</tr>
<tr>
<td>$C_{robust}$</td>
<td>0.991</td>
<td>0.979</td>
<td>0.941</td>
</tr>
<tr>
<td>$C_{normal}$</td>
<td>0.965</td>
<td>0.944</td>
<td>0.927</td>
</tr>
</tbody>
</table>

Table 2.3: Results of single-pulse rotation experiments. The ability to include robustness against RF inhomogeneity into the pulse design yields measurable improvements in the attenuated correlation.

|          | $\pi/2|_{1}^{1}$ | $\pi/2|_{1}^{2}$ | $\pi/2|_{1}^{12}$ | $\pi/2|_{1}^{123}$ | $\pi|_{1}^{12}$ | $\pi|_{1}^{23}$ |
|----------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| $P_{robust}$ | 0.991           | 0.992           | 0.991           | 0.986           | 0.994         | 0.993         | 0.992         |
| $P_{normal}$ | 0.996           | 0.994           | 0.996           | 0.994           | 0.996         | 0.995         | 0.995         |
| $A_{robust}$ | 0.990           | 0.989           | 0.987           | 0.988           | 0.986         | 0.984         | 0.986         |
| $A_{normal}$ | 0.954           | 0.953           | 0.948           | 0.951           | 0.942         | 0.952         | 0.941         |
| $C_{robust}$ | 0.981           | 0.981           | 0.978           | 0.974           | 0.980         | 0.977         | 0.979         |
| $C_{normal}$ | 0.950           | 0.948           | 0.944           | 0.945           | 0.938         | 0.947         | 0.936         |

2.5 Conclusion

The ability to implement faithfully a desired unitary transformation is at the heart of any future implementation of a quantum computer. Any control technique should minimize the effects of decoherent errors while retaining the required addressability. We have demonstrated a method to find control sequences that use detailed knowledge of the system's Hamiltonian and of experimental imperfections to generate desired gates. The sequences employ high-power pulses that strongly modulate the system's dynamics. These gates are short in duration yet selective, implementing the correct unitary transformation. The effect of these control sequences has been simulated under various conditions and experimentally demonstrated by NMR. Finally, avenues for future improvements are within the reach of current technologies.
Chapter 3

Applications

3.1 Disentanglement Eraser

One of the most intriguing effects in quantum mechanics is the "quantum eraser" [57, 58, 59, 60, 61, 62, 63, 64]. Given an ensemble of identically prepared quantum systems, this effect is described by the loss or gain of interference in a subensemble that is determined by the outcome of the measurement of one or the other of a pair of noncommuting binary observables, respectively. Thus a quantum eraser demonstrates the principle of complementarity without making use of the corresponding uncertainty relation. Quantum erasers have previously been demonstrated by optical [65] as well as atom [66] interferometry. In this Letter we use liquid-state NMR spectroscopy on pseudo-pure states [67] to demonstrate a novel "disentanglement" eraser, due to Garisto and Hardy [68], in which not only interference, but also entanglement, is lost or gained in a subensemble. An analogous quantum erasure procedure operating on a pair of Bell states has recently been used by Zeilinger's group to prepare an entangled three-photon state [69].

An important goal of our group is to design and build increasingly more powerful experimentally controllable devices capable of precisely simulating the dynamics of any quantum system with an equal or smaller Hilbert space dimension. Previously we have addressed the issues of coherent control [70] and pseudo-pure state preparation [71], and we are now developing methods for non-unitary quantum operations. The disentanglement eraser is of particular interest in this regard, because it allows us to show that NMR on pseudo-pure states is capable of reproducing even the decoherent dynamics associated with strong (projective) measurements on the members of the ensemble, which are needed to create or destroy entanglement in this eraser (cf. [71]).

It should be understood that the density matrices of the highly mixed macrostates involved in liquid-state NMR experiments can always be rationalized in terms of ensembles of disentangled micro-states [72]. Consequentially, the ensemble-average observations on pseudo-pure states reported here do not prove the existence of the

\footnote{Most of this section was extracted from G. Teklemariam, E.M. Fortunato, M.A. Pravia, T.F. Havel, and D.G. Cory, "NMR analog of the quantum disentanglement eraser," Physical Review Letters, 86:5845-49, 2001.}
corresponding entangled micro-states in the sample. Nevertheless, because pseudo-pure states provide an equivalent representation of the underlying quantum dynamics, our experiments created exactly the same ensemble-average coherences that would have been observed if the same operations had been applied to the corresponding pure state ensemble, and this is sufficient for our purposes.

In the disentanglement eraser two of the spins (qubits) in a GHZ (Greenberger-Horne-Zeilinger) state [73, 74] are regarded as the components of a Bell state labeled by the state of an additional "ancilla" spin \#1 (left-most), i.e.

$$|\psi_{GHZ}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle).$$

Assuming that the computational basis corresponds to the eigenvectors of the \(\sigma_z\) spin 1/2 operator, a projective measurement of the ancilla along \(z\) yields a mixture of separable states \(|00\rangle\) and \(|11\rangle\) labeled by the ancilla spin. This corresponds to the ensemble

$$\rho_z = E_z^1|00\rangle\langle 00| + E_z^1|11\rangle\langle 11|,$$

where \(E_z^1 = \frac{1}{2}(I \pm \sigma_z^1)\) expresses the density matrices \(|0\rangle\langle 0| \otimes \sigma_z \otimes \sigma_z = E_z^1\) and \(|1\rangle\langle 1| \otimes \sigma_z \otimes \sigma_z = E_z^1\) in terms of the Pauli matrix \(\sigma_z^1 = \sigma_z \otimes \sigma_z \otimes \sigma_z\), where \(\sigma_z = |0\rangle\langle 0| + |1\rangle\langle 1|\) and \(I = \sigma_1 \otimes \sigma_1 \otimes \sigma_1\) is the 8 \(\times\) 8 identity matrix.

Alternatively, expressing the GHZ state in terms of the \(x\) eigenstates of the ancilla spin and the Bell states of the other two spins yields

$$|\psi_{GHZ}\rangle = \frac{1}{\sqrt{2}}(|x_+\rangle|\phi_+\rangle + |x_-\rangle|\phi_-\rangle),$$

where \(|x_\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}\) and \(|\phi_\pm\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}\). Thus a projective measurement along the \(x\)-axis followed by a rotation of the ancilla back to \(z\) gives

$$\rho_x = E_x^1|\phi_+\rangle\langle \phi_+| + E_x^1|\phi_-\rangle\langle \phi_-|.$$

This is a mixture of complementary Bell states each labeled by the state of the ancilla. Note that the partial trace over the ancilla in \(|\psi_{GHZ}\rangle\langle \psi_{GHZ}|\), \(\rho_z\) and \(\rho_x\) are all equal to \(\sigma_z \otimes (|00\rangle\langle 00| + |11\rangle\langle 11|) = E_z^2E_x^2 + E_x^2E_z^2\), so that these states can be distinguished only if the information contained in the state of the ancilla is used.

These effects were demonstrated by liquid-state NMR using as the qubits the three spin 1/2 carbons in a \(^{13}\text{C}\)-labeled sample of alanine in deuterated water. With decoupling of the protons [75], this spin system exhibits a weakly coupled spectrum corresponding to the Hamiltonian of Eq. (2.18) with the coupling and chemical shift values specified in Fig. 2-1. The \(T_1\) relaxation times for the three spins are 21, 2.5 and 1.6 s, while the \(T_2\) times are 550, 420 and 800 ms, respectively.

The pseudo-pure ground state was prepared from the thermal equilibrium state by the procedure summarized in Table 3.1, which uses magnetic field gradients (denoted by \([\nabla]\)) to dephase off-diagonal elements of the density matrix at strategic points along the way [67]. Letting \(\rho_{eq} = \sigma_z^1 + \sigma_z^2 + \sigma_z^3\) be the traceless part of the equilibrium density matrix (with all physical constants set to unity), the first two transformations in the table yield the state \((\sqrt{3}/\sqrt{3})(\sigma_z^2 + (\sigma_z^1 + \sigma_z^3)E_z^2\). Spins 1 and 3 may then be
Transformations

1) \( |\nabla| e^{-\frac{i}{2} \cos^{-1}(\frac{\sqrt{3}}{4\sqrt{2}})\sigma_z^2} \)
2) \( |\nabla| e^{-i\frac{\pi}{4}(\sigma_1^y + \sigma_3^y)}E_z \)
3) \( e^{i\frac{\pi}{4}\sigma_z^2}e^{-i\frac{\pi}{4}\sigma_z^2\sigma_z^2}e^{-i\frac{\pi}{4}(\sigma_1^y + \sigma_3^y)}e^{-i\frac{\pi}{4}\sigma_1^z\sigma_z^2}e^{-i\frac{\pi}{8}(\sigma_z^2 + \sigma_3^2)} \)
4) \( |\nabla| e^{i\frac{\pi}{12}(\sigma_1^y + \sigma_3^y)}e^{-i\frac{\pi}{4}\sigma_z^2\sigma_z^2}e^{-i\frac{\pi}{8}(\sigma_z^2 + \sigma_3^2)} \)

Table 3.1: Three-spin pseudopure state creation sequence. The table shows the transformations used to obtain the initial state \( |000\rangle \) from the thermal state, \( \rho_{\text{eq}} \) transformed into the state \( (\sqrt{3}/\sqrt{2})(\sigma_1^1 + \sigma_2^3 + \sigma_3^3) \) by the efficient two-spin pseudopure state preparation procedure described in Ref. [71] (Eq. (47)), yielding the three-spin pseudo-pure ground state

\[
\dot{\rho}_{\text{int}} = \frac{\sqrt{3}}{\sqrt{2}} \left( E_+^1 E_+^2 E_+^3 - \frac{1}{8} \right) \equiv \left( |000\rangle \langle 000| - \frac{1}{8} \right).
\] (3.5)

The logic network shown in Fig. 3-1 transforms this state into the pseudo-pure GHZ state, and then decoheres the ancilla as indicated. The GHZ state is obtained by rotating spin 2 (since \( J_{13} \ll J_{12}, J_{23} \)) to the axis in the rotating frame with a \( \pi/2 \) y-rotation \( R^y_2(\pi/2) \equiv \exp(-i\sigma_3^y\pi/4) \), and then using it as the control for a pair of c-NOT (controlled-NOT [76]) gates to the other two spins. This pair of c-NOT's was implemented by the propagator \( N^{13|2} \equiv e^{i(\sigma_1^1 - \sigma_2^2)E^2_2\pi/2} = e^{i\sigma_1^1 E^2_2\pi/2}e^{-i\sigma_2^2 E^2_2\pi/2} \) (ensuring cancellation of the phases \( \pm i \) between the two factors). The overall sequence of transformations on the corresponding state vector is thus:

\[
|000\rangle \xrightarrow{R^y_2(\pi/2)} |0\rangle(0\rangle + |1\rangle)|0\rangle)/\sqrt{2} \xrightarrow{N^{13|2}} (|000\rangle + |111\rangle)/\sqrt{2} \equiv |\psi_{\text{GHZ}}\rangle
\] (3.6)

Implementations of these operations in NMR by RF (radio-frequency) pulse sequences may be found in Refs. [67, 71, 77]. The resulting pseudo-pure GHZ state is written in product operator notation as [77]

\[
\dot{\rho}_{\text{GHZ}} = \frac{\sqrt{3}}{4\sqrt{2}}(\sigma_1^1 \sigma_3^2 + \sigma_2^2 \sigma_3^3 + \sigma_3^1 \sigma_3^3 \\
+ \sigma_1^1 \sigma_3^2 \sigma_z^2 - \sigma_1^1 \sigma_3^2 \sigma_z^2 - \sigma_3^1 \sigma_3^2 \sigma_z^3 - \sigma_3^1 \sigma_3^2 \sigma_z^3),
\] (3.7)

and has previously been studied by NMR in Refs. [78, 79].

The coherences of \( \rho_{\text{GHZ}} \) can be dephased, exactly as they would be by strong measurements of \( \sigma_z \) on all the individual systems in the ensemble, by means of magnetic field gradients similar to those used to prepare the initial pseudo-pure state (cf. [71]). Specifically, a constant gradient \( \nabla = \partial B_z/\partial z \) applied for a period \( t \) along the static field axis \( z \) causes spin evolution under the Hamiltonian \( \gamma \nabla B_z \sum_{j=1}^3 \sigma_j^z \), where \( \gamma \) is the gyromagnetic ratio of all the spins. This multiplies each coherence \( \rho_{kl}(k \neq l) \) with a spatially dependent phase \( \exp(-i\gamma m_{kl} \nabla x t/2) \), where \( m_{kl} \) is the coherence or-
Figure 3-1: **Logic network for the disentanglement eraser.** Initially, a pseudopure state on spins 1, 2 and 3 is created, \( \rho_{\text{ini}} = |000\rangle\langle 000| \equiv E_+^1 E_+^2 E_+^3 \). A \( \frac{\pi}{2} \) y-pulse is then applied to spin 2, followed by two controlled-not (c-NOT) gates to create the GHZ state (see text). Conditionality on the second spin being in the \( |1\rangle \) state is represented in the network by a filled circle on its time line. Finally, the two complementary measurements, \( \sigma_z^1 \) and \( \sigma_z^2 \), are applied to spin 1. State tomography was performed to fully reconstruct the density matrices at the positions indicated.
der [12] (i.e. the difference in the \( z \)-component of the angular momentum in units of \( \hbar \) between the \( |k \rangle \) and \( |\ell \rangle \) states [75]). Thus after such a gradient pulse the density matrix averaged over the sample volume satisfies \( \rho_{k\ell} = 0 \) for all \( k \neq \ell \) save for the zero quantum coherences \( (m_{kl} = 0) \). Because only one spin is dephased in the eraser experiments, only single quantum coherences are of consequence.

