The Quantum Fourier Transform and Quantum Chaos

by

Yaakov Shmuel Weinstein

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Abstract

In this thesis I study control of quantum systems while implementing complex quantum operations. Through experimental implementations of such operations, I test the accuracy of control and provide methods for identifying the type and strength of experimental errors. The centerpiece of this work is the quantum Fourier transform (QFT), an essential gate for quantum algorithms and quantum simulations. Experiments are performed on a three qubit liquid-state nuclear magnetic resonance quantum information processor, and demonstrate salient features of the QFT in both of these venues.

The first experiment exhibits the ability of the QFT to extract periodicity, a necessary process for many quantum algorithms. As an example of a quantum simulation, I implement a three qubit quantum baker's map, which is composed of QFTs, and discuss how various conjectures of quantum chaos could be experimentally realized on a quantum computer.

Another example of complex quantum operations are 'pseudo-random' maps. These are operators which pass statistical tests of randomness but can be efficiently implemented on a quantum computer. I explore the importance of pseudo-random maps for the study of quantum chaos and a host of quantum information processing protocols. I also implement a set of such maps experimentally.

In order to determine the type and strength of the errors effecting our implementations, quantum process tomography is done on the QFT. From the constructed QFT superoperator and Kraus forms I show how best to analyze the data in order to extract information about coherent, incoherent, and decoherent errors.

Finally, I explore fidelity decay as a signature of quantum chaos. The simulations performed concentrate on the exact determination of fidelity decay behavior for quantum chaotic systems, and attempt to identify properties of the evolution operator that cause the observed fidelity decay behavior.

Thesis Supervisor: David G. Cory
Title: Professor, Dept. of Nuclear Engineering
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Chapter 1

Introduction to Quantum Information Processing

Successful quantum information processing promises a revolution in computation, cryptography and the way we interact with information. A computer comprised of qubits, two-level systems governed by quantum mechanics, could factor large numbers [75] and search data bases [36] faster than their classical counterparts. Quantum cryptography would allow the transfer of information protected from eavesdropping by the laws of physics [86], and quantum simulators would be capable of efficiently simulating other quantum systems [30, 54].

Although no one currently has a quantum computer, quantum information processing has become an increasingly popular area of research. In this introduction I explore some of the vital differences between classical and quantum information processing. These include exotic quantum phenomena that have the positive potential to speed up algorithms, but can also lead to errors that have no parallel in classical computation.

1.1 Bits versus Qubits

Claude Shannon [74] postulated that information as a quantifiable metric is a function of the number of possible states. The more states a system can be in the less
we know about the actual state of the system, and the more information we learn when told the state of the system. For example, we know less about the outcome of the die toss (which has six possibilities) than a coin flip (which only has two possibilities). Thus, learning the die state reveals more information than learning the coin state. The logarithmic relationship between possible states and information can be seen intuitively as follows. We would expect two pages in a book to hold twice the information of one page. However, there are twice as many characters on two pages then one page, meaning there are a power of two more possible states. To turn this power into addition requires a logarithm.

The fundamental unit of information, the bit, is defined as representing a distinction between two equal possibilities: 0 / 1, yes / no, true / false, heads / tails, capacitor charged / capacitor uncharged. The logarithmic relation between possible states and information is chosen to be base 2 such that the flip of a fair coin possesses \( \log_2 2 = 1 \) bit of information. In general, information, \( I \), is equal to \( \log_2 \) (number of possibilities). Thus, the roll of a fair six sided die generates \( \log_2 6 \) bits of information.

