

# NMR Quantum Computing

John Klingner, Sean McKenna, and Suzie Wood

February 2, 2012

## 1 Introduction

The goal of this project is to do ‘proof of concept’ quantum information processing. The basic elements needed for this are a quantum system and a way to control and measure its state. Our quantum system is a solution of C-13 Chloroform, and we interacted with system’s state using Cornell College’s Nuclear Magnetic Resonance (NMR) spectrometer. By mapping certain aspects of the quantum state to binary values, we can start to replicate familiar operations from electrical computation in the quantum system.

### 1.1 Motivation

In addition to abstract concepts like furthering human knowledge, the primary motivation for research in quantum information processing is the allure of faster computing. One major source of the desired speed increase is quantum parallelism. According to Jones, a quantum computer with  $n$  qubits as inputs can evaluate the function over all  $2^n$  inputs in one step [5]. Though, the result of this will have the quantum state as a superposition of the possible outputs. As with parallelism in classical computers, this isn’t always useful. There are also quantum logic gates with no classical analogue. By exploiting quantum parallelism and using these operations, researchers have been able to develop quantum algorithms faster than any classical counterpart [10]. Of particular note is the work of Peter Shor, who developed a polynomial time quantum algorithm for prime factorization that will threaten the basis of many modern cryptosystems as quantum computers mature [8]. A more direct application of quantum computing is to simulate other quantum systems.

## 2 Background

### 2.1 Quantum Mechanics and NMR Spectroscopy

According to quantum mechanics, all elementary particles have spin. Of particular interest to us are fermions, all of which have spin  $\frac{1}{2}$  and which include protons, neutrons, and electrons. We use Chloroform with a C-13 Carbon isotope, called C-13 Chloroform, because the extra neutron gives the molecule an intrinsic spin. This spin in turn gives the molecule a small magnetic moment and causes it to line up with the NMR’s powerful magnetic field. Our NMR works by hitting the solvent with an electromagnetic pulse and measuring the free induction decay (FID) as the solvent returns to a relaxed state. Figure 1 shows the FID and resultant proton spectra for a solution of 7% regular chloroform. The tall peak is the response of the Hydrogen in the chloroform. Barely visible are two tiny peaks on either side. These peaks are due to the small amount of naturally occurring C-13 chloroform in the solution. The rest of the results in this paper will only show the Fourier transformed spectra, and will be centered on the frequency of the solution. Different pulse shapes and timings effect the quantum system in different ways; quantum logic gates are implemented by sending certain pulse sequences.

### 2.2 Quantum Logic Gates

A quantum logic gate represents a predictable transformation from one quantum state to another in a predictable way. To emphasize the connection with classical computing, I generally refer to quantum states in the notation of 0s and 1s familiar from elec-