This dephasing operation was made specific to those coherences involving transitions of the ancilla spin 1 by applying a \( \pi \) pulse to the other two spins, after which a second gradient pulse of the same amplitude and duration “refocuses” all the other coherences. At the same time it is necessary to also refocus the evolution under the internal Hamiltonian using \( \pi \) pulses selective for single spins. A sequence of RF and gradient pulses which accomplishes this is (in temporal order):

\[
P_z^1 = \frac{[\nabla]_z - [\pi]^2_z - [\nabla]_z - [\pi]^{3,3}_z - [\nabla]_z - [\pi]^{3,3}_z}{[\nabla]_z - [\pi]^{2,3}_z - [\nabla]_z - [\pi]^{3,3}_z}
\]  

The corresponding effective (average) propagator is simply \( e^{-i\nabla \sigma_z 1/2} \). This dephases the ancilla spin in the same way as would a strong measurement of \( \sigma_z^1 \) on every member of the ensemble. To dephase the ancilla in the same way as would a strong measurement of \( \sigma_z^1 \), one need only rotate the ancilla to the \( z \)-axis with a \( \pi/2 \) \( y \)-rotation \( R_{-y}^1(\pi/2) \), as follows:

\[
P_z^1 = [\pi/2]_{-y}^1 - P_z^1
\]  

The ancilla is left along \( z \) for subsequent tomography.

The results of \( P_z^1 \) and \( P_z^1 \) applied to \( \hat{\rho}_{GHZ} \) are

\[
\hat{\rho}_{GHZ} \overset{P_1}{\to} \frac{\sqrt{3}}{4\sqrt{2}}(\sigma_2^1 \sigma_z^2 + \sigma_2^2 \sigma_z^3 + \sigma_2^3 \sigma_z^3),
\]

\[
\hat{\rho}_{GHZ} \overset{P_1}{\to} \frac{\sqrt{3}}{4\sqrt{2}}(\sigma_2^2 \sigma_z^3 + \sigma_2^3 \sigma_z^2 - \sigma_1^2 \sigma_z^2 \sigma_y^2).
\]

These states were confirmed by full tomography [80]. Because only the single quantum \( (m_{kl} = 1) \) coherences give rise to observable (dipolar) magnetization, it is necessary to collect spectra not only following the dephasing operation, but also following additional \( \pi/2 \) pulses selective for single spins, to rotate the \( m_{kl} = 0 \) and \( m_{kl} > 1 \) coherences, as well as the populations (diagonal elements), into observable single quantum coherences. Tomography was performed at the points of the procedure indicated in Fig. 3-1; the real parts of these four density matrices are shown in Fig. 3-2 (the imaginary parts were essentially zero).

The overall precision of quantum information transmission was quantified by an extension of Schumacher’s fidelity [47], which takes into account not only systematic errors, but also the net loss of magnetization due to random errors. This measure, called the attenuated correlation, is given by

\[
C(\hat{\rho}^{exp}) = \frac{\text{Tr}(\hat{\rho}_{\text{the}}^{\text{exp}})}{\text{Tr}(\hat{\rho}_{\text{the}}^{\text{the}})}.
\]
Figure 3-2: Disentanglement eraser experimental density matrices. The rows are enumerated in the standard computational basis, where for example 000 represents the state label $|000\rangle$. Although not shown, the columns are similarly labeled with the leftmost end representing $|000\rangle$ and the rightmost end representing $|111\rangle$. $\rho_{\text{ini}}$ is the three-spin pseudo-pure ground state, and $\rho_{\text{GHZ}}$ is the pseudo-pure GHZ state. The last two plots are $\rho_z$, which is $\rho_{\text{GHZ}}$ after decoherring spin 1 about the z-axis, and $\rho_x$, which is after decoherring it about the x-axis. (Note: $\rho_{\text{GHZ}}$, $\rho_z$, and $\rho_x$ have been magnified by a factor of two for clarity). An amount of identity, chosen to optimize the input projection, was added to all experimentally measured density matrices.
Here, \( \hat{\rho}^{\text{the}} \) is the measured pseudo-pure ground state \( \hat{\rho}_{\text{ini}}^{\text{exp}} \), transformed on a computer by the same sequence of unitary and non-unitary (measurement) operations to which it was subjected on the spectrometer to get \( \hat{\rho}^{\text{exp}} \). Note that, since \( Tr(\hat{\rho}^{\text{exp}}\hat{\rho}^{\text{the}}) \leq Tr(\hat{\rho}^{\text{the}}\hat{\rho}^{\text{the}}) \), the Cauchy-Schwarz inequality implies that \(-1 \leq c(\hat{\rho}^{\text{exp}}) \leq 1\).

The values of the correlation for each of the four tomographic readouts were 
\[ c(\hat{\rho}_{\text{ini}}^{\text{exp}}) = 1 \text{ (by definition), } c(\hat{\rho}_{\text{GHZ}}^{\text{exp}}) = 0.88, \quad c(\hat{\rho}_{x}^{\text{exp}}) = 0.92 \text{ and } c(\hat{\rho}_{z}^{\text{exp}}) = 0.93. \]
Although not included here for brevity, tomography on the state \( |0\rangle (|00\rangle + |11\rangle)/\sqrt{2} \) yields an attenuated correlation of 0.93, showing that spins 2 and 3 were entangled before the GHZ state was created. The increases in \( c \) are not unexpected, since the additional \( \pi \) and gradient pulses needed to mimic measurements on \( \rho_{\text{GHZ}} \) are easily implemented with high precision, and the tomographic errors are estimated at \( \pm 5\% \).

The leading candidates for the loss of correlation are pulse imperfections arising from RF field inhomogeneity, less than perfect RF pulse calibrations, and relaxation. The total time before data collection in the complete experiments was ca. 65 ms; the time required to prepare the GHZ state from the initial state was 21 ms. Since the \( T_2 \) relaxation times of the spins varied from 400 – 800 ms, the net loss of magnetization due to relaxation in going from \( \hat{\rho}_{\text{ini}} \) to \( \hat{\rho}_{\text{GHZ}} \) was 3 – 5\%. Thus, the additional loss due to pulse imperfections etc. was about another 5\% or so, confirming the high precision of the strongly modulated pulse sequences used in these experiments.

In conclusion, we have used a three-spin liquid-state NMR quantum information processor to obtain a high-precision implementation of the dynamics, both coherent and decoherent, underlying Garisto and Hardy’s “disentanglement eraser”, and have found that the experimental results confirm the theoretically predicted conditional expectation values. This shows that we can judiciously and selectively render phase information macroscopically inaccessible in a way that precisely mimics the decoherence attendant on strong measurements. It should be noted that during this dephasing operation all interactions among the spins were refocused, and that only the \textit{macroscopically accessible} information contained in the ancilla spin due to its earlier interactions with the other two was changed. This was nevertheless sufficient to convert the net triple-quantum coherence in \( \rho_{\text{GHZ}} \) into a pair of double-quantum coherences, conditional on the state of the ancilla representing this information. Unlike previous eraser implementations, it was not necessary to explicitly read out this information in each member of the ensemble in order to see the conditional coherence, because this was done for us by the coupling of the ancilla to the other two spins while the spectra were being measured. This ability to convert macroscopic correlations into one another via well-defined microscopic (molecular) interactions is the essence of ensemble quantum computing.
3.2 Quantum Fourier Transform

A key subroutine of algorithms for factoring and simulation \cite{81, 5, 6} is the quantum Fourier transform (QFT) \cite{82, 83, 84}. In essence, the QFT takes a 'position' state $|x\rangle$ to the corresponding 'momentum' state $|p\rangle$, and it is defined as

$$QFT_q|x\rangle \rightarrow \frac{1}{\sqrt{q}} \sum_{p=0}^{q-1} e^{2\pi ip/q} |p\rangle. \quad (3.13)$$

where $q$ is the dimension of the system's Hilbert space. The $QFT_q$ transforms a general input state as

$$QFT_q \sum_x f(x)|x\rangle \rightarrow \sum_p \tilde{f}(p)|p\rangle, \quad (3.14)$$

where the coefficients $\tilde{f}(p)$ are

$$\tilde{f}(p) = \frac{1}{\sqrt{q}} \sum_x e^{2\pi ip/q} f(x). \quad (3.15)$$

For example, the two qubit QFT corresponds to the unitary operator,

$$QFT_4 = \frac{1}{2} \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & i & -1 & -i \\
1 & -1 & 1 & -1 \\
1 & -i & -1 & i
\end{pmatrix}. \quad (3.16)$$

The operator separates the input states by 0 degrees in the first row and column, and then by 90 degrees, 180 degrees and 270 degrees.

Equation (3.15) shows that the QFT, which was modeled after the discrete Fourier transform and is itself discrete, has effects similar to that of the classical discrete Fourier transform. In particular, if $f(x)$ is periodic with period $r$, then $\tilde{f}(p)$ will exhibit a peak at $p = q/r$. This feature of the QFT is at the heart of Shor's algorithm for factoring numbers in polynomial time. The classical Fourier transform reveals the periodicity in functions, just as the QFT reveals periodicity of wavefunctions.

As formulated by Coppersmith \cite{82}, the QFT can be constructed from two basic unitary operations, the Hadamard gate operating on the $j$th qubit,

$$H_j = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 1 \\
1 & -1
\end{pmatrix}. \quad (3.17)$$

\footnote{Most of this section was extracted from Y.S. Weinstein, M.A. Pravia, E.M. Fortunato, S. Lloyd, and D.G. Cory, “Implementation of the quantum fourier transform,” Physical Review Letters, 86:1889-91, 2001.}
and a conditional phase shift operating on the \( j \)th and \( k \)th qubits,

\[
B_{jk} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & e^{i\theta_{jk}} \\
0 & 0 & 0
\end{pmatrix},
\]

where \( \theta_{jk} = \pi/2^{k-j} \).

To implement the QFT, the gates,

\[
B_{j,1}B_{j,2}...B_{j,j-1}H_j
\]

are implemented on each bit as \( j \) is indexed from 1 to \( L \). A bit reversal at end completes the QFT. The bit reversal can be achieved by relabeling bits or by performing swap operations.

This sequence of quantum logic gates can be realized using NMR. As an example, we implement the 8-dimensional QFT on the three-spin system alanine. The internal Hamiltonian of alanine is accurately described by Eq. (2.18) with the coupling and chemical shift values specified in Fig. 2-1. The pulse program is conveniently derived from an idempotent or projection operator description of the propagators. The operators \( E \) are defined as \((1 \pm \sigma_z)/2 \). The \( H_j \) matrix can be broken down into \( E_+ - E_- + \sigma_x (E_+ + E_-) \). The pulse sequence [77] of the \( H_j \) gate is,

\[
H_j = \left( \frac{\pi}{2} \right)^j_y - \left( \pi \right)^j_x.
\]

This pulse program reads: apply a pulse that rotates spin \( j \) 90 degrees about the \( y \)-axis, followed by a pulse that rotates \( j \) 180 degrees about the \( x \)-axis. Magnetization along the \( z \)-axis would be rotated to the positive \( x \)-axis. The \( B_{jk} \) gate, can be implemented using the coupling between qubits. In terms of projection operators the \( B_{jk} \) gate is \( 1 - E_- E_- E_+ + e^{i\varphi} E_- E_+ E_- \), and the following pulse sequence:

\[
\begin{align*}
B_{jk} &= (\pi)^j_y - (\theta_{2\pi J_{jk}})^j_y - (\pi)^j_x - (\theta_{2\pi J_{jk}})^j_x \\
&= (\pi)^j_y - (\theta_{2\pi J_{jk}})^j_y - (\pi)^j_x - (\theta_{2\pi J_{jk}})^j_x.
\end{align*}
\]

The notation \( \theta_{2\pi J_{jk}} \) represents an interval of spin evolution between spins \( j \) and \( k \) while refocusing chemical shifts and couplings between all other spins. The final three pulses effectively perform a rotation around the \( z \)-axis.

A bit reversal can be achieved by simply renaming the bits. In our experiment, however, we actually perform the bit reversal with a swap gate to fully observe the extraction of periodicity by the QFT. A bit reversal can be achieved by a series of nearest-neighbor swap gates. \( SWAP_{jk} \) gates can be implemented with the following
Figure 3-3: QFT input state. The plot shows the real part of the QFT input density matrix. This state, created by Hadamards on the first and second bit after the three bits were put into a pseudo-pure state, is a superposition of the |000⟩ + |010⟩ + |100⟩ + |110⟩ states. Note that the input state has a periodicity of r = 2.

pulse sequence:

\[
\text{SWAP}_{jk} = \left( \frac{\pi}{2} \right)^{j,k}_y - \left( \frac{1}{2J_{jk}} \right) \left( \frac{\pi}{2} \right)^{j,k}_{-y} - \left( \frac{1}{2J_{jk}} \right) \left( \pi \right)^{j,k}_x - \left( \frac{\pi}{2} \right)^{j,k}_{-x}.
\]  

(3.22)

The complete gate sequence for the three qubit QFT is:

\[H_1B_{12}H_2B_{13}B_{23}H_3\text{SWAP}_{13}\]  

(3.23)

The complete pulse program for the QFT is the compilation of the pulse programs for each of the gates listed above. Pulses were combined when possible without affecting the overall unitary operator. In addition, since the J_{13} coupling is small, any J_{13} couplings were replaced by a series of J_{12} and J_{23} couplings that would perform the exact same operations, so called relayed experiments [85]. For example, the SWAP_{13} gate was replaced by SWAP_{12}SWAP_{23}SWAP_{12} which enacts the exact same unitary transformation. The pulses used for the implementation were self-refocusing for all J-couplings and chemical shifts.