When the states of the system are not equally likely, the definition of information must be modified to include the likelihood of the system being in a particular state. For a random variable \( X \) with possible values \( x \) each with probability \( p(x) \) is defined as

\[
I(X) = -\sum_x p(x) \log_2 p(x). \tag{1.1}
\]

In parallel to the classical bit, a quantum bit, or qubit [71], is the amount of quantum information that can be registered by a two state quantum system. However, unlike a classical bit which can be in only one of two states, a qubit can be in a superposition of states. A paradigmatic example of a qubit is a spin \( \frac{1}{2} \) particle which has two possible spin states: spin up \( (m_z = +\frac{1}{2}, \ |\uparrow\rangle) \), and spin down \( (m_z = -\frac{1}{2}, \ |\downarrow\rangle) \), but can also be in a superposition of these two states, \( \alpha |\uparrow\rangle + \beta |\downarrow\rangle \), where \( \alpha \) and \( \beta \) are complex amplitudes such that \( |\alpha|^2 + |\beta|^2 = 1 \). The ability of qubits to exist in superposition states allows for increased computing power, as will be discussed subsequently. For ease of comparison to classical bits, let us rename the possible

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states of our qubits $|\uparrow\rangle = |0\rangle$ and $|\downarrow\rangle = |1\rangle$.

1.2 Classical and Quantum Information Processing

All algorithms of classical information processing and computing can be expressed as sequences of one and two-bit gates. For universal computation it is necessary to be able to perform NOT, OR, AND, and COPY operations. The NOT operation simply flips and 0 to a 1 and a 1 to a zero. The AND operation has two input bits and will output a 1 if and only if both input bits are 1. Similarly, OR will output a 1 if either of the input bits are 1. Quantum information processing and computing can be described by a sequence of one and two-qubit gates [26]. However, unlike classical gates, quantum gates must be reversible [51], a consequence of the requirement for unitary dynamics in quantum mechanics. Reversibility means that the input state can be uniquely determined from the output state. The classical NOT gate is reversible. If the output state is a 1 we know that the input state must have been a 0. The classical AND gate is not reversible. Given the output 0 the input bits could have been 00, 01, or 10. To construct a reversible AND gate requires three qubits. Such a gate is known as the Toffoli and is defined by the following truth table

<table>
<thead>
<tr>
<th>input</th>
<th>output</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 0 0</td>
<td>0 0 0</td>
</tr>
<tr>
<td>0 0 1</td>
<td>0 0 1</td>
</tr>
<tr>
<td>0 1 0</td>
<td>0 1 0</td>
</tr>
<tr>
<td>0 1 1</td>
<td>0 1 1</td>
</tr>
<tr>
<td>1 0 0</td>
<td>1 0 0</td>
</tr>
<tr>
<td>1 0 1</td>
<td>1 0 1</td>
</tr>
<tr>
<td>1 1 0</td>
<td>1 1 1</td>
</tr>
<tr>
<td>1 1 1</td>
<td>1 1 0</td>
</tr>
</tbody>
</table>
Each of the outputs on the right side of the table matches up with one and only one input. In addition, the Toffoli gate can perform any of the above operations necessary for universal computation.

1.3 The Power of Qubits

A classical bit can exist in one of two possible states, 0 or 1. A qubit can exist in a superposition of both $|0\rangle$ and $|1\rangle$. Two classical bits can exist in one of four possible states, but two qubits can be in a superposition of all four of those states. In general, $n$ qubits can exist in a superposition of $2^n$ possible states. Therefore, while a classical computer can apply an algorithm to one input state, a quantum computer, acting on a superposition state, can apply the same algorithm to all states simultaneously. Unlike classical systems, measuring the output state will irreversibly change the state of the system, forcing it into one term of the superposition. Only by properly crafting quantum algorithms can superposition be used to speed up certain computations [75, 36, 30, 55].