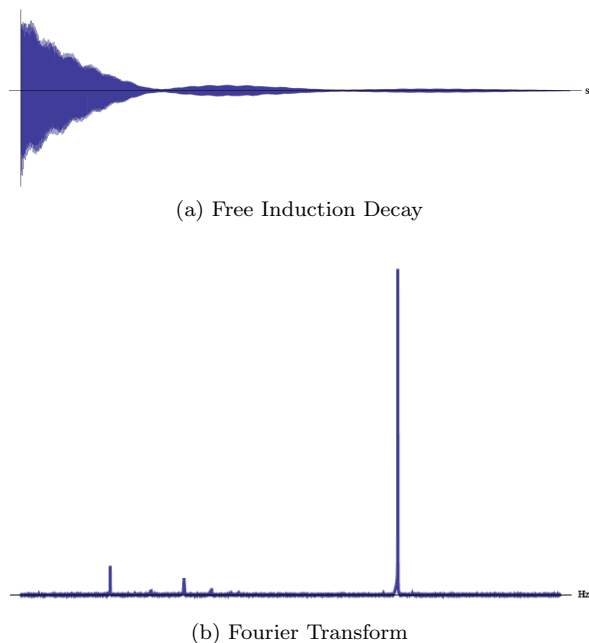


Figure 1: 7% Chloroform Solution, Raw FID and Spectra

tronic bits. The correspondence between the quantum state and the qubit representation is shown in figure 3 . Quantum principles require that any of these transformations preserve information, ie. be reversible. The controlled not, or c-not gate, is one example of a two qubit reversible transformation. Its truth table is shown in table 2 . Using the c-not gate and a few other simple logic gates it is possible to reproduce all logic gates used in classical computing, and even some gates classically impossible. Unfortunately, we were preoccupied with more fundamental questions of implementing quantum NMR at Cornell and thus did not get the chance to explore these transformations.

### 2.3 Effective Pure State

At 0 K, our sample would naturally be in the lowest energy state ( $\uparrow\uparrow$ ), which corresponds to the 00 qubit state. Unfortunately, chilling our sample at all is impractical on our equipment. However, it is pos-

In		Out	
A	B	A	B
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

Figure 2: Truth table for a controlled-not gate

Qubits	Spin
00	$\uparrow\uparrow$
01	$\uparrow\downarrow$
10	$\downarrow\uparrow$
11	$\downarrow\downarrow$

Figure 3: The first qubit/arrow is for the Carbon system, the second for the Proton system.

sible [10] to prepare what’s called an ‘effective’ pure state, where multiple experiments are run with different parameters and the results are averaged such that the effects of undesired quantum states cancel each other out. More details on our specific methods for producing the effective pure state will follow.

## 3 Pulse Programming

Once we had prepared our sample, the bulk of our work was on programming and understanding pulse sequences. One obstacle we faced was inconsistency in how two different papers might describe the same pulse sequence (see the INEPT sequence in [9] and [3] for an example of this). As I’ve said, a pulse sequence is just a chain of pulses. A pulse rotates the quantum system around a certain axis and has three properties of interest: duration, frequency, and phase. The phase controls the axis, the frequency controls whether the carbon or hydrogen is effected, and the duration controls how far it rotates. We have two gates from which to send pulses and use one to send at the carbon frequency and the other at the proton. For each system, a certain duration is selected to produce  $90^\circ$  rotations, and that duration is doubled for  $180^\circ$  rotations. These durations were built in to Delta [4] software, and we validated

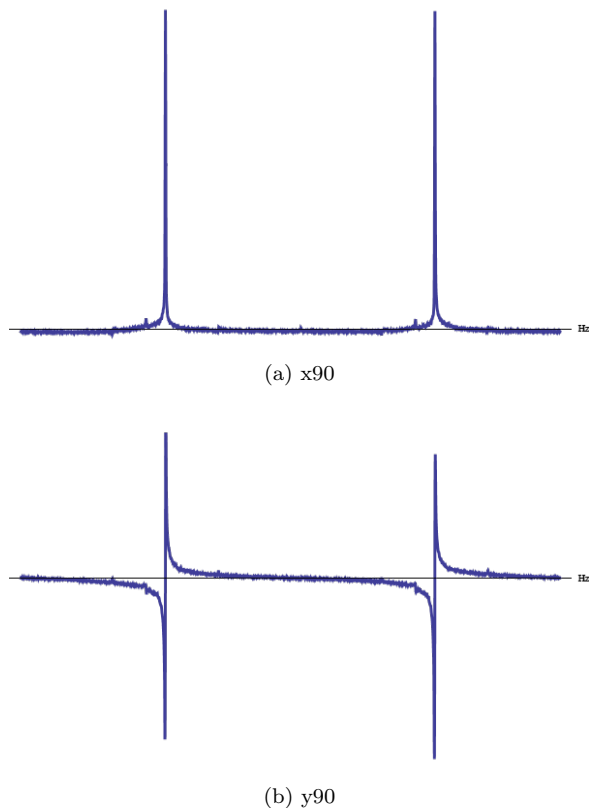


Figure 4: Results of two single-pulse experiments

them as outlined in [7]. We send pulses in the x or y plane, normal to each other and both normal to the axis of the static magnetic field. Thus, an x90 pulse on a given channel rotates that channel's system  $90^\circ$  around the x axis.