The implemented QFT will give the correct results to any input state. To show the ability of the QFT to extract periodicity, we created a periodic input state of periodicity r = 2 and implemented the QFT on that state. The periodic input state was created by performing a Hadamard on the first and second bits of the |000⟩ pseudo-pure state. The density matrix of the input state is shown in Fig. 3-3.

Fig. 3-4 shows the density matrix after implementation of the QFT minus the
Figure 3-4: **Output of QFT minus the swap gate.** The plot shows the real part of the density matrix after implementation of the QFT without the final swap gate. The attenuated correlation is 0.78

bit reversal. Fig. 3-5 shows the density matrix after subsequent implementation of a $SWAP_{13}$ which performs the necessary bit reversal. Clearly, the density matrix is now periodic with a periodicity of $q/r = 4$ thus showing that the QFT did indeed extract the periodicity of our input state.

The attenuated correlation of the implementation of the QFT is 0.78 not including the swap gate and 0.61 with the swap gate. This measure reflects both imperfections in the applied pulses and delays, as well as decoherence. Spin lattice relaxation ($T_1$) is not an important factor over the time scale of the experiment. Robust pulses where not used in the implementation of the QFT, but their use could significantly reduce the attenuations from RF inhomogeneity.

In conclusion, using NMR, the QFT has been used on a three bit quantum system to extract periodicity of an input state. In addition, the correlation has been measured. The values for the correlation are high enough to permit studies on small quantum systems, possibly including quantum simulations. A particularly straightforward use of the QFT is in quantum chaos: as Balazs and Voros [86] pointed out, a simple version of the quantum baker's map can be performed by QFTs and Schack [87] has shown how such a quantum map might be realized on a quantum computer.
Figure 3-5: Output of QFT. The plot shows the real part of the density matrix after the implementation of the complete QFT. Notice there is now a periodicity of \( q/r = 4 \) in the density matrix. This shows that the QFT extracted the periodicity of the input state. The attenuated correlation is 0.61.
3.3 Entanglement Swap

Entanglement is one of the most striking features of quantum mechanics and a key requirement for many procedures in QIP. Entangled pairs of particles are usually obtained by having both particles emerging from a common source, or bringing them together and letting them interact in a tightly controlled fashion[88]. It has recently been demonstrated that entanglement can be teleported from one pair of photons to another when the quadruple contains two singlet states among disjoint pairs [88] — an effect which has been argued to show that quantum correlations are as nonlocal as the quantum states themselves [89]. This report demonstrates the dynamics of entanglement transfer by a relatively simple liquid-state NMR experiment, in which two swap operations from the two qubits of a (pseudo-pure [71, 72]) Bell state to two other qubits are performed. Despite its simplicity, this form of transfer provides a means of shuttling data between quantum memory (with long decoherence time) and a fast processor (capable of applying a universal set of gates), thereby simplifying the programming of a quantum computer in a fashion similar to that proposed with the aid of quantum teleportation [90].

An overview of the experiment is given in Fig. 3-6. From an information point of view, it consists of initializing two qubits out of four in a known state, entangling them, and finally transferring this entanglement to the two remaining ones via two swap gates.

This demonstration was carried out on a liquid-state NMR quantum information processor [70, 71], using as the qubits the four $^{13}$C nuclei in a sample of crotonic acid (Fig. 2-1). Because liquid-state NMR deals with a highly mixed ensemble of spin systems (molecules) in thermal equilibrium, the state of which can always be described by an ensemble of unentangled systems [72], the experiment described here does not depend on the existence of entanglement in the individual molecules. Nevertheless, the use of pseudo-pure states provides a macroscopic representation of exactly the same unitary dynamics to which the microscopic systems are subject [29, 30]. Pseudo-pure states can be created by introducing an incoherent interaction into the spin dynamics, usually by means of magnetic field gradients. The thermal equilibrium density matrix [91][67], given by

$$\rho_{eq} \approx \frac{I}{2^n} + \frac{\hbar \beta}{2 \cdot 2^n} \sum_{k=1}^{n} \omega_k \sigma_z^k,$$  

(3.24)

can thereby be transformed into a pseudo-pure ground state

$$\rho = \frac{1 - \epsilon}{2^n} I + \epsilon |0000\rangle \langle 0000|,$$  

(3.25)

where $\beta = 1/k_B T$ is the Boltzmann factor, $n$ is the number of spins, $\omega_k$ are their

---

Figure 3-6: Logic network for the entanglement transfer experiment. The four spins are represented by the four horizontal control lines, where each line is labeled on the left by the input state superscripted by the spin's index (where "1" indicates that the spin is depolarized and $E_+$ indicates that it was part of the pseudopure state). The pseudo-pure ground state on spins 2 and 3, $\rho_{pp}^{23} \leftrightarrow |00\rangle \langle 00|$, is converted by an entanglement operation on the same spins to obtain $\rho_{Ent}^{23} \leftrightarrow (|00\rangle + |11\rangle)(\langle 00| + \langle 11|)$. This state is then transferred to spins 1 and 4 by using swap gates.

chemical shifts, $I$ is the identity matrix and $\sigma_z^k$ is a Pauli matrix for the $k$th spin.

With decoupling of the protons, the internal spin Hamiltonian of crotonic acid in the weak coupling limit is given by Eq. (2.18) with the coupling and chemical shift values specified in Fig. 2-1. The $T_1$ relaxation times for the carbons are all greater than 2 s, while the $T_2$ times are longer than 500 ms. The experiments were performed on a Bruker Avance 300 MHz spectrometer, using strongly modulating pulses optimized to implement all the single spin rotations required with relatively high speed and precision while simultaneously refocusing evolution under the internal Hamiltonian. Robustness against RF inhomogeneity was not incorporated into the pulse design.

The states created at each stage in Fig. 3-6 will be denoted by $\rho_{pp}^{23}, \rho_{Ent}^{23}, \rho_{Ent}^{14}$ and are given explicitly by

$$\rho_{pp}^{23} = \lambda I + \epsilon \sum_{a,b=0}^1 |a00b\rangle \langle a00b|,$$

$$= \lambda I + \epsilon(0000\rangle \langle 0000| + 0001\rangle \langle 0001| + 1000\rangle \langle 1000| + 1001\rangle \langle 1001|),$$

$$\rho_{Ent}^{23} = \lambda I + \frac{\epsilon}{2} \sum_{a,b=0}^1 (|a00b\rangle + |a11b\rangle)(\langle a00b| + \langle a11b|),$$

56
\[ \rho_{\text{Ent}}^{14} = \lambda I + \frac{\epsilon}{2} \sum_{a,b=0}^{1} (|0ab0\rangle + |1ab1\rangle)(\langle 0ab0| + \langle 1ab1|). \]

where \( \lambda = \frac{1-\epsilon}{2\epsilon} \). Here and throughout the paper the computational basis |0\rangle and |1\rangle corresponds to the spins being aligned parallel or anti-parallel to the z-axis. Once the pseudo-pure state was created, the subsequent pulse sequences were:

\[
P^{23}_{\text{Ent}} = \left[ \frac{\pi}{2} \right]_x - \left[ \frac{\pi}{2} \right]_y - \left[ \frac{1}{2J_{23}} \right] - \left[ \frac{\pi}{2} \right]_y,
\]

\[
P^{12,34}_{\text{SWAP}} = \left[ \frac{\pi}{2} \right]_x - \left[ \frac{1}{2J} \right] - \left[ \frac{\pi}{2} \right]_y - \left[ \frac{1}{2J} \right] - \left[ \frac{\pi}{2} \right]_y
\]

These sequences are written in left-to-right temporal order. Radio-frequency pulses are indicated by \( [\text{angle}]^{\text{spins}}_{\text{axis}} \), and are applied to the spins in the superscript, along the axis in the subscript, by the angle in brackets. No superscript indicates a pulse applied on all the spins. Evolution for the indicated periods under the system's internal couplings is denoted by \( [\frac{1}{2J_{kl}}] \), where \( J_{kl} \) represents the coupling constant between spins \( k \) and \( \ell \). During these free precession periods, only the specific coupling term in the internal Hamiltonian evolves, while the other terms are refocussed by \( \pi \) pulses [53, 50]. The unsubscripted evolution \( [\frac{1}{2J}] \) denotes a sequence of \( \pi \)-pulses designed to allow the evolutions \( [1/(2J_{12})] \) and \( [1/(2J_{34})] \) to occur while refocussing all other interactions. Because the two swap gates commute, they were performed simultaneously in order to reduce decoherence. The details of translating logic gates to pulse sequences can be found in [92] and [93].

The density matrices were reconstructed by state tomography [54]. Since only single quantum coherences can be directly observed, tomography involves repeating the experiment several times followed by a different readout pulse sequence each time. A total of eighteen readout sequences were used to rotate all density matrix elements into single quantum coherences. These sequences were of the order of 500 \( \mu \)s and therefore did not introduce significant decoherent errors. The attenuated correlations at the different steps were respectively 0.99, 0.92 and 0.65 while the corresponding reconstructed density matrices are given in Fig. 3-7.

This demonstrates a substantial degree of coherent control over a four-qubit homonuclear system. Furthermore, the correlation of 0.65 at the end of the experiment shows that the deviation part of the density matrix describes, to a significant extent, a pseudo-pure entangled state, demonstrating the dynamics of entanglement transfer. The decrease in the correlations in the course of the experiment can be attributed to imperfect pulses, RF inhomogeneities, and intrinsic decoherence (the total duration of the experiment was 75 ms).

In summary, we have demonstrated entanglement transfer by liquid-state NMR on a homonuclear four-spin system. The density matrices were reconstructed and the correlations calculated, illustrating the control available in NMR with the use of strongly modulating pulses. It should be noted that the (relatively small) \( J_{14} \) term
Figure 3-7: Reconstructed density matrices showing entanglement transfer. From left to right are shown the real part of the reconstructed density matrices of the initial pseudo-pure $\rho_{pp}^{23}$, spins 2&3 entangled $\rho_{Ent}^{23}$ and spins 1&4 entangled $\rho_{Ent}^{14}$ (in normalized units). The bottom row of density matrices is obtained from the top row after having traced over the two ancilla spins. The rows and columns represent the standard computational basis in binary order, with $|0000\rangle$ starting on the leftmost column and $|1111\rangle$ being the rightmost column.
in the internal spin Hamiltonian was always refocussed, so that no direct interaction
between spins 1 and 4 was used for this entanglement transfer [88, 94]. Since the cou-
pling networks available in larger molecules are generally quite sparse, this technique
is expected to be useful in future demonstrations of quantum information processing
by NMR, as well as in many potential implementations of quantum computers.
3.4 Noiseless Subsystem

Quantum information is represented in terms of superposition states of elementary two-level systems, known as qubits. The coherence properties of such superpositions are essential to the extraordinary capabilities that quantum mechanics promises for quantum simulation [4], computation [95], and communication [96]. At the same time, they are also extremely vulnerable to the decoherence processes that real-world quantum devices undergo due to unwanted couplings with their surrounding environment [97]. Thus, achieving noise control is indispensable for practical quantum information processing (QIP). While a variety of strategies have been devised to meet this challenge, no single method can compensate for a completely arbitrary noise process. Rather, constructing a reliable QIP scheme depends crucially on the the errors that occur. If the interaction with the environment is sufficiently weak, then to a good approximation a restricted set of errors dominates the information loss, and active quantum error correction (QEC) [98] can be successfully implemented. Another instance where the relevant errors belong to a subset of all the possible errors is realized when the system-environment interaction, no matter how strong, exhibits a symmetry. Taking advantages of symmetries motivated passive noise control schemes based on encoding quantum information into "noiseless" (or "decoherence-free", DF) subspaces [99, 100, 101, 102]. A DF subspace is spanned by states of the system that, up to a possible common phase factor, experience no evolution under the noise. In spite of the intuitive appeal, the invariance properties needed for a DF subspace imply strong symmetry constraints, which restrict the applicability of the approach to exceptionally favorable situations. The notion of a noiseless subsystem (NS) [103] removes such constraints, opening the way for exploiting symmetries in full generality. The basic insight is that protecting quantum information need not demand protecting the entire physical quantum state. Because symmetries generally imply the existence of conserved quantities, encoding information into the abstract subsystems corresponding to such preserved degrees of freedom suffices to guarantee noiselessness – although, typically, errors will evolve the overall system's state. Thus, NSs can be built from physical states displaying non-trivial transformation properties under the noise – encompassing the invariance of DF subspaces as a limiting case. Unlike QEC, which only compensates for a finite numbers of errors, information encoded in a NS is protected with "infinite-distance", against arbitrarily large noise strength and/or order in time.

The fact that NSs cover the full range of possibilities for error-free storage has immediate practical significance: not only can NSs exist in the absence of noiseless subspaces, but they ensure the same degree of protection via more efficient encodings[103]. These advantages are explicitly witnessed by the present work. Even in a scenario where memory resources are not a concern, NSs allow for a major conceptual advance in realizing noise control in QIP. The identification of appropriate

\footnote{Most of this section was extracted from I. 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, 293:2059-63, 2001.}
NSs provides the key for linking passive stabilization schemes with active error control based on either QEC or quantum error suppression [104] – resulting in a unified picture of noise control strategies that is not achievable in terms of DF subspaces alone [103, 104, 105]. In particular, although a correspondence exists between degenerate QEC codes and DF subspaces, establishing a similar duality for arbitrary codes requires the more powerful NS formalism [103, 105, 106]. In fact, the deepest implication behind the NS idea is to point to the ultimate structure – a logical subsystem – where quantum information can reside. While the full impact of subsystems in QIP is still to be appreciated, this is likely to be substantial beyond noise protection itself. For instance, the approach of “encoded universality” [106] aims at achieving universality via subsystem-encodings that are naturally supported by the intrinsic interactions of the physical system – thereby enabling for enhanced flexibility in designing universal quantum computing architectures [107]. Also, NSs have been shown to provide the basic exemplification for the emergence of “virtual” subsystems [108] whose understanding may shed light on quantum entanglement in QIP.