Superposition states typically lead to entanglement, a quantum phenomenon that allows quantum systems to exhibit correlations beyond what is possible for classical systems. A maximally entangled state can be created starting with a (control) qubit in the superposition state $\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$ and applying a controlled-NOT gate, which flips another (target) qubit only if the control qubit is in the state $|1\rangle$. However, the control qubit is in a superposition part of which says flip the target qubit and part of which says do not. Thus, the output state of this operation is the entangled state $\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$. Measurement on one of the qubits will give $|0\rangle$ or $|1\rangle$ each with a probability of .5. But once one qubit is measured, we know with certainty the state of the other qubit. If measurement of the first qubit is a $|1\rangle$ the measurement has changed the state of the system to $|11\rangle$ and the second qubit must be in the state $|1\rangle$. An entangled state such as this one cannot be written in the form $|\varphi\rangle_A \otimes |\chi\rangle_B$. The increased correlations between the two qubits in such states allows for various quantum operations that have no classical parallel.
1.4 Errors and Decoherence

While the ability of qubits to be in superposition states and become entangled give quantum information processing an advantage over classical information processing, these phenomena also introduce new challenges. Quantum information can go wrong in ways not possible classically. Such peculiarly quantum errors go under the name of decoherence. To understand decoherence we must first review quantum measurement.

As seen above, measurement of a quantum system in a superposition of states, changes the state of the system. The probability of which state the superposition will be forced into is the value of the complex amplitude squared. For example, measurement on a qubit in the state $\alpha|0\rangle + \beta|1\rangle$, will cause the state of the qubit to become $|0\rangle$ with probability $|\alpha|^2$ and $|1\rangle$ with probability $|\beta|^2$. Since the probabilities must add to 1, $|\alpha|^2 + |\beta|^2 = 1$.

Measurement of this kind is irreversible and nonunitary. Once the measurement has taken place the information inherent in the relative phase between $\alpha$ and $\beta$ is lost. Successful quantum information processing must transfer information without measurement by making two quantum systems interact in a coherent, non-destructive manner. Quantum information processing can also instruct how to make measurements that will reveal the desired information.

We can now understand the basic workings of decoherence. Evolution of an isolated quantum system is described by the Schrödinger equation

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle$$

(1.2)

where $H$ is a Hermitian operator, $H = H^\dagger$, called the Hamiltonian. The time evolution induced by the Schrödinger equation is ‘unitary’ $|\psi(x)\rangle = U(t)|\psi\rangle$ where $U(t)|\psi\rangle \to e^{-iHt/\hbar}$ and $U^\dagger U = UU^\dagger = 1$ since $H = H^\dagger$. However, no quantum system can be said to be truly isolated from its environment. Let us single out the quantum system we are interested in $Q$, and call everything else the environment $E$. Interactions between $Q$ and $E$ typically entangle the two systems, as if $E$ is performing measurements on $Q$ [94]. If we restrict our attention to $Q$ alone its evolution looks
non-unitary due to its interactions with $E$. This non-unitary evolution known as decoherence tends to destroy the superpositions within $Q$. Decoherence is a major barrier to successful quantum information processing because of the difficulty in isolating the quantum systems of interest.

1.5 Outline

In this work we discuss our experimental control of complex quantum operations. These operations include the quantum Fourier transform (QFT), a Fourier transform appropriate for qubits, quantum chaotic maps, quantized versions of classically chaotic maps, and pseudo-random maps. We will discuss experimental implementations of each of these examples. Our main goal in performing these experiments is to see how accurately these operations can be implemented and to identify and characterize experimental errors.

The thesis is structured as follows: the next two chapters are introductions to NMR, the system used to implement our experiments, and quantum chaos. Chapters four, five, and six discuss the actual experiments and the import of the specific operations. Chapter four introduces the QFT and shows how it can extract the periodicity of a state, a characteristic making it invaluable for quantum algorithms. Chapter five discusses the quantum baker’s map which, besides being a complex operator itself, exhibits the QFT as an element of quantum simulations. Chapter 6 discusses the importance and implementation of pseudo-random maps, maps which can be implemented efficiently on a quantum computer, but, nevertheless, pass certain statistical tests of randomness. Recipes for extracting error information are given in the chapter on the QFT superoperator. The final two chapters canvass fidelity decay as an indicator of quantum chaos.
Chapter 2

Nuclear Magnetic Resonance as a Paradigm for Quantum Information Processing

2.1 Why NMR?

A prototypical system used as a test bed for many aspects of QIP is liquid-state nuclear magnetic resonance (NMR)[22, 33]. In liquid state NMR an ensemble of identical systems are operated on simultaneously allowing for readout of expectation values without the loss of information associated with a direct measurement. NMR also has a decoherence time on the order of seconds allowing for the implementation of a few operations.