## 4 Results

By the end of the block we were able to prepare an effective pure state for each of the four possible states of our two qubit system. To get the effective pure state, we used the temporal averaging techniques described in [6]. Figure 5, from that paper, describes the pulse sequences we used for two of the three temporal averaging experiments. We chose these sequences over others because of their relative simplicity and the fact

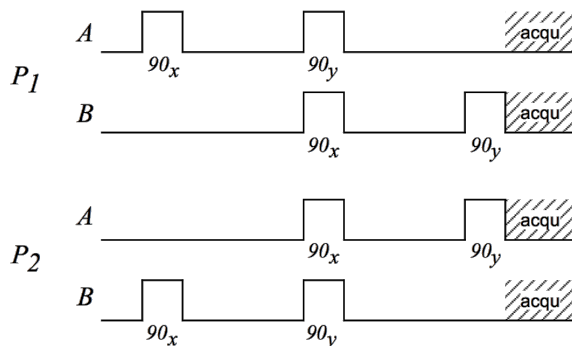


Figure 5: Pulse Sequences for Two Temporal Averaging Experiments.  $A$  is Hydrogen channel &  $B$  is Carbon channel. The delay between pulses is about  $2.3ms$

that [6] was significantly better-cited than other papers.

The third experiment is a simple thermal state obtained by sending an x90 pulse on both channels simultaneously. Figure 6 shows the results of these experiments, with normalized amplitudes. The amplitude is normalized because the relevant part of each spectra is the relative amplitude of the two peaks. The 'average', then, is just the sum of the three normalized spectra. As you can see, the other quantum states aren't completely eliminated, but the positive and negative components of the right-hand peak largely cancel out in the integral.

We have two primary concerns in our data and analysis. The first is that we were able to produce an arbitrary quantum state by adjusting the Delta program's [4] phasing parameters. To avoid the program doing any 'cheating' for us, we disabled all automatic phasing and did none ourselves. The second concern relates to the baseline for the integral calculations; the x-axis, such that higher values increase the integral and lower values decrease it. Naively, this baseline would be a straight line, but even then the question of where to put that line is non-trivial. The ACD NMR [1] software we used has several automatic baseline methods built in that adjust the baseline to eliminate curves in the spectra, such as those visible on