A relevant symmetry arises when the environment couples to the qubits without distinguishing between them i.e., in the “far field”. The resulting “collective” noise behavior provides the paradigmatic situation for discussing passive noise control. Experimental effort to date has been limited to demonstrate the existence of protected subspaces under special types of collective noise – a single DF state of two photons [109] and a DF subspace of two trapped ions [28]. Here, we realize the minimal, three-qubit NS that guarantees the preservation of one qubit against the most general collective noise.

Our physical system is composed of three spin 1/2 particles. Under collective noise conditions, only global angular momentum operators $S_{\alpha} = (\sigma_{\alpha}^{(1)} + \sigma_{\alpha}^{(2)} + \sigma_{\alpha}^{(3)})/2$, $\alpha = x, y, z$, contribute to the system-environment interaction. If the spins are initially in a pure state $\varrho_{in}$, the effect of the environment may be depicted in terms of a quantum operation that leaves them in a mixed state, $\varrho_{in} \mapsto \varrho_{out} = \mathcal{E}(\varrho_{in}) = \sum_a E_a \varrho_{in} E_a^\dagger$, for a set of error operators $\{E_a\}$ satisfying $\sum_a E_a^\dagger E_a = 1$. The possible errors that the error generators $S_{\alpha}$s can induce belong to the “interaction algebra” $\mathcal{A}$ [103], which contains all the linear combinations of arbitrary products of the $S_{\alpha}$s and the identity. Error operators involving products of any number of the basic first-order errors $S_{\alpha}$s occur whenever the exposure to noise is sufficiently long or sufficiently strong. The interaction algebra $\mathcal{A}$, for general collective noise consists of all the totally symmetric operators – which reflects the permutation-symmetry of the noise. For three qubits, the dimension of the symmetric operators’ subspace is 20, so an error basis for describing an arbitrary collective noise process involves up to 20 error operators. Simpler collective noise models, like the ones probed in [109, 28], correspond to smaller error algebras. For instance, collective dephasing with arbitrary strength, $\mathcal{E}_z$, is described by an abelian subalgebra $\mathcal{A}_c$ spanned by 4 elements, $1, S_z, S_x^2, S_y^2$ – and similarly for any fixed axis. The full, non-abelian $\mathcal{A}_c$ can be induced by cascading noise processes along at least two non-commuting spatial directions e.g., $\varrho_{out} = \mathcal{E}_{zz} (\varrho_{in}) = \mathcal{E}_z (\mathcal{E}_z (\varrho_{in}))$.

The NS reported here lives in the four-dimensional subspace $\mathcal{H}_{1/2}$ of states carrying total angular momentum $S = 1/2$ [103, 1]. Basis states for $\mathcal{H}_{1/2}$ are specified by two quantum numbers, $|\lambda, s_z\rangle$, where $s_z = \pm 1/2$ is the eigenvalue of $S_z$ and
\( \lambda = 0, 1 \) accounts for the existence of two distinct pathways leading to total angular momentum \( S = 1/2 [1, 106] \). Because each error generator \( S_{\alpha} \) acts equivalently and non-trivially only within each path, the quantum number \( \lambda \) is preserved under the action of arbitrary errors in \( A_c \). Thus, the logical subsystem \( L \) supported by \( \lambda \) is a NS under general collective noise. In other words, \( \mathcal{H}_{1/2} \) can be pictured as the state space of two abstract qubits - \( L \), which is fully protected against collective errors, and \( Z \), which carries all the entropy inserted by the noise. The stability of information encoded in \( L \) against all error operators in \( A_c \) characterizes \( L \) as an infinite-distance QEC code for collective noise [103]. Since four physical qubits are required for attaining the same goal via a DF subspace [99], the three-qubit NS realizes the smallest one-bit noiseless quantum memory under \( A_c \).

The outline of our experiment is given in Fig. 3-8. In terms of the single-qubit input \( \rho_{in} \) and output \( \rho_{out} \) for the data spin alone, the overall effect of the procedure is described by a one-bit quantum operation that maps \( \rho_{in} \mapsto \rho_{out} = \mathcal{Q}(\rho_{in}) \). Ideally, \( \rho_{out} = \rho_{in} \). In the presence of unavoidable imperfections, we invoke the entanglement fidelity \( F_e [47] \) as the appropriate measure for quantifying the preservation of the quantum data. For a given process \( \mathcal{Q} \), \( F_e(\mathcal{Q}) \) equals one if and only if \( \mathcal{Q} \) perfectly preserves every input state. A complete characterization of \( \mathcal{Q} \) from experimentally available data can be obtained via "quantum process tomography" [55], which relies on measuring the output states generated from a complete set of independent input states. Let \( |+\rangle = (|0\rangle + |1\rangle)/\sqrt{2} \) and \( |+i\rangle = (|0\rangle + i|1\rangle)/\sqrt{2} \), respectively. Under the assumption that \( \mathcal{Q} \) describes a "unital" process for which \( \mathcal{Q}(1) = 1 \), \( F_e(\mathcal{Q}) \) can be calculated as [110]

\[
F_e(\mathcal{Q}) = \left( F_{|0\rangle} + F_{|+\rangle} + F_{|+i\rangle} - 1 \right) / 2
\]

where \( F_{|\psi_{in}\rangle} = Tr\{|\psi_{in}\rangle\langle\psi_{in}| \mathcal{Q}(|\psi_{in}\rangle\langle\psi_{in}|)\} \) is the input-output fidelity for the intended one-bit pure input state \( |\psi_{in}\rangle \).

Our implementation was performed via liquid-state nuclear magnetic resonance (NMR) on a sample of \(^{13}\)C labeled alanine (Fig. 2-1) in \( D_2O \) solution, using a 300 MHz Bruker Avance spectrometer. NMR QIP has been extensively discussed in the literature [70]. Room temperature NMR qubits exist in highly mixed, separable states. Thus, NMR QIP relies on "pseudo-pure" (p.p.) states whose traceless (or "deviation") component is proportional to that of the corresponding pure state. The identity component of the density matrix is unobservable and can be treated as a constant under the assumption of unital dynamics\(^2\). Initialization of the qubits in one of the p.p. input states \( \rho_{in}^{pp} = |0\rangle_1 \langle 0| \otimes |0\rangle_2 \langle 0| \otimes |\psi_{in}\rangle_3 \langle \psi_{in}| \), where \( |\psi_{in}\rangle = |0\rangle, |+\rangle, |+i\rangle \), was accomplished using standard gradient-pulse techniques. A sequence of transformations generating the above states from the 3-spin thermal equilibrium state, as well as other implementation details, can be found in Table 3.1. State preparation was verified by tomographically reconstructing the resulting 3-spin deviation den-

\(^2\)We explicitly verified this assumption by tomographically reconstructing the super-operator corresponding to the processes \( Q_{0,m} \). We found a maximum absolute deviation from identity, \( \max|1 - Q_{0,m}(1)| \sim 4\% \).
Figure 3-8: **Logical quantum network for the NS experiment.** The information is initially stored in qubit 3, while qubits 1 and 2 are initialized in the state $|0\rangle$. A unitary encoding transformation $U_{\text{enc}}$ is applied to map the initial input state space into the NS $|1\rangle$. A time delay follows, during which the qubits are stored in the NS memory. Applying the unitary transformation $U_{\text{dec}}$ returns the information to the state of carbon 2. Encoding and decoding networks are expressed in terms of controlled rotations. $U_{\text{enc}}$ is a simplified version of $U_{\text{dec}}^{-1}$ obtained by exploiting the knowledge of the initial non-data bits. For $|\psi_{in}\rangle = \alpha|0\rangle + \beta|1\rangle$ with arbitrary complex $\alpha, \beta, |\alpha|^2 + |\beta|^2 = 1$, $U_{\text{enc}}$ implements a transformation $U_{\text{enc}}(|0\rangle_1 \otimes |0\rangle_2 \otimes |\psi_{in}\rangle_3) = |\psi_{in}\rangle_L \otimes |1/2\rangle_Z$. A collective noise process $\mathcal{E}_{\text{coll}} = \{E_a\}$ only affects the Z subsystem. $U_{\text{dec}}$ decodes a generic noisy state $E_a(|\psi_{in}\rangle_L \otimes |1/2\rangle_Z)$ in $\mathcal{H}_{1/2}$ to the computational basis, $U_{\text{dec}}[(\alpha|0\rangle_L + \beta|1\rangle_L) \otimes (c_a|1/2\rangle_Z + d_a|1/2\rangle_Z)] = \alpha c_a|000\rangle + \beta c_a|010\rangle + \alpha d_a|001\rangle + \beta d_a|011\rangle$ for appropriate coefficients. This produces the intended state of qubit 2 upon discarding spins 1 and 3 i.e., $\text{Tr}_{1,3}[U_{\text{dec}}[\mathcal{E}_{\text{coll}}(|\psi_{in}\rangle_L \langle\psi_{in}| \otimes |1/2\rangle_Z \langle -1/2|)]U_{\text{dec}}^\dagger] = |\psi_{in}\rangle_2 \langle\psi_{in}|$. 


sity matrix. An amount of identity component able to optimize the fidelity with the intended 3-spin p.p. state was added to the experimental $\rho_{\text{pp}}$, and maintained throughout the analysis\(^3\). The evolution of a p.p. state is equivalent to the corresponding pure-state evolution under unital dynamics. The logical manipulations involved in the NS encoding and decoding were mapped into ideal pulse sequences via standard quantum network methods [70]. Conditional gates between qubits 1 and 3 were replaced by compositions of operations between pairs (1,2), (2,3) to avoid employing the slow (1,3)-coupling. Once the logical operations were translated into sequences of RF pulses and delays, complete pulse programs for $U_{\text{enc}}, U_{\text{dec}}$ resulted from the compilation of the partial pulse programs for individual gates. Consecutive pulses were combined whenever possible to allow for a faster implementation. Pulses were implemented by modulating the internal Hamiltonian of the alanine molecule (Fig. 2-1) with externally controlled RF magnetic fields, as described in chapter 2. Robust pulses were not used in the implementation, but the pulses were corrected with the RF feedback procedure.

To investigate the NS performance in a controlled way, the time delay between encoding and decoding is designed to implement a net evolution of the spins under a desired collective noise model. Unwanted, symmetry-breaking dynamics generated by the molecule’s internal Hamiltonian were refocused via standard average Hamiltonian techniques [70]. A variety of collective noise processes can be engineered through gradient-diffusion methods [12, 111]. A pulsed magnetic field gradient $\partial B_z/\partial z$ parallel to the static quantizing field $B_z$ causes the spins to precess with a $z$-dependent Zeeman rate – thereby acquiring a phase factor that is identical\(^4\) for each species but varies linearly with $z$. These spatially dependent phases add incoherently to zero when the integrated signal from the sample is measured. Thus, the action of a strong gradient pulse over the ensemble amounts to an incoherent implementation of all the possible collective phase errors, emulating the error algebra $\mathcal{A}_z$ of the strong dephasing regime. Collective noise along an arbitrary axis is induced by sandwiching a $z$-noise between RF pulses effecting a collective rotation of the spin state to the desired axis [111]. The incoherent action of a single gradient pulse could be refocused by a second inverse gradient. A truly irreversible, decoherent implementation of collective noise is obtained by allowing for molecular diffusion to take place for a time $\Delta t$ before applying an inverse gradient. Because the molecules have moved, the spins’ phases are not returned to their original values but are randomly modified. Thus, the combined gradient-diffusion action results in an exponential signal loss whose effective decay rate $1/\tau$ is proportional to the diffusion constant and tunable with the gradient intensity [12].

Decoherent collective noise of variable strength was engineered by stepping the

\(^3\)Optimization of the fidelity with respect to the intended 1-spin p.p. state for the data carbon alone results in an amount of identity component that is equal to the one based on the corresponding 3-spin p.p. state within the experimental accuracy.

\(^4\)For a given species, e.g. $^{13}$C, the gradient action is symmetric to an accuracy substantially better than 0.1%. By contrast, dephasing processes naturally occurring in alanine are dominated by non-collective effects reflecting the different chemical environment of each carbon.
gradient amplitude from 0 to the maximum achievable value of about 0.5 T/m, and applied for a fixed evolution time $t_{ev}$. All noise strengths $1/\tau$ were calibrated by independent measurements using a gradient stimulated echo sequence [12]. The attained ratios $t_{ev}/\tau$ are sufficient to push the evolution beyond the weak-noise regime dominated by first-order phase errors that can be compensated for by QEC [34]. Separate experiments were performed to expose the NS-encoded qubit and the un-encoded data spin, $C_3$, to single-axis collective $z$ and $y$ noise (Fig. 3-9). Both the un-encoded and NS-encoded data are fit to a decaying exponential model\(^5\), $F_e = A_1 \exp(-t_{ev}/\tau) + B$. The asymptotic $F_e$ value given by $B$ is a relevant figure of merit for lower-bounding the entanglement fidelity attainable for single-axis noise of arbitrary strength. The test data is expected to decay under a single-qubit dephasing channel along $y$, i.e. $A_1 = B = 0.50$ – as opposed to the observed values of $A_1 = 0.51 \pm 0.04$, $B = 0.43 \pm 0.03$. For the NS data, the theory predicts a constant unit $F_e$. In the experiment, both a constant term, $B = 0.64 \pm 0.02$ ($y$) and $B = 0.64 \pm 0.02$ ($z$), and a small decaying contribution, $A_1 = 0.03 \pm 0.03$ (both $y$ and $z$) are seen. For both the NS- and the un-encoded cases, departures from the ideal values are explained by pulse imperfections and by natural relaxation processes, whose action is assumed to be independent of the applied noise strength. Several remarks are in order concerning the NS data. First, the fact that $A_1$ is compatible with zero suggests that the measured signal predominantly originates from the NS, as signal from other locations would necessarily decay with increasing applied noise. Second, because $B$ well exceeds the threshold 0.50, the implementation guarantees entanglement preservation for arbitrary noise strength [112]. Finally, even with the current implementation errors, the fidelities achieved for sufficiently strong noise imply an actual improvement in preserving quantum information via the NS code.