The liquid-state NMR system is made up of a sample placed in a large magnetic field $B_0 \hat{z}$. Atoms in the sample that have non-zero spin (such as hydrogen or carbon-13) tend to align with the magnetic field. In the high temperature limit, only a fraction $\frac{1}{2} + \epsilon$ of spins will align parallel to the magnetic field, while $\frac{1}{2} - \epsilon$ will align anti-parallel to the magnetic field. At room temperature and magnetic fields on the order of 10 Tesla $\epsilon \simeq 10^{-6}$. Nevertheless, due to the large number of spins in the sample, this excess magnetization is detectable and is the observed NMR signal.
2.2 Describing the State of an NMR Sample

The magnetic state of the NMR ensemble is conveniently defined using the density matrix formalism [76]. If a system is in a state $|\psi_1\rangle$ with probability $p_1$ or a state $|\psi_2\rangle$ with probability $p_2$, the density matrix of the system is

$$\rho = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|. $$

Such a system is said to be in a mixed state. If the system is in a definite state, $|\psi_1\rangle$, with probability 1, the state is said to be in a pure. The expectation value of an operator $A$ can be directly calculated from the density matrix as follows

$$\langle A \rangle = \text{tr} \rho A = p_1\langle\psi_1|A|\psi_1\rangle + p_2\langle\psi_2|A|\psi_2\rangle.$$  \hspace{1cm} (2.1)

The density matrix is non-negative, Hermitian, and has a trace of 1. For a closed system, the density matrix obeys a Schrödinger equation

$$\frac{d\rho}{dt} = i[\rho, H].$$  \hspace{1cm} (2.2)

In liquid state NMR, tumbling of the molecules averages out dipolar interactions between the systems leaving each individual quantum system effectively isolated from its surroundings. Each molecule can be treated as an individual, isolated, quantum system. Hence, rather then requiring a wave function of dimension $2^n \times q$ to describe the state of the system, where $n$ is the number of spins in each molecule and $q$ is the number of molecules in the sample, the NMR ensemble can be described by a reduced density matrix $\rho = \frac{1}{q} \sum_{i}^{q} |\psi_i\rangle\langle\psi_i|$ where each $|\psi_i\rangle$ describes the state of one molecule and has dimension $2^n$.

The reduced density matrix includes a large identity term from cancellation of spins having opposite polarizations, $\rho = 1 + \epsilon \rho$, where $\epsilon$ is defined above. In NMR it is customary to subtract the trace due to this identity term since only the traceless part of the reduced density matrix is observed. The remainder of the reduced density matrix is scaled to have integer elements and is known as the deviation density matrix. From this point on, ‘density matrix,’ $\rho$, will refer to the reduced, shifted, scaled density matrix.

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2.3 NMR as a Controllable System

The idea of using nuclear spins for the realization of a quantum computer was first suggested by Lloyd [54] in 1993. Later, Cory et al. [22] and Gershenfeld and Chuang [33] realized that liquid state NMR is an ideal way to explore many aspects of quantum computing and QIP.

The general Hamiltonian governing a three spin liquid-state NMR system is

$$H = \omega_1 I_x^1 + \omega_2 I_x^2 + \omega_3 I_x^3 + 2\pi J_{12} I^1_x \cdot I^2_x + 2\pi J_{13} I^1_x \cdot I^3_x + 2\pi J_{23} I^2_x \cdot I^3_x$$  \hspace{1cm} (2.3)

where $\omega_i = \gamma_i (1 - s_i) B_0$ is the Larmor frequency, the frequency of the spins precession around the large magnetic field. $\gamma_i$ is the spins gyromagnetic ratio and $s_i$ is the shielding tensor caused by electrons surrounding the spin. The difference between the Larmor frequencies of the spins is called the chemical shift. $I$ is equal to $\sigma/2$ where $\sigma$ are the Pauli spin matrices. $J_{ij}$ is the coupling constant between spins $i$ and $j$. The particular interaction described by the liquid state NMR Hamiltonian is known as $J$-coupling.