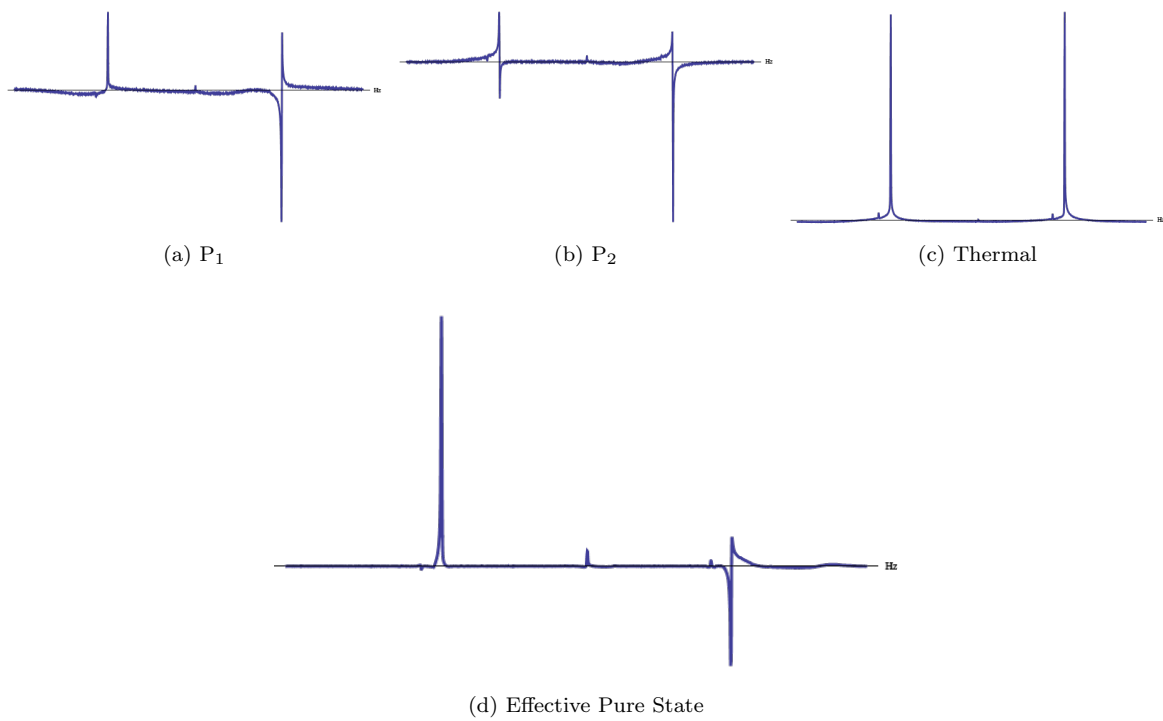


Figure 6: Results of the three experiments for and their average, our Effective Pure State

the right side of the effective pure state in figure 6. All integrals reported are with baselines automatically calculated using the same method.

To get from the 00 effective pure state to any of the four possible states, we needed a pulse to act as a ‘not’ gate to flip the state of either the carbon system, proton system, or both. [3] shows us that the DEPT pulse sequence acts as a not gate for the hydrogen channel, and we were able to successfully implement the sequence as described in [3] and get the anticipated 01 state as a result. By this point, we were developing an understanding of pulses and were able to get a 10 state with a simple x180 pulse on the carbon channel after some unsuccessful guesses. The 11 state was prepared by chaining these two together, preparing first a 01 state from the 00 and then using the x180 pulse to get the 11 state. Figure 7 has the spectra and normalized peak integrals after the various preparation sequences described. It is entirely possible that different pulse sequences for preparing 01 and 10 states would produce cleaner results with smaller integrals for undesired peaks, but we chose to test a simple quantum logic gate rather than trying to improve these results.

This logic gate was the c-not gate, shown earlier (2). We chose this gate because it was widely discussed in many different papers, and pulse sequences for it are fairly available. The c-not pulse sequence we chose to implement was provided in [2], and we implemented it by appending those pulses on the end of our existing preparation pulses. The resulting outputs and normalized integrals are available in figure 8. The states in the cNot gate output are less clear than the simple preparations, but we did not have time to experiment with other c-not gate implementations or other methods. The worst case peak, for the 10 input state, still has one integral twice as large as the other, but this is not the state given by the truth table - we should instead see the 11 state, given by negative peak on the right hand side. The outputs were as predicted for the other three input states.

## 5 Conclusion

The most important achievement of our work this block was demonstrating the possibility of further research in quantum information processing at Cornell College. The JEOL NMR spectrometer and software available here proved able to transmit pulses on multiple channels simultaneously, and we were able to control the frequency, duration, and plane of the pulses on each channel to a sufficient degree to implement pulse sequences described in literature.

Future work in this area should focus on an increased understanding of quantum logic gates as matrix transforms, and ways to implement such transforms as a pulse sequence. Now that we know with confidence how to send certain elementary pulse types, a good deal of experimentation with simple combinations of these elementary pulses would probably help with the implementation step. In order to implement more interesting quantum algorithms, future researchers in this area may wish to experiment with quantum systems featuring more qubits. I would like to wish any successors reading this the best of luck, and encourage you to contact me with any questions at jklingner12@cornellcollege.edu.