A variety of incoherent collective error processes were also implemented to explore exhaustively the NS robustness under strong single- and multiple-axes noise that fully probe the non-abelian error algebra of general collective noise. Incoherent implementations have the advantage that full-strength error models can be induced quickly compared to the natural relaxation time scales. The experimental data for both un-encoded and NS-encoded evolutions are summarized in Table 3.2. As in the decoherent case, the $F_e$ values for single-axis noise, $E_\alpha$, $\alpha = x, y, z$, demonstrate the infinite error-correcting behavior of the NS code against errors in the corresponding abelian subalgebra $A_\alpha$. Robustness against the full $A_c$ is verified through the composite processes ($Q_{xx}$, $Q_{zy}$, $Q_{pzz}$) obtained by sequentially implementing evolution periods corresponding to single-axis error models along different directions. The measured input-output and entanglement fidelities are consistent with the expectation that single-axis and composite noise processes induce full phase-damping and full depolarization on the data bit – with predicted fidelities of 0.50 and 0.25, respec-

\(^5\)We initially fit the data to a multi-exponential model, $F_e = \sum_n A_n \exp(-n^2 t_{ev}/\tau) + B$, that accounts for the possible single, double, and triple ($n = 1, 2, 3$) decay modes of quantum coherences in a three spin system. From the resulting best estimates we confirm that contributions from double ($A_2$) and triple ($A_3$) quantum coherence terms, arising from unintentionally populated states outside $\mathcal{H}_{1/2}$, are negligibly small.
Figure 3-9: Experimentally determined entanglement fidelities for the decoherent implementation of single-axis collective error models. We used a diffusion time $\Delta t \sim 34$ ms and gradient times $\delta \sim 5$ ms, giving a fixed $t_{ev} = 2\delta + \Delta t \sim 44$ ms. Variable-strength collective noise along either the y axis (NS-encoded (squares) and un-encoded data (triangles)) or the z axis (NS-encoded data only (circles)) was applied during $t_{ev}$. The decay of the un-encoded spin, $C_3$, was measured by turning off the NS-encoding and decoding sequences. Both the un-encoded and encoded data are fit to an exponential decay, with the interpolated (solid) and extrapolated (dashed) lines shown in the plot. Best estimates and uncertainties of the parameters are also given. The relatively large error bars of the data arise from a conservative estimate of the uncertainties associated with the noise strength determination.
| Quantum process | $F_{|0\rangle}$ | $F_{|+\rangle}$ | $F_{|+\rangle}$ | $F_e$ |
|----------------|----------------|----------------|----------------|-------|
| $Q_{x,un}$     | 0.50           | 0.97           | 0.49           | 0.48  |
| $Q_{0,ns}$     | 0.84           | 0.74           | 0.78           | 0.68  |
| $Q_{x,ns}$     | 0.79           | 0.74           | 0.78           | 0.66  |
| $Q_{y,ns}$     | 0.81           | 0.77           | 0.82           | 0.70  |
| $Q_{z,ns}$     | 0.86           | 0.72           | 0.76           | 0.67  |
| $Q_{xx,un}$    | 0.49           | 0.50           | 0.50           | 0.24  |
| $Q_{00,ns}$    | 0.80           | 0.79           | 0.80           | 0.70  |
| $Q_{zz,ns}$    | 0.78           | 0.80           | 0.82           | 0.70  |
| $Q_{zy,ns}$    | 0.79           | 0.80           | 0.82           | 0.70  |
| $Q_{000,ns}$   | 0.77           | 0.79           | 0.78           | 0.67  |
| $Q_{yzz,ns}$   | 0.75           | 0.80           | 0.77           | 0.66  |

Table 3.2: Summary of experimental data for the incoherent implementation of various collective error models. The first column lists the one-bit quantum processes realized in the experiment. Gradient fields with maximum strength $\sim 0.5 \text{ T/m}$ were applied during a fraction $\delta \sim 0.5 \text{ ms}$ of the evolution period, $t_{ev} \sim 3, 6, 9 \text{ ms}$ for single-, double-, and triple-axes error models, respectively. In addition to the applied error model, $E_x, E_y, E_z, E_{xy}, E_{xz}, E_{yz}, E_{xzz}$, the channel label specifies whether (ns) or not (un) encoding and decoding procedures were implemented. The processes $Q_{0,ns}$, $Q_{00,ns}$, $Q_{000,ns}$ differ in the length of the evolution period over which they apply the trivial error model (i.e., the identity evolution). For each process, the input-output fidelities $F_{|\psi_0\rangle}$ involved in the process tomography as well as the resulting entanglement fidelities $F_e$ are listed. Statistical uncertainties are $\sim 2\%$, arising from errors in the tomographic density matrix reconstruction.

Infinite-distance error-correcting behavior with respect to $A_e$ is established by the unchanged fidelity levels observed in the presence of the applied noise relative to the corresponding no-error case. The data show a substantial increase in the amount of information retained under the action of the applied error models.

NSs provide extremely efficient means of preserving quantum information whenever a dominant symmetry occurs in the noise. Therefore, symmetry should be a leading criterion for engineering future QIP. We have shown that the implementation of NSs is within the reach of current quantum information technologies. Although the attained fidelities are less than ideal and point to the need for improved quantum control capabilities, our implementation demonstrates for the first time improvement in error-correcting a class of both abelian and non-abelian error models via an infinite-distance one-qubit quantum code. The encoding, decoding, and verification techniques used here are readily exportable to other quantum information devices, where the dominant noise mechanisms are collective in nature. Besides providing the chief source of ambient noise in trapped ion QIP [28], collective noise behavior is also expected to be predominant in solid-state architectures at low temperatures.
[113]. NS coding, possibly combined with appropriate fault-tolerant and active control methods, can thus play a practical role for both reliable storage and manipulation of quantum information in future QIP.
Figure 3-10: Alanine spins as system and environment. The carbons represent the system and the protons the environment. In the array, the diagonals contain the corresponding chemical shifts, while the other terms are the coupling constants between the spins. All values are listed in Hz.

### 3.5 Quantum Error Correction with Dynamical Decoupling

One of the crucial tasks in realizing Quantum Information Processing (QIP) is to develop methods for counteracting the nonunitary features of open quantum systems like decoherence and dissipation. Schemes such as quantum error correction (QEC) [114, 115, 116], decoherence-free subspaces [117, 101], noiseless subsystems [103] and decoupling [118, 119, 41] have aimed at protecting against such effects. All these techniques have been tested and verified experimentally using ion traps [28] or nuclear magnetic resonance [35, 44, 34]. While QEC is a general method of counteracting decoherence, it requires extra quantum bits (or qubits) called ancillae[120]. For a known noise source with a correlation time significantly longer than the inverse of the available system modulation rate, decoupling saves significant ancillae resources. The key requirements for effective decoupling are that the procedure has to be performed quickly compared to the correlation time of the environment, and that the external Hamiltonian introducing the modulation must not commute with the noise operator [121, 122, 8]. Recently, questions have been raised concerning the validity of QEC when environmental correlation times are long [123]. In such a case, the noise acts non-locally and memory effects result in a non-Markovian evolution. Although it is not clear that these problems have been fully addressed theoretically, this report demonstrates the utility of decoupling concatenated with QEC to protect both against coherent noise with memory effects and small random phase errors.

The specific problem we address in this paper is the following: given a coupling

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5This section was extracted from N. Boulant, M. A. Pravia, E. M. Fortunato, D. G. Cory, and, T. F. Havel, “Experimental Concatenation of Quantum Error Correction with Dynamical Decoupling,” submitted for publication, 2002.

69
Figure 3-11: **Logic network for the concatenation code.** Note that the protons are included in the network but no operation is applied on them since an environment is by definition inaccessible.

Hamiltonian between the system and the local environment of the form $\sigma_z \otimes \sigma_z$, can we save costly ancillae qubits using decoupling while still protecting a qubit $\psi$ for a given amount of time? While QEC techniques alone could correct for these errors, decoupling is more efficient but can only correct for part of the errors. We show in detail how to combine these two approaches to achieve the best of each. This demonstration was carried out on a liquid-state NMR quantum information processor [70, 71], using the $^{13}C$ spin $\frac{1}{2}$ nuclei in a sample of alanine (Fig. 3-10) as qubits. An overview of the experiment is given in Fig. 3-11. The QEC code implemented has been studied previously [34, 124], and is designed to correct for independent small random phase errors. In addition to the stochastic environmental noise modulated by random molecular motions (natural relaxation), we permit the protons to act as an environment with a long correlation time. Experimentally, the relevant correlation time ($T_1$) of the protons is 2.8s for "H" and 1.5s for "M" (the methyl group). Two experiments were performed: in the first the system evolved under the $\sigma_z^C \otimes \sigma_z^H$ coupling, after the qubit to be protected has been properly encoded. The fidelity of state preservation was measured after the decoding sequence and the error correction. In the second experiment, coherent evolution between the system and the local environment was refocused by decoupling during the storage time.

In room temperature liquid-state NMR, one can coherently manipulate the internal states of the coupled spin $\frac{1}{2}$ nuclei in each of an ensemble of molecules subjected to a large external magnetic field. Although the system's density matrix is highly mixed, it has been shown that it can be transformed into a pseudo-pure state whose deviation part mimics a pure state [29, 30]. In the experiments to be described, the $^{13}C$ labeled nuclei were taken as the open quantum system, and the coupled protons represented the environment. Since the protons are coupled to the carbon spins, for times short compared to the proton spin-lattice relaxation time the coupled dynamics can be described by a Hamiltonian,

$$N = \sum_{i=1}^{3} \sigma_{i}^C \cdot (\alpha_{iH} \sigma_{i}^H + \alpha_{iM} \sigma_{i}^M)$$  \hspace{1cm} (3.26)
where the $\sigma$ are the Pauli spin operators, $\alpha_{iH}$ and $\alpha_{iM}$ are coupling constants, and the $^{13}C$ and $H$ atoms have been labeled according to Fig. 3-10. The values of the coupling constants are listed in Fig. 3-10. During the storage time, for demonstration purposes we wish to implement a "noise" involving the coupling $\sigma_z^i \otimes \sigma_z^e$ of qubit $i$ to environmental qubit $e$, while suppressing the remainder of the internal Hamiltonian. Further we wish to accomplish this through control of the system qubits only. One method of implementing this noise is shown in Fig. 3-12. In such a case, the evolution of the initial open system alone is not Markovian, the proton-carbon interaction is coherent and will yield recurrences. Such memory effects can be removed using decoupling methods provided the correlation time between the system and the environment is long compared to the time necessary to perform the refocussing sequence. In general, for a fluctuating field $< B^2(t) >$ with correlation time $\tau_c$, one can average out the unwanted interactions provided the system is modulated faster than $1/\tau_c$. Average Hamiltonian theory (AHT) [8] provides a systematic method for describing any unitary propagator $U(T)$ resulting from the evolution under the time-varying Hamiltonian $H_S = H_{\text{int}} + H_{\text{ext}}$ in terms of an effective Hamiltonian $\overline{H}$ applied over the same time interval. The basic idea is to apply on the system a cyclic train of pulses $P = \{P_j\}_{j=1}^M$ with $\Pi_{j=1}^MP_j = 1$ which, in the simplest setting, are assumed to be infinitely short and equally spaced by $\Delta t > 0$. The net controlled evolution over the period $T = M\Delta t$ can then be expressed as

$$e^{-i\overline{H}T} = \prod_{k=0}^M e^{-iH_k \Delta t} ,$$

where the "toggling-frame" Hamiltonians $H_k$ are determined as $H_k = U_k^\dagger H_{\text{int}} U_k$, in terms of the composite pulses $U_k = \Pi_{j=1}^k P_j$, $k = 1, \ldots, M$, $U_0 = 1$ [8]. By appropriately designing the pulse sequence $P$, unwanted interactions in the internal Hamiltonian can be averaged out. Of course, if QEC were repeated fast enough, then it would also correct the coherent errors. For a coupling value of 100 Hz, a period of 1ms suffices to decrease the fidelity by 0.001. This would require four cnot gates and one resetting of the ancillae (qubits 1 and 3) in less than 1ms to correct for these errors using QEC. Therefore, although QEC can correct for such coherent errors, decoupling techniques can be a more efficient approach. However, nothing so far would require a concatenation of both techniques since either could in this case correct for the same sort of errors. We therefore show that decoupling techniques can be used to correct for most of the phase errors using only four pulses on the system, but that QEC can still be used to correct for the remaining stochastic phase errors, coming from natural relaxation. In other words, the high frequency components of the noise sources will survive [118, 119], but can be removed by QEC. Armed with these control methods we now experimentally explore the suppression of decoherence via a combination of decoupling and QEC.