In the weak coupling regime, $\omega_i - \omega_j >> J_{ij}$. In this regime the terms $I_x^i I_x^j$ and $I_y^i I_y^j$ are non-commuting perturbations to the large chemical shift terms, $I_x^i - I_x^j$. First order perturbation theory tells us that such terms do not significantly effect the energy levels. Hence, the Hamiltonian in the limit of weak coupling is

$$H = \omega_1 I_x^1 + \omega_2 I_x^2 + \omega_3 I_x^3 + 2\pi J_{12} I_x^1 I_x^2 + 2\pi J_{13} I_x^1 I_x^3 + 2\pi J_{23} I_x^2 I_x^3.$$  \hspace{1cm} (2.4)

The first three terms in the Hamiltonian correspond to three qubits. The large chemical shift allows them to be individually addressed. The last three terms are the interaction terms. They allow for conditional rotations between qubits, such as those necessary for controlled-NOT and Toffoli gates.

We note that quantum observables (which are not necessarily terms that can be directly observed on an NMR spectrum) such as $I_z$ are used to denote both operators and expectation values. Thus, when describing the state of a spin (the spin is in the
"state" $I_z$, what is in fact meant is that the expectation value of the operator $I_z$, $Tr(\rho I_z)$ is equal to one.

2.4 Single Qubit Rotations

Radio frequency (RF) pulses applied at a spins Larmor frequency will rotate that spins magnetization into the transverse plane. For example, a 90-degree RF pulse along the $x$-axis will rotate a spin originally along the $z$-axis onto the $y$-axis (following the left-hand rule). An RF pulse along $x$ that will rotate the spin by an angle $\theta$ is described as [76]

$$U = e^{i I_z \theta}.$$  

(2.5)

The effect of a rotation on a density matrix is

$$U \rho U^\dagger.$$  

(2.6)

If the initial magnetization is along $z$ the effect of the RF pulse described above is

$$e^{i I_z \theta} I_z e^{-i I_z \theta} = I_z \cos(\theta) + I_y \sin(\theta).$$  

(2.7)

In general we will denote RF pulses in this way

$$(\theta)_k^i$$  

(2.8)

which we take to mean a rotation of angle $\theta$ about the $k$ direction applied to spin $i$.

2.5 Two Qubit Interactions

Evolution under the coupling terms of the internal Hamiltonian will cause interactions between the spins. The coupling between two spins can be described as follows.
Recalling that the Pauli spin matrices square to 1,

\[ e^{-iaI_1^1I_2^2t}I_y^{1}I_y^{1}e^{iaI_1^1I_2^2t} = I_y^{1}\cos\left(\frac{at}{2}\right) + 2I_x^{1}I_z^{2}\sin\left(\frac{at}{2}\right) \]  

(2.9)

where \( t \) is the amount of time under the evolution of the coupling term in the Hamiltonian and \( a = 2\pi J \).

Of course, simply allowing the internal Hamiltonian to evolve will cause coupling of all the spins and evolution by the chemical shift terms. To pick out only one of the coupling terms requires refocusing the other terms by applying a series of \( \pi \)-pulses. For example, in a three spin system, spins 1 and 2 can be coupled for a time \( t \) via the following sequence

\[ (\pi)_x^{1,2} - \left(\frac{t}{4}\right) - (\pi)_x^{3} - \left(\frac{t}{4}\right) - (\pi)_x^{1,2} - \left(\frac{t}{4}\right) - (\pi)_x^{3} - \left(\frac{t}{4}\right). \]

(2.10)

This sequence will refocus the unwanted couplings and the chemical shifts. In general, we will denote a coupling between spins 1 and 2 for a time \( \theta / J_{ij} \) as

\[ \left(\frac{\theta}{J_{ij}}\right) \]

(2.11)

with the understanding that all other terms of the internal Hamiltonian have been refocused.