## References

- [1] ACD/Labs. ACD/NMR processor. *12.0.0*.
- [2] Neil A. Gershenfeld and Isaac L. Chuang. Bulk spin-resonance quantum computation. *Science*, pages 350–356, January 1997.
- [3] A. Güleç and S. Bahçeli. Quantum gates based on polarization transfer NMR spectroscopy. *Acta Physica Polonica A*, 107:983, June 2005.
- [4] JEOL. Jeol Delta. *4.3.6*.
- [5] J. A. Jones. NMR quantum computation. *Chem-Inform*, 32(29):288–288, 2001.
- [6] E. Knill, I. Chuang, and R. Laflamme. Effective pure states for bulk quantum computation. *Phys. Rev. A*, 57:3348–3363, May 1998.

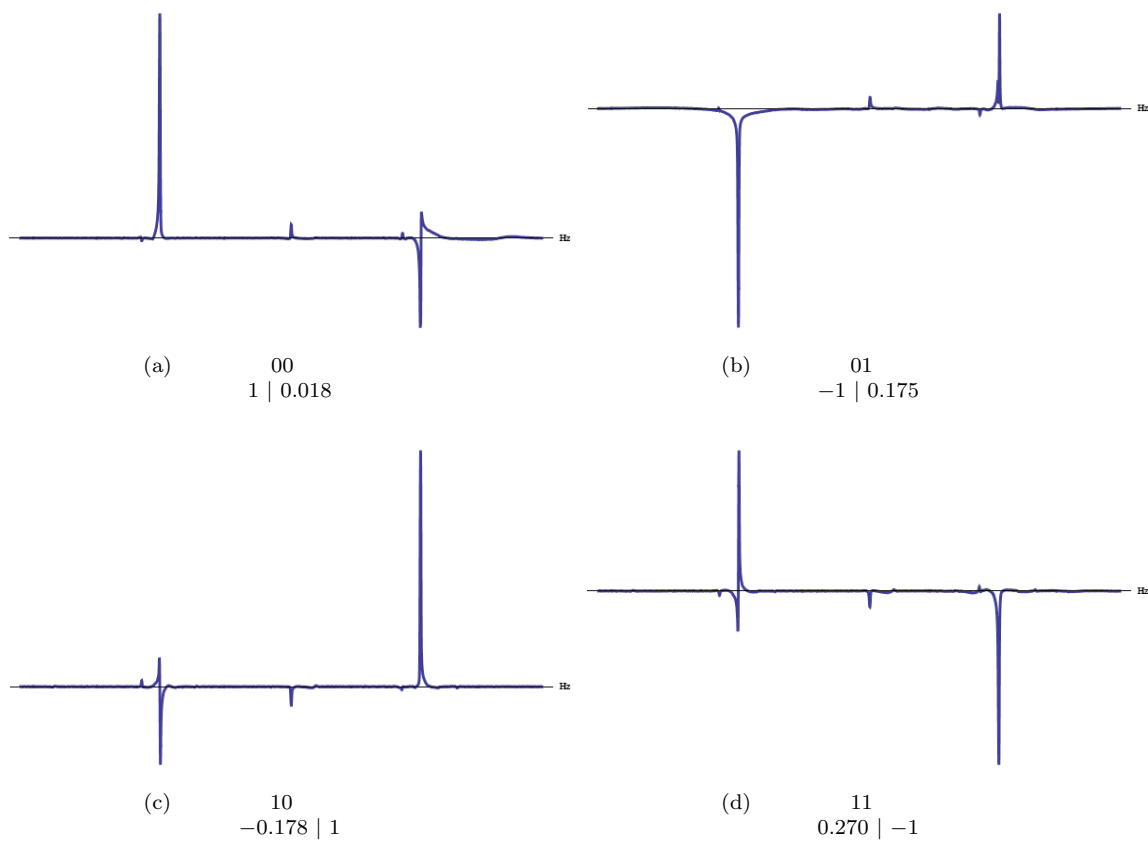


Figure 7: Four possible effective pure states and normalized peak integrals

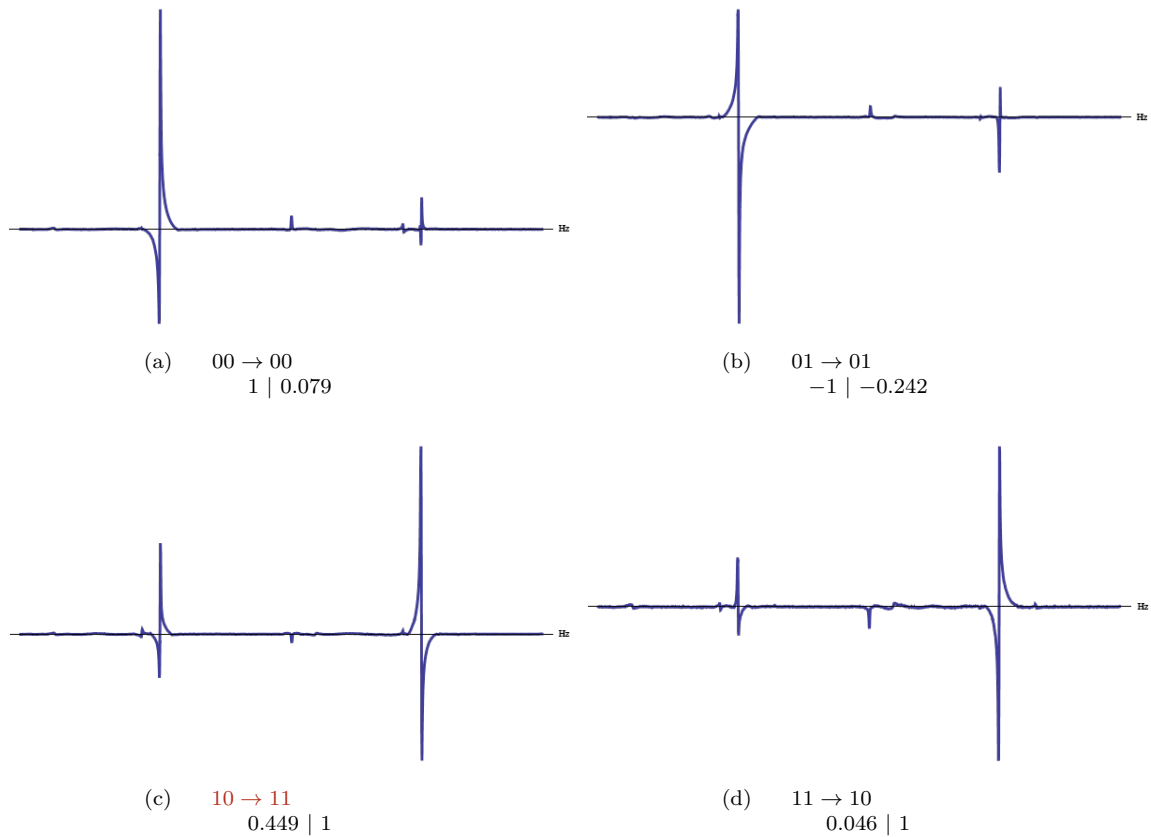


Figure 8: Spectra after performing a c-not pulse sequence on each of the four input states in  $??$ . The labels for each spectra show the anticipated transformation and normalized peak integrals.

- [7] MIT Department of Physics. Quantum information processing with NMR. August 2010.
- [8] Peter W. Shor. Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer. *SIAM Review*, 41(2):pp. 303–332, 1999.
- [9] Deniz Türkpençe, İrfan Şaka, and Azmi Gençten. INEPT NMR spectroscopy of  $^{14}\text{ND}_n$  groups: product operator theory and simulation. *Turk J Phys*, 34:139–148, 2010.
- [10] Lieven M. K. Vandersypen, Isaac L. Chuang, and Dieter Suter. *Liquid-State NMR Quantum Computing*. John Wiley & Sons, Ltd, 2007.