The experiments were performed on a Bruker Avance 300 MHz spectrometer, using the robust strongly modulating pulses described in chapter 2. We stress that, once the NMR spectrometer had been calibrated and the strongly modulating pulses programmed into it, no further adjustments of any kind were required during the course
Figure 3-12: **Scheme for implementing the noise operator.** The whole sequence is split into 3 equal parts of duration $T$. For each period, one qubit evolves with the protons under the scalar coupling term but also under the chemical shift term of the internal Hamiltonian. Each block represents a selective $\pi$ pulse about the X or Y axis while the three last pulses are individual Z rotation pulses to refocus the chemical shift evolution mentioned above.

of the many measurements that made up this study. The scheme used to exclusively implement the evolution of the coupling between the carbons and the protons, or to refocus it, was derived from [53, 50]. Because at the end of the experiment we were interested in how well the state of the data qubit was preserved, we implemented a modified Toffoli gate, i.e. a gate whose net result on the latter qubit is the same as when one does apply a Toffoli, but which changes the states of the ancillae qubits [124]. To measure the effects of the interaction Hamiltonian between the system and the environment in addition to our ability to refocus these interactions, we calculated the metric used in [44], derived from the entanglement fidelity defined in [47],

$$F = \frac{(F(\psi_0) + F(\psi_+)+ F(\psi_{++}) - 1)/2}{2} \tag{3.27}$$

where $F(\psi) = \langle \psi | \rho | \psi \rangle$ is the input-output fidelity and measures the amount of information retained in the system, $\rho$ is the final density matrix and $\psi_0 = |0\rangle$, $\psi_+ = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $\psi_{++} = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$ are the eigenfunctions of the $\sigma_z$, $\sigma_\xi$ and $\sigma_y$ operators respectively. Here, the computational basis $|0\rangle$ and $|1\rangle$ corresponds to the spins being parallel or anti-parallel to the $z$-axis. The experiment was repeated for each eigenstate and for each noise scenario. In all cases, the two ancillae qubits were initialized to $|00\rangle$. The pulse sequences to prepare the initial states and to implement the encoding and decoding sequences can be found in [124, 43, 93, 92]. The density matrices were reconstructed by state tomography [54, 125]. Since only single quantum coherences can be directly observed, tomography involves repeating the experiment several times followed by a different readout pulse sequence each time. Only two readout sequences each composed of a single pulse were needed since only the state of spin 2 is of interest. However, for the sake of completeness, a three-spin density matrix reconstruction was carried out using seven readout pulses [126], right before the encoding sequence to verify and measure the quality of the initialization.
Figure 3-13: Short time information loss. The plots show the entanglement fidelity as a function of the evolution time (from 1 up to 15ms) with and without decoupling, but with QEC in both cases. In the absence of decoupling, the coherent scalar coupling between the proton “environment” and carbon qubits introduces the observed oscillation.

$F(\psi)$ was measured to be 0.99 for $\psi_0$, $\psi_+$ and $\psi_{+t}$, demonstrating relatively good state preparation. The results of the experiment are summarized in Figs. 3-13 and 3-14.

Fig. 3-13 shows the entanglement fidelity with respect to time for QEC with and without decoupling the protons. In the absence of decoupling, an oscillatory behavior is seen due to the coherent evolution with the environmental protons. This can also be seen as recurrences due to the finiteness of the number of coupled spins in the environment. In this case, information flows back and forth between the system and the local reservoir so the evolution of the system is non-Markovian. With decoupling, the fidelity remains high and the large oscillation is removed. The average entanglement fidelity over the whole time interval in this case is 0.79. Here the effective modulation frequency of decoupling is 4 kHz, well above the inverse correlation time (proton $T_1$).

Fig. 3-14 demonstrates the improvement in fidelity available from QEC, beyond that available with decoupling alone. Since decoupling removes only the slowly varying environmental terms we rely upon QEC to remove the remainder (mostly dipolar interactions modulated by the random molecular motions). The improvement in performance is evident from the relative flatness of the plot (with QEC). The difference in the implementation between “with and without QEC” is only whether or not we applied the final correction, i.e. the modified Toffoli gate. The encoding and decoding sequences were implemented in both cases. Note that in related work [126] we have developed strongly modulating control sequences that rely on coherent averaging to remove unwanted evolution during the pulses, including that of an environment with long correlation times and weak strengths compared to the control resources. As a result, decoupling is also used during the control pulses.

Fig. 3-14 therefore shows the effect of concatenating both methods. In the long time regime, one can see the effect of using QEC. The solid lines in the figure were obtained by fitting an exponential function (without QEC) and fitting the short time
Figure 3-14: Long time information loss. The plot shows the entanglement fidelity with respect to the evolution time (20 time points equally spaced from 20ms) between the carbons and the protons with the decoupling scheme, with and without QEC. For the sake of clarity, the last plot shows the two fitted curves.
data points (up to 100ms) with the function presented in [124] for uncorrelated errors, i.e.

\[ f = \gamma + \frac{1}{2}(3\exp(\alpha t) - \exp(-3\alpha t)) \]  

(3.28)

and then extrapolating (\(\chi^2/DOF = 1.38\) and number of degrees of freedom=18). Clearly, QEC decreases the initial slope substantially. This is expected in that the QEC code implemented is able to correct for stochastic random phase errors included in the natural noise that the decoupling scheme was not able to counteract. The last plot of Fig. 3-14 shows on a logarithmic scale for the Y axis the difference between the implementation or not of QEC to emphasize the initial slope, and the improvement in the long time regime when the QEC is implemented, in spite of the higher initial entanglement fidelity when the QEC was not implemented.

In conclusion, we have explored the experimental concatenation of a decoupling scheme and of a quantum error-correcting code designed to correct for small random phase errors. We showed that provided with some knowledge about the noise, one can concatenate both QEC and decoupling methods to protect more efficiently quantum information against an undesired coherent evolution and stochastic phase errors. The relevant three and one spin density matrices were reconstructed and the entanglement fidelities calculated. Such procedure could become useful in future quantum information processing devices that would need to be protected against a wide variety of noise.
Chapter 4

Quantum Lattice Gas Computation

The field of quantum information processing (QIP) has made steady progress in the past decade, driven in part by the realization that some quantum algorithms offer a computational advantage over the best-known classical counterparts[127]. To reach a practical improvement, however, quantum algorithms require precise control in a large Hilbert space, making physical implementations difficult. Recently, it has been suggested that some interesting problems might be solvable by a hybrid classical-quantum device defined as a type-II quantum computer[128]. A type-II quantum computer is essentially a parallel lattice of small quantum information processors that share information through classical channels. Such a device offers the experimental simplification that quantum coherences only exist within each small quantum processor. Using this architecture, it might be possible to increase the range of problems that small quantum processors can tackle by classically stringing many of them together. A type-II quantum computer may thus serve as an intermediate architecture between few-qubit and large-scale quantum computers.

Here, we explore the experimental aspects of building a type-II quantum computer using nuclear magnetic resonance (NMR) techniques[50]. QIP experiments utilizing NMR typically employ a liquid sample of molecules containing spin-$\frac{1}{2}$ nuclei. The sample is subjected to a strong magnetic field $B_0$ of order $\sim 10$ T creating an energy difference $\Delta E$ between the aligned and antialigned spin states that results in an equilibrium state with net magnetization. At room temperature, $\Delta E/k_BT$ is about $10^{-5}$, so that the net magnetization is relatively small, but, given the large number of molecules in the sample ($\sim 10^{18}$), it is still easily detectable. The entire spin ensemble is accurately described by a reduced density matrix of only the intramolecular spin degrees of freedom. The ensemble nature of the NMR sample thus makes it inherently applicable to parallel computation. A type-II architecture can be mapped onto an NMR sample by creating a correspondence between the sites of the lattice and spatially distinct spin ensembles. Using magnetic field gradients and radio frequency (RF) pulses, information in the lattice can be encoded, manipulated, and read out.

\footnote{This section was extracted from M. A. Pravia, Z. Chen, J. Yepez, D. G. Cory, "Experimental Demonstration of Quantum Lattice Gas Computation," submitted for publication, 2002.}
4.1 Lattice Gas Algorithms

The lattice gas method is a tool of computational physics used to model complex hydrodynamical flows that are too large for a standard low-level molecular dynamics treatment and that contain discontinuous interfacial boundaries that prevent a high-level partial differential equations description. [129, 130, 131, 132] The basic idea underlying the lattice gas method is to statistically represent a macroscopic scale time-dependent field quantities by “averaging” over repeated instances of a system of artificial microscopic particles scattering and propagating throughout a lattice of interconnected sites. A particular instance of the system has many particles distributed over the lattice sites. Multiple particles may coexist at each site at a given time, and each particle carries a unit mass and a unit momentum of energy. Particles interact on site by an artificial collision rule which is locally invariant under the point-group symmetries of the lattice, and, furthermore, which exactly conserves the total mass, momentum, and energy at that site. The movement of particles along the lattice is prescribed by a streaming operation that shifts particles to nearest neighboring sites, thus endowing the particles with the property of momentum. In a maximally discrete way, the algorithm encapsulates the microscopic scale kinematics of the particles scattering on site and moving along the lattice. The mean-free path length between collisions is about one lattice cell size and the mean-free time between collision elapses after a single update. This is computationally simple in comparison to molecular dynamics where many thousands of updates are required to capture such particle interactions.

The mesoscopic evolution is obtained by taking the ensemble average over many instances of microscopic realizations. At the mesoscopic scale, the average presence of each particle type is defined by a real-valued occupation probability. In addition, the microscopic collision and streaming rules translate into the language of kinetic theory. The behavior of the system is described by a transport equation for the occupation probabilities, and this equation is a discrete Boltzmann equation called the lattice Boltzmann equation.

The lattice Boltzmann equation further translates into a macroscopic, continuous, effective field theory by letting the cell size approach zero (the limit of infinite lattice resolution called the continuum limit). At the macroscopic scale, partial differential equations describe the evolution of the field, admitting solutions such as propagating sound wave modes and diffusive modes. The passage of the Boltzmann equation to the effective field theory begins by expanding the occupation probabilities, which have a well-defined statistical functional form, in terms of the continuous macroscopic variables, such as the mass density $\rho$ (and the velocity or energy field if they are defined in the model). This expansion usually is carried out perturbatively in a small parameter such as the Knudsen number (ratio of mean-free path to the largest characteristic length scale) or the Mach number (ratio of the sound speed to the largest characteristic flow speed) in a fashion analogous to the Chapman-Enskog expansion of kinetic theory. Conversely, and self-consistently, the macroscopic field quantities can also be expressed as a function of the mesoscopic occupation probabilities—for example, the mass density at some point is a sum over the occupation probabilities

78
in that vicinity.

Quantum lattice gas (QLG) algorithms are generalizations of the classical lattice gas algorithms described above where quantum bits are used to encode the occupation probabilities and where the principle of quantum mechanical superposition is added to the artificial microscopic world. In this quantum case, the mesoscopic occupation probabilities are mapped onto the wave functions of quantum mechanical sites. In the case where the quantum lattice gas describes a hydrodynamic system when the time evolution of the flow field is required, we must periodically measure these occupation probabilities and the quantum lattice gas algorithm becomes suited to a type-II implementation. Such type-II algorithms have been shown to solve dynamical equations such as the diffusion equation [133], the Burgers equation [134], and magnetohydrodynamic Burgers turbulence [135]. As a first exploration of a type-II architecture using NMR, we implemented a QLG model of diffusive dynamics in one dimension.

4.2 Solving the 1-D Diffusion Equation

The quantum lattice gas algorithm that solves the 1-D diffusion equation derives from a classical lattice gas of particles moving up and down a 1-D lattice[133]. The motion of the particles occurs in discrete steps (streaming phase), and the particles have a probability of changing directions (collision). When the collisions are such that the particles reverse directions half of the time, then the continuum effective field theory that emerges obeys diffusive dynamics. In this case, the motion of an individual particle is a random walk, and an arbitrary initial distribution of particles will diffuse isotropically as a function of time.

The lattice gas described above is summarized by the Boltzmann equation

\[ f_{1,2}(z \pm \Delta z, t + \Delta t) = f_{1,2}(z, t) + \Omega_{1,2}(z, t), \]  

(4.1)

where the left-hand side denotes the occupation of the lattice as a function of the previous lattice configuration and where the collision term is

\[ \Omega_{1,2} = \pm \frac{1}{2} [f_1 (1 - f_2) - f_2 (1 - f_1)] \]  

(4.2)

The variables \( f_1 \equiv f_1(z,t) \) and \( f_2 \equiv f_2(z,t) \) are the occupation probabilities for finding upward- and downward-moving particles, respectively, at the site location \( z \) and time \( t \). The time step is denoted by \( \Delta t \), while the lattice spacing is given by \( \Delta z \). The collision term changes the direction of some particles, and it is responsible for the diffusive behavior.

The interesting macroscopic quantity of the lattice gas is the mass density field, \( \rho \), defined as the sum of upward- and downward-moving particles

\[ \rho(z, t) = f_1(z, t) + f_2(z, t). \]  

(4.3)
The ambiguity in assigning the mass density between the two occupation probabilities is resolved by a constraint for local equilibrium demanding that the mass density be initially distributed equally

$$f_1^{\infty}(n, 0) = f_2^{\infty}(n, 0) = \frac{1}{2} \rho(n \Delta z, 0).$$  \hspace{1cm} (4.4)

After a single time step, the occupation probabilities $f_1$ and $f_2$ evolve according to (4.1), resulting in a new mass density

$$\rho(z, t + \Delta t) = \frac{1}{2} \left[ \rho(z + \Delta z, t) + \rho(z - \Delta z, t) \right].$$  \hspace{1cm} (4.5)

The first finite-difference in time of the mass density field is then written as

$$\rho(z, t + \Delta t) - \rho(z, t) = \frac{1}{2} \left[ \rho(z + \Delta z, t) - 2\rho(z, t) + \rho(z - \Delta z, t) \right].$$  \hspace{1cm} (4.6)

In the limit where the lattice cell size and the time step approach zero ($\Delta z \to 0$ and $\Delta t \to 0$), the mass density field becomes continuous and differentiable. The second-order Taylor expansion of equation (4.6) about $z$ and $t$ can thus be written in the differential form

$$\frac{\partial \rho(z, t)}{\partial t} = \frac{\Delta z^2}{2\Delta t} \frac{\partial^2 \rho(z, t)}{\partial z^2}$$  \hspace{1cm} (4.7)

where it is now evident that $\rho$ evolves according to the diffusion equation with a constant transport coefficient $\frac{\Delta z^2}{2\Delta t}$.