### 2.6 Quantum State Tomography

Not all of the terms of the density matrix are observable in an NMR spectra. Only transverse dipolar magnetization can be detected by the detection coil of the spectrometer. This allows only \( 2n \) (binomial expansion to \( n \) terms) out of the \( 2^{2n} \) (where \( n \) is the number of spins) terms to be observed in any given spectra. To read out all the terms of the density matrix it is necessary to repeat the experiment a number of times and after each experiment rotate different terms into observables. This process is known as quantum tomography.
There are an infinite number of readout pulse sequences that can be used to reveal the exact quantum state. The experiments described here used the two different sequences described in [82] and [81].

2.7 Errors in NMR QIP

A nuclear spin system is also subject to natural decoherence. Each term decays at its own specific rate and the general relaxation superoperator also couples terms.

Besides decoherent errors there are coherent and incoherent errors that can occur during an NMR QIP implementation. Coherent, or unitary, errors emerge due to inexact pulses and waiting times. The operations are still unitary, they just are not the unitary operators that were desired. Incoherent errors arise because not all of the spins in the finite size sample will see the exact same magnetic fields. This causes the spins to evolve in slightly different ways. Although each individual spin undergoes unitary evolution, when observing the signal from the entire sample this effect will look non-unitary.

2.8 Pseudo-Pure States

As explained above, the NMR system is not in a pure state. In fact, it is in a highly mixed state due to the small percentage of spins that are polarized along the direction of the magnetic field. In many situations it is desirable to begin experiments in a pure state. Therefore it is necessary to create, pseudo-pure states, states whose deviation density matrix evolve as pure states [22][33]. The creation of these states require the use of a non-unitary gradient a varying magnetic field across the sample, and must include a small, uniquely determined amount of the identity operator, necessary for reconstructing a positive state operator. The amount of identity included is fixed for each set of experiments [79, 81].
2.9 Measures of Accuracy for NMR QIP Experiments

Room temperature NMR is always very close to the fully mixed state and only the deviation density matrix can undergo interesting evolution and hold information. However, the deviation density matrix has a relative weight one millionth the weight of the fully mixed state. We define two measures of accuracy appropriate for almost fully mixed density matrices [23]. The projection:

\[ P = \left( \frac{\text{Tr}(\rho_{\text{theory}}\rho_{\text{exp}})}{\text{Tr}(\rho_{\text{theory}}^2)^{1/2}\text{Tr}(\rho_{\text{exp}}^2)^{1/2}} \right) \] (2.12)

also called the unattenuated correlation, and the correlation,

\[ C = \left( \frac{\text{Tr}(\rho_{\text{theory}}\rho_{\text{exp}})}{\text{Tr}(\rho_{\text{theory}}^2)^{1/2}\text{Tr}(\rho_{\text{exp}}^2)^{1/2}} \right) \left( \frac{\text{Tr}(\rho_{\text{exp}}^2)}{\text{Tr}(\rho_{\text{initial}}^2)} \right). \] (2.13)

The first term in \( C \) is the projection and it measures the correlation between the desired experimental outcome \( \rho_{\text{theory}} \) and the actual outcome \( \rho_{\text{exp}} \). The second term modifies the projection by taking into account the reduction in signal over the course of the experiment, where the initial amount of signal is recorded by \( \rho_{\text{initial}} \). \( C = 1 \) means that the theoretical and experimental deviation density matrices are totally correlated and there has been no signal attenuation during the experiment. \( C = -1 \) means the matrices are fully anti-correlated, and \( C = 0 \) means the matrices are totally uncorrelated.