Finally, in this implementation we consider an initial mass density $\rho(z, t = 0)$ whose evolution obeys the periodic boundary condition $\rho(z, t) = \rho(z + L, t)$, where $L$ is the length of the lattice. As a result, the initial mass density diffuses until the total mass is evenly dispersed throughout the lattice.

The corresponding quantum lattice gas algorithm description begins by encoding the occupation probabilities, and thus the mass density, in the states of a lattice of quantum objects. The streaming and collision operations are then a combination of classical and quantum operations, including measurements. The aim of the algorithm is to take an initial mass density field and to evolve its underlying occupation probabilities according to the Boltzmann equation (4.1). A schematic of the entire quantum algorithm is shown in Fig. 4-1. A single time step of the algorithm is decomposed into four sequential operations:

1. encoding of the mass density
2. application of the collision operator $\hat{C}$ at all sites
3. measurement of the occupation numbers
4. streaming to neighboring sites.

These operations are repeated until the mass density field has evolved for the desired number of time steps. In the first time step, the encoding operation specifies
the initial mass density profile, while in all the subsequent steps the encoding writes the results of the previous streaming operation. The final time step ends with the readout of the desired result, so operation 4 is not performed.

Each occupation probability is represented as the quantum mechanical expectation value of finding a two-level system, or qubit, in its excited state \(|1\rangle\). As a result, the state of the qubit encoding the value \(f_a(z, t)\) is

\[
|f_a(z, t)\rangle = \sqrt{f_a(z, t)}|1\rangle + \sqrt{1 - f_a(z, t)}|0\rangle.
\] (4.8)

It follows that a single value of the mass density is recorded in two qubits, one for each occupation number. The combined two-qubit wave function for a single node becomes

\[
|\psi(z, t)\rangle = \sqrt{f_1f_2}|11\rangle + \sqrt{f_1(1 - f_2)}|10\rangle + \sqrt{(1 - f_1)f_2}|01\rangle + \sqrt{(1 - f_1)(1 - f_2)}|00\rangle.
\] (4.9)

The kets \(|00\rangle\), \(|01\rangle\), \(|10\rangle\), and \(|11\rangle\) span the joint Hilbert space of the two qubits, and this is the largest dimension space over which quantum superpositions are allowed. As with the classical algorithm, the constraint for local equilibrium (4.4) forces the initial occupation probabilities at a node to be half of the corresponding mass density value.

The occupation numbers encoded in the two-qubit wave function \(|\psi(z, t)\rangle\) can be recovered by measuring the expectation value of the number operator \(\hat{n}_a\), as given in

\[
f_a(z, t) = \langle \psi(z, t) | \hat{n}_a | \psi(z, t) \rangle,
\] (4.10)

where \(\hat{n}_1 = \hat{n} \otimes \mathbf{1}, \hat{n}_2 = \mathbf{1} \otimes \hat{n}\), where \(\mathbf{1}\) is the 2 \times 2 identity matrix, and where the action of the single-qubit number operator \(\hat{n}\) returns 1 if qubit is in its excited state and 0 for the ground state.

The encoded occupation probabilities evolve as specified by the Boltzmann equation by the combined action of the collision operator, the measurement, and streaming. The collision operator contributes by taking the local average of the two occupation probabilities. This averaging (not to be confused with statistical coarse-grain averaging, time averaging, or ensemble averaging) is done by choosing the the collision operator \(\hat{C}\) to be the “square-root of swap” gate, written as

\[
\hat{C} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{2} + \frac{i}{2} & \frac{1}{2} - \frac{i}{2} & 0 \\
0 & \frac{1}{2} - \frac{i}{2} & \frac{1}{2} + \frac{i}{2} & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\] (4.11)

in the standard basis. The propagator \(\hat{C}\) induces local quantum entanglement. The same collision is applied simultaneously at every site, resulting in

\[
|\psi'(z, t)\rangle = \hat{C}|\psi(z, t)\rangle
\] (4.12)
Figure 4-1: **Quantum lattice gas algorithm for solving the 1-D diffusion equation.** The algorithm employs $N$ two-qubit sites to encode the discretized mass density. Each site codes for a single value of the mass density using the quantum state of the two qubits. The encoded information is subjected to a series of local transformations that evolve the system. The collision operator $C$ is the only entangling operation in the algorithm, and it creates quantum coherences limited to each two-qubit system. The streaming is executed by classical communication, and it moves the occupation numbers up and down the lattice as denoted by the arrows. The sectioned cylinder depicts the position of the sites in the NMR sample. Each site is physically realized as an addressable slice of isotopically-labeled Chloroform solution.
Using (4.10), the intermediate occupation probabilities of the wave function $|\psi'(z, t)\rangle$ are

$$f'_a(z, t) = \frac{1}{2} (f_1 + f_2) \quad (4.13)$$

as required for $a = 1, 2$. The third operation physically measures these intermediate occupation probabilities $f'_a(z, t)$ at all the sites. If the algorithm is performed on individual quantum systems, then the values are obtained by averaging over many strong quantum measurements of identical instances of each step. However, when the algorithm is performed using a large ensemble of quantum systems, as in the case of NMR, then a single weak measurement of the entire ensemble can provide sufficient precision to obtain $f'_a(z, t)$. A single time step is completed with the streaming of the occupation probabilities to the nearest neighbors, according to the rule

$$f_1(z - \Delta z, t + \Delta t) = f'_1(z, t) \quad (4.14)$$
$$f_2(z + \Delta z, t + \Delta t) = f'_2(z, t) \quad (4.15)$$

The information on the two qubits is shifted to the neighboring sites in opposite directions. The streaming operation is a classical step causing global data shifting, and it is carried out in a classical computer interfaced to the quantum processors. Together, the last three operations result in

$$f_{1,2}(z \pm \Delta z, t + \Delta t) = \frac{1}{2} [f_1(z, t) + f_2(z, t)]$$

which is the exact dynamics described by the Boltzmann equation (4.1).

### 4.3 NMR Implementation

#### 4.3.1 Spin System and Control

The goal of the NMR implementation is to experimentally explore the steps outlined by the diffusion QLG algorithm. For this two-qubit problem, we chose a room-temperature solution of isotopically-labeled chloroform ($^{13}$CHCl$_3$), where the hydrogen nucleus and the labeled carbon nucleus served as qubits 1 and 2, respectively. The chloroform sample was divided into 16 classically-connected sites of two qubits each, creating an accessible Hilbert space larger than would be available with 32 non-interacting qubits.

The internal Hamiltonian of this system in a strong and homogeneous magnetic field $B_0$ is

$$H_{\text{internal}} = -\frac{1}{2} (\gamma_H B_0) \sigma_1^1 - \frac{1}{2} (\gamma_C B_0) \sigma_2^2 + \frac{\pi J}{2} \sigma_1^1 \sigma_2^2 \quad (4.17)$$

where the first two terms represent the Zeeman couplings of the spins with $B_0$ and the last term is the scalar coupling between the two spins. The operators of the form $\sigma_k^a$ are Pauli spin operators for the spin $a$ and the Cartesian direction $k$. The choice
of chloroform is particularly convenient because the different gyromagnetic ratios, \( \gamma_H \) and \( \gamma_C \), generate widely spaced resonant frequencies. As a result, a RF pulse applied on resonance with one of the spins does not affect, to a good approximation, the other spin. In the 7 T magnet utilized for the implementation, the hydrogen and carbon frequencies were about 300 MHz and 75 MHz, respectively. The widely spaced frequencies allow us to write the two RF control Hamiltonians as acting on the two spins independently. More concretely, the externally-controlled RF Hamiltonians are written as

\[
H_{RF}^a(t) = -\frac{1}{2} \left[ w_x^a(t)\sigma_x^a + w_y^a(t)\sigma_y^a \right]
\]  

(4.18)

The RF Hamiltonians generate arbitrary single-spin rotations with high fidelity when the total nutation frequencies

\[
\nu_{RF}^a = \frac{1}{2\pi} \sqrt{|w_x^a|^2 + |w_y^a|^2}
\]

(4.19)

are much stronger than \( J \), the scalar coupling constant. The scalar coupling Hamiltonian and the single-spin rotations permit the implementation of a universal set of gates, and they are the building blocks for constructing more involved gates such as the collision operator \( \hat{C} \).

The lattice of quantum information processors is realized by superimposing a linear magnetic field gradient on the main field \( B_0 \), adding a position dependent term to the Hamiltonian having the form

\[
H_{\text{gradient}}(z) = -\frac{1}{2} \left( \gamma_H \frac{\partial B_z}{\partial z} \right) \sigma_z^1 - \frac{1}{2} \left( \gamma_C \frac{\partial B_z}{\partial z} \right) \sigma_z^2
\]

(4.20)

The variable \( z \) denotes the spatial location along the direction of the main field, while the constant \( \frac{\partial B_z}{\partial z} \) specifies the strength of the gradient. The usefulness of this Hamiltonian can be appreciated by noticing that the offset frequencies \( \Delta \Omega_{H,C} = \gamma_H, C \left( \frac{\partial B_z}{\partial z} \right) z \) of the spins vary with position when the gradient field is applied. Spins at distinct locations can thus be addressed with RF fields oscillating at the corresponding frequencies. In this way, the magnetic field gradient allows the entire spin ensemble to be sliced into a lattice of smaller, individually addressable sub-ensembles.

Using the coupling, RF, and gradient Hamiltonians described above, together with the appropriate measurement and processing tools, we can now describe in detail how the four steps of the diffusion QLG algorithm translate to experimental tasks. The lattice initialization step (1) uses the magnetic field gradients to establish sub-ensembles of varying resonant frequency addressable with the RF Hamiltonians. The collision step (2) makes use of both the RF and the internal coupling Hamiltonians to generate the desired unitary operation \( \hat{C} \). The readout (3) is accomplished by measuring the spins in the presence of a magnetic field gradient. And finally, the streaming operation (4) is performed as a processing step in a classical computer in conjunction with the next initialization step.
4.3.2 Lattice Initialization

The initialization of the lattice begins by transforming the equilibrium state of the ensemble into a starting state amenable for quantum computation. At thermal equilibrium, the density matrix is

\[ \sigma_{\text{thermal}} = \frac{1}{Z} \exp \left[ -\frac{H_{\text{internal}}}{k_B T} \right] \approx \frac{1}{2^2} + \epsilon \left[ \frac{\gamma_H}{\gamma_C} \sigma_z^1 + \sigma_z^2 \right] \]  

(4.21)

where \( \epsilon \) has a value on the order of \( 10^{-5} \) and \( Z \) is the partition function. The equilibrium state is highly mixed and the two spins have unequal magnetizations. To perform quantum computations, it is convenient to transform the equilibrium state into a pseudopure state [29, 30], a mixed state whose deviation part transforms identically to the corresponding pure state and, when measured, returns expectation values proportional to those that would be obtained by measuring the underlying pure state. Two transformations create the starting pseudopure state \(|00\rangle\) from the thermal state. First, the magnetizations of the two spins are equalized,

\[ \sigma_{\text{thermal}} \xrightarrow{\text{Equalize}} \sigma_{\text{equal}} = \frac{1}{2^2} + \frac{\epsilon}{2} \left( 1 + \frac{\gamma_H}{\gamma_C} \right) \left[ \sigma_z^1 + \sigma_z^2 \right] \]  

(4.22)

followed by a pseudopure state creation sequence that results in

\[ \sigma_{\text{equal}} \xrightarrow{\text{Pseudopure}} \sigma_{pp} = \frac{1}{2^2} + \frac{\epsilon \sqrt{3}}{4 \sqrt{2}} \left( 1 + \frac{\gamma_H}{\gamma_C} \right) \left[ \sigma_z^1 + \sigma_z^2 + \sigma_z^1 \sigma_z^2 \right] \]  

(4.23)

The equalization and pseudopure state creation sequences are described in detail in reference [136]. For clarity, we define the constant in front of the brackets to be \( \epsilon' \), allowing us to write the pseudopure state \( \sigma_{pp} \) in terms of the desired spinor \(|00\rangle\) as

\[ \sigma_{pp} = \left( \frac{1}{4} - \epsilon' \right) |00\rangle \langle 00| + \epsilon' |00\rangle \langle 00| \]  

(4.24)

Expressed in this manner, it is now more easily seen how a unitary transformation applied to \( \sigma_{pp} \) acts trivially on the term proportional to the identity, but it evolves the term \(|00\rangle \langle 00|\) as it would a pure state.

Individually addressing the sites of the lattice, as depicted in Fig. 4-1, is accomplished by selectively addressing slices of the cylindrical sample. The procedure is related to slice-selection in magnetic resonance imaging (MRI)[137], and it works by applying the gradient Hamiltonian in the presence of suitably shaped RF pulses. First, consider the Hamiltonian for a one-spin system subjected to a linear magnetic field gradient in the \( z \)-direction and to a time-dependent RF pulse applied in the \( y \)-direction. In this case, the Hamiltonian is

\[ H_{RF,G}(z, t) = -\frac{1}{2} \left( \gamma \frac{\partial B_z}{\partial z} \right) \sigma_z - \frac{1}{2} w_y(t) \sigma_y \]  

(4.25)
where the $\sigma_z$ term is the linearly-varying static field and the $\sigma_y$ term is the time-dependent RF. The Hamiltonian $H_{RF,G}(z, t)$ does not commute with itself at all times, so a closed-form and exact solution cannot be easily given without specifying the function $w_y(t)$. A valuable approach, however, is to consider the approximate evolution generated by $H_{RF,G}(z, t)$ during infinitesimal periods of the RF pulse. To first order, the evolution during the initial period $\Delta t$ becomes

$$U_{RF,G}(z, t = \Delta t) \approx \exp \left[ i \frac{1}{2} \left( \gamma \frac{\partial B_z}{\partial z} \Delta t \right) z \sigma_z \right] \exp \left[ i \frac{w_y(\Delta t) \Delta t}{2} \sigma_y \right]$$

By defining the term in the parenthesis as $\Delta k_z \equiv \gamma \frac{\partial B_z}{\partial z} \Delta t$, the evolution of an initial density matrix $\sigma_z$ through a single period becomes

$$U_{RF,G}\sigma_z U_{RF,G}^\dagger \approx \exp \left[ i \frac{\Delta k_z z}{2} \sigma_z \right] \sigma_z \exp \left[ -i \frac{\Delta k_z z}{2} \sigma_z \right] w_y(\Delta t) \Delta t + \sigma_z$$

where small angle approximations have been made. The first term is a spatial helix of the $x$ and $y$ magnetizations having a wavenumber $\Delta k_z$. The second term is the first order approximation to the magnetization remaining in the state $\sigma_z$. Another period of evolution will affect the $\sigma_z$ term as described, creating a new magnetization helix with wavenumber $\Delta k_z$. In addition, the initial helix will have its wavenumber increased by an amount $\Delta k_z$. The final result over many periods is the formation of a shaped magnetization profile having many components

$$\sigma_z \rightarrow \sum_{n=1}^{N} \exp \left[ i \frac{n \Delta k_z z}{2} \sigma_z \right] \sigma_z \exp \left[ -i \frac{n \Delta k_z z}{2} \sigma_z \right] w_y(n \Delta t) \Delta t + \sigma_z$$

Each term in summation can be interpreted as a cylindrical Fourier component of the $x$-$y$ magnetization weighted by the RF nutation rate $w_y(n \Delta t)$. The RF waveform specifies the magnitude of each spatial Fourier component, and the resulting spatial profile is the Fourier transform of the RF waveform[12]. An equivalent description is to say that, for weak RF pulses, the excited magnetization of the spins at a given resonance frequency is, to first order, proportional to the Fourier component of the RF waveform at that frequency. As a result, control of the appropriate RF Fourier component essentially translates to selective addressing of spatial frequencies, which in turn allows the excitation of particular spatial locations.

The Fourier transform approximation allows encoding of arbitrary shapes on the various spatial locations of one uncoupled nuclear species. For QIP, however, coupled spins are required to implement entangling operations. In particular, the chloroform carbons and protons are coupled together via the scalar coupling. Given that the required RF waveforms should be weak, the coupling interferes with the desired evolution. The effect of the coupling present while encoding on spin 1 is removed by applying a strong RF decoupling sequence on the second spin\textsuperscript{2}. The decoupling modulates the $\sigma_z^2$ operator in the interaction Hamiltonian, making its average over a cycle

\textsuperscript{2}The decoupling was accomplished by applying the pulse cycle $Q\bar{Q}Q\bar{Q}$ during the pos-
period equal to zero. As a result, the second spin feels an identity operation during the decoupling. Fig. 4-2 shows the complete RF and gradient pulse sequence. As can be seen from the diagram, the first encoding on qubit 1 was subsequently swapped to qubit 2, followed by a re-encoding of qubit 1. We chose this method because the smaller gyromagnetic ratio of $^{13}$C causes a narrower frequency dispersion in the presence of the gradients, making the carbon decoupling simpler.

As described above, the encoding process writes the desired shapes in the spatial dependence of each spin’s $x$-magnetization. The occupation numbers, however, are proportional to the $z$-magnetization, as can be seen when the number operator in the equation

$$f_a(n, m) = \langle \psi(n, m) | \hat{n}_a | \psi(n, m) \rangle,$$

(4.29)

is replaced with $\hat{n}_a = \frac{1}{2} (1 + \sigma_a^z)$ resulting in

$$f_a(n, m) = \frac{1}{2} [1 + \langle \psi(n, m) | \sigma_a^z | \psi(n, m) \rangle].$$

(4.30)

where second term in the brackets represents the $z$-magnetization. The encoding process is followed by a $\pi/2$ pulse that rotates the excited $x$-magnetization to the $z$ direction.

### 4.3.3 Collision and Swap Gates

After initialization, the next step is to apply the collision operator. For the QLG algorithm solution to the diffusion equation, the collision operator $\hat{C}$ is the square-root of swap gate. Expressed in terms of the Pauli operators, it is

$$\hat{C} = \exp \left[ -i \frac{\pi}{8} \left( \sigma_1^x \sigma_2^z + \sigma_3^y \sigma_2^2 + \sigma_3^1 \sigma_2^1 \right) \right]$$

(4.31)

where an irrelevant global phase has been ignored. Written in this form, the operation $\hat{C}$ can be decomposed into a sequence of implementable RF pulses and scalar coupling evolutions[67, 138] by noticing that the product operators in the exponent commute with each other, resulting in

$$\hat{C} = \exp \left[ -i \frac{\pi}{8} \sigma_3^y \sigma_2^z \right] \exp \left[ -i \frac{\pi}{8} \sigma_3^1 \sigma_2^1 \right] \exp \left[ -i \frac{\pi}{8} \sigma_3^2 \sigma_2^2 \right]$$

(4.32)

Expanding the first and last exponentials as scalar couplings sandwiched by the appropriate single-spin rotations results in

$$\hat{C} = \exp \left[ i \frac{\pi}{4} \sigma_3^1 \sigma_2^z \right] \exp \left[ i \frac{\pi}{4} \sigma_3^2 \sigma_2^2 \right] \exp \left[ i \frac{\pi}{4} \sigma_3^1 \sigma_2^1 \right] \exp \left[ i \frac{\pi}{4} \sigma_3^2 \sigma_2^2 \right].$$

Expansive and negative gradients. The element $Q$ is a composite $\pi$ pulse implemented with four sequential pulses having nutation angles $80.4^\circ, 362.0^\circ, 181.6^\circ, 180.8^\circ$ and respective phases $271.3^\circ, 132.4^\circ, 292.3^\circ, 200.4^\circ$. This composite pulse was chosen over more commonly used pulse sequences for its relatively short total nutation angle and good decoupling, allowing the cycle to fit within a gradient period.
Figure 4-2: NMR methodology for QLG algorithm. The NMR implementation consists of four main sections, each corresponding to the prescribed QLG algorithm step. The top two lines in the diagram correspond to RF pulses applied to the proton and carbon qubits, respectively. The third line shows the application of magnetic field gradients. In the encoding section, the initial carbon magnetization is recorded on the protons before being transferred to the carbons. The starting magnetization is specified by using a RF pulse shaped as the Fourier transform of the desired magnetization. The shaped pulses are applied in the presence of gradients so that each site can be addressed. A carbon decoupling sequence prevents the scalar coupling from interfering with the low power shaped pulses. The $\pi/2$ at the end of the encoding move the information form the x-axis to the z-axis, as required by the QLG algorithm. The collision operator follows the encoding, and it is implemented without gradients to ensure that all of the sites in the sample feel the same transformation. The results are observed in two experiments, each time using the more sensitive proton channel. A swap gate is added when measuring the carbon magnetization. Finally, the streaming operation is applied by shifting the frequencies of the carbon and proton shapes in opposite directions.
\[ \exp \left[ -i \frac{\pi}{8} \sigma_z^2 \right] \exp \left[ -i \frac{\pi}{4} \sigma_y^1 \right] \exp \left[ -i \frac{\pi}{4} \sigma_y^2 \right] \exp \left[ -i \frac{\pi}{8} \sigma_z^1 \sigma_z^2 \right] \exp \left[ i \frac{\pi}{4} \sigma_y^1 \right] \exp \left[ i \frac{\pi}{4} \sigma_y^2 \right] \]  

(4.33)

The exponents of terms proportional to \( \sigma_z^1 \sigma_z^2 \) represent internal Hamiltonian evolutions lasting for a time \( t_{zz}^{col} = 1/(4J) \). The exponents of terms with single-spin operators are implemented by \( \pi/2 \) rotations. They were generated by RF pulses whose nutation rate was about 50 times greater than \( J \). All of the pulses and delays were applied without a magnetic field gradient in order to transform all of the sites identically.

As shown in Fig. 4-2, swap gates were utilized both in the lattice initialization and in the measurement of the carbon magnetization. The pulse sequence for the swap gates was almost identical to the sequence for \( \hat{C} \). The only difference was that the internal evolution delay was set to \( t_{zz}^{swap} = 1/(2J) \).

### 4.3.4 Measurement

The occupation numbers resulting from the collision were obtained by measuring the \( z \)-magnetizations and using equation (4.30). Since only the \( \sigma_x^a \) and \( \sigma_y^a \) operators are directly observable, a “read out” \( \pi/2 \) pulse transformed the \( z \)-magnetization into \( x \)-magnetization. The proton magnetization was measured directly after the collision, while the carbon magnetization was first swapped to the protons before observation. Measurements of both the \( ^{13}C \) and \( ^{1}H \) magnetizations were carried out separately, and in both cases via the more sensitive proton channel. The measurements were made in the presence of a weak linear magnetic field gradient, causing signals from different sites to resonate with distinguishable frequencies. The observed proton signal was digitized and Fourier transformed to record an image of the spatial variation of the spin magnetization. The observed spectrum was then processed to correct the baseline and to obtain the resulting magnetization at each site. Because each site is composed of a slice of the sample with spins resonating in a band of frequencies, the occupation number for each site was obtained by averaging over all spins in the corresponding band.

### 4.3.5 Streaming

The final step involves classically streaming the results of the measurements according to equations (4.14) and (4.15). The streaming operation is applied in conjunction with the next lattice initialization step by adding a linearly varying phase to the Fourier transform of the desired shape. The added phase causes a shift in the frequency of the pulse determined by the slope of the phase. When the frequency-shifted pulse is applied in the presence of the magnetic field gradient, the shift results in spatial translation of the encoded shape. The streaming operation is thus implemented as a signal processing step in the lattice initialization procedure.
Figure 4-3: QLG algorithm experimental results. The experimental mass densities are plotted in the figure, together with plots of the analytical solution and the numerical simulation of the NMR experiment. Seven steps of the algorithm were implemented on 16 two-qubit sites. The simulations were performed using the actual RF mutation rates and times of the experimental setup. The calculations closely match the data, suggesting that the deviation between the analytical results and the data can be attributed imperfections in the methodology. As a result, the simulations promise to be useful in exploring the errors from alternate methods.

4.4 Results and Discussion

The results of the experiment are shown in Fig. 4-3, together with plots of the analytical solution and of numerical simulations of the NMR experiment. In total, 7 steps of the algorithm were completed using a parallel array of 16 two-qubit ensemble NMR quantum processors. The observed deviations between the data points and the analytical plots can be attributed to imperfections in the various parts of the NMR implementation.

To explore the source and relative size of these errors, we simulated perfect experiments, each time adding controlled errors in four sections of the implementation:

- Fourier transform approximation in the initialization
- Decoupling during the initialization
- Encoding swap gate and $\pi/2$ pulse errors
- Collision gate errors

The Fourier transform approximation executes a correct writing of the desired magnetization to first order in the overall flip angle. To explore errors introduced by the
approximation, we simulated NMR experiments using nutation angles ranging from \( \pi/2 \) to \( \pi/20 \). In this range, angles smaller than \( \pi/4 \) resulted in accurate encodings of the desired Gaussian shapes through the ten steps of the implementation. The errors in the three remaining sections were simulated by using RF pulses with the actual time and nutation rate that were used on the spectrometer. By using a finite power, errors from imperfect averaging of the scalar coupling could be observed. Errors in the collision gate caused the least impact to the mass density, followed by errors originating from the imperfect decoupling sequence. The largest deviations originated from realistic simulations of the swap gate and the \( \pi/2 \) pulses in the encoding. It is important to note that the simulated gate fidelities for the swap and collision gates, although imperfect, are still about 0.995. This suggests that the observed deviations are caused by the coherent buildup of errors through a few iterations, and not just by the individual errors from a single gate. The complete simulation, using realistic RF pulses everywhere and a shaped pulse nutation angle of \( \pi/4 \), is plotted in Fig. 4-3. The calculated mass densities closely match the experimental results, suggesting that the observed errors are accurately modeled.

Other potential sources of errors include signal to noise, the state fidelity of the starting pseudo pure state, and gradient switching time. In addition, the random self-diffusion of the liquid molecules in the presence of a strong gradient can result in a substantial loss of signal. Although these errors were not significant in our implementation, they are likely to become important as more complicated algorithms are executed on larger lattices.

4.5 Conclusion

Ensemble NMR techniques have been used to study the experimental details involved in quantum information processing. The astronomical number of individual quantum systems (~ \( 10^{18} \)) present in typical liquid-state spin ensembles greatly facilitates the problem of measuring spin quantum coherences. In addition, the ensemble nature has been successfully utilized to create the necessary pseudopure states\[29, 30\] and to systematically generate nonunitary operations over the ensemble\[111\]. In this experiment, we again exploit the ensemble nature, but this time as a means of realizing a parallel array of quantum information processors. The novel architecture is then used to run a quantum lattice gas algorithm that solves the 1-D diffusion equation.

The closeness of the data to the analytical results is encouraging, and it demonstrates the possibility of combining the advantages of quantum computation at each node with massively parallel classical computation throughout the lattice. Currently, commercial MRI machines routinely take images with \( 256 \times 256 \times 256 \) volume elements. As a result, the large size of the NMR ensemble provides, in principle, sufficient room to explore much larger lattices. However, in moving to implementations with more computational power, several challenges remain. The limited control employed here is sufficient for a few time steps of the algorithm, but refinements are necessary to increase the number of achievable iterations. In addition, although complicated operations have been done in up to 7 NMR qubits, the problem of efficiently initializing a
large lattice of few-qubit processors still remains. Our results provide a first advance in this direction, and they provide confirmation that NMR techniques can be used to test these new ideas.
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