2.10 The Alanine System

The sample used for the experiments discussed in this work is carbon-13 labeled alanine. The three carbon-13 spins shown in figure (2-2), are used as qubits. The J-couplings between the three spins are \( J_{12} = 54.1 \), \( J_{13} = -1.3 \), and \( J_{23} = 35.0 \).
Figure 2-1: The theoretical density matrix $\rho_{\text{theory}}$ is calculated by applying the theoretically perfect operator, $U_{\text{theory}}$, to the initial density matrix, $\rho_{\text{initial}}$. The experimental density matrix, $\rho_{\text{exp}}$, is the result of the experiment, that is, the initial density matrix after the experimentally applied operator, $U_{\text{experimental}}$.

Figure 2-2: Chemical structure of the alanine system. The qubits used for the NMR QIP experiments are the three carbons. The chart shows the J-coupling constants between the qubits and the placement of the qubits (in frequency space) compared to the RF transmitter during experiments.

The chemical shift differences between the carbon spins of alanine on a 300 MHz spectrometer (the Larmor frequency of protons are 300 MHz) are 9454.28 Hz between spins 1 and 2, and 2594.91 Hz between spins 2 and 3.
Chapter 3

Introduction to Quantum Chaos

There is no unambiguous definition of chaos for quantum systems. Quantum systems are governed by the linear Schrödinger and thus cannot exhibit the sensitivity to initial conditions of classical chaotic systems. Instead numerous conjectures have been offered as to appropriate indicators of quantum chaos. These conjectures may be some aspect of the evolution operator or the reaction of the system to perturbation. To test these conjectures, quantized versions of classically chaotic systems are devised. These are shown to fulfill the proposed conjecture while quantized versions of classically regular systems do not.

Quantum chaotic operators are another example of the complex quantum operators we are using to demonstrate control. Additionally, many of these evolution operators can be implemented with one or more quantum Fourier transforms. We will discuss the implementation of the quantum baker’s map an operator made up of a QFT on half of Hilbert space followed by an inverse QFT on all of Hilbert space.

In this chapter we give a short general introduction to the field of quantum chaos. We start with a quick review of the Lyapunov approach to classical chaos and examine why quantum systems cannot be described by this classical approach. Then we examine various conjectured signatures of quantum chaos.
3.1 Does Quantum Chaos Exist?

Chaos is a phenomenon in which nonlinear systems exhibit extreme sensitivity to initial conditions. Two initially close points in phase space diverge at an exponential rate as the chaotic dynamics evolve. The rate of divergence is quantified by the Lyapunov exponent [53]. Let $\Delta x$ be the distance between two points on phase space. We define $\xi = lim_{\Delta x(0) \to 0} \left( \frac{\Delta x(t)}{\Delta x(0)} \right)$, to describe how far apart two initially arbitrarily close points on phase space become at some time $t$. Generally, $\xi(t)$ is the solution to the differential equation

$$\frac{d\xi(t)}{dt} = \lambda \xi(t),$$  \hspace{1cm} (3.1)

giving the solution

$$\xi(t) = e^{\lambda t}$$  \hspace{1cm} (3.2)

where $\lambda$ is the Lyapunov exponent. As seen from the above equation when the Lyapunov exponent is positive two arbitrarily close points on phase space diverge at an exponential rate. Thus, the dynamics described by $\xi(t)$ is strongly sensitive to initial conditions and we have chaotic dynamics.

While the Lyapunov exponent description of chaos works well for points on a classical phase space it cannot hold true for quantum mechanical states or wavefunctions. A measure of distance between quantum wavefunctions is the overlap $O = \langle \Psi | \Phi \rangle$. However, the overlap between two quantum wavefunctions remains unchanged under evolution governed by the linear Schrödinger equation as seen from

$$O(n) = \langle \Psi(U^n) | U^n | \Phi \rangle = O_1,$$  \hspace{1cm} (3.3)

where $U$ is the unitary system evolution. Hence, the distance between two arbitrarily close quantum mechanical wavefunctions, like the distance between two Liouville probability densities, does not diverge as a function of time and cannot be described by the Lyapunov exponent picture. This seeming lack of correspondence between classical and quantum physics has led to the study of ‘quantum chaos,’ the search for characteristics of quantum dynamics that manifest themselves as chaotic in the
classical realm [12, 13, 37, 14].

3.2 Classical and Quantum Chaotic Maps

Classical chaos studies and simulations are extremely difficult given their non-linear equations of motion and extreme sensitivity to small errors, such as roundoff errors. Chaotic maps were introduced in attempt to study chaotic phenomenon without having to solve the equations of motion. A map is a simple discrete algorithm instructing the evolution of points in phase space. The map is applied discretely and, as time increases, relatively simple maps can exhibit a host of classical chaotic phenomena.

To test the various conjectures of quantum chaos, researchers turned to quantum chaotic maps. Quantum chaotic maps are quantized versions of classical maps known to exhibit chaotic dynamics. There is no unique way to quantize a map. One oft used method requires quantizing the underlying phase space, be it a cylinder, torus, or sphere, and then rewriting the dynamics of the classical map in terms of unitary operations on the quantized phase space.

Many chaotic maps, such as the bakers maps, cat maps and kicked tops, have been quantized, some in multiple fashions. These quantized maps are used to test conjectures of quantum chaos. For a conjecture to pass the test, the proposed characteristic should be evident in quantized chaotic maps but not found in quantized versions of regular, non-chaotic maps.

3.3 Quantum Signatures of Chaos

Many characteristics, quantum signatures of chaos, have been conjectured, are detailed in the literature, and have been tested on quantum analogs of classically chaotic systems. These signatures can be divided into two broad categories, static signatures and dynamic signatures. Static signatures look at characteristics of the Hamiltonian or unitary operator governing the system. It is conjectured that the evolution operator of quantum chaotic systems have statistical properties similar to those of
Figure 3-1: Eigenvalue (left) and eigenvector (right) statistics for the chaotic quantum kicked top (QKT). $U_{QKT} = e^{-i\pi J_y/2\hbar} e^{-i k J_z^2/2J^2 \hbar}$ where $\hat{J}$ is the operator associated with the irreducible representation of angular momentum, and $k$ is the ‘kick’ strength. Depending on the value of $k$, the QKT operator is the quantized version of a system with regular, chaotic, or mixed (having a phase space with both regular and chaotic regions) dynamics. Here we use a kick strength $k = 6$ which in the chaotic realm of the QKT. The distribution of $y = \eta N$, where $\eta$ is the squared modulus of an element of a QKT eigenvector, is shown on the left. The solid line shows the $\chi^2_\nu$ distribution expected for random matrices. The right figure shows the eigenvalue spacing distribution, where $s$ is the difference between two neighboring eigenvalues. The solid lines show the Gaussian and Poissonian distributions expected for random and integrable systems, respectively. The agreement between the distributions for the QKT and random matrices is remarkable.

random matrices. Hence, it is expected that quantum analogs of classically chaotic systems show level repulsion, that is, if the energy eigenvalues of the system are ordered, the difference between nearest neighbors would result in a histogram with a Wigner-Dyson distribution [14] and not the Poissonian distribution expected for regular systems. Additional, the distribution of the squared modulus of the elements of the eigenvectors of quantum chaotic operators follow $\chi^2_\nu$ distributions[39] from appropriate random matrix ensemble. Similarly, each column of the unitary operator itself should follow the statistics appropriate for random states.

Dynamic signatures of quantum chaos look at the evolution of a state under a quantum chaotic operator compared to evolution under the same operator with some slight perturbation. In this sense, these signatures are analogous to the Lyapunov exponent description of classical chaos, except that the sensitivity resides in the Hamil-
Figure 3-2: Eigenvalue (left) and eigenvector (right) statistics for the chaotic quantum kicked top (QKT) with \( k = 1 \). For this kick strength the system is regular and therefore the distribution of eigenvector elements does not follow the distribution appropriate for random matrices. Also, the eigenvalue spacings follow the Poisson distribution expected for integrable systems.
	onian of the system rather than the initial state of the system. An example of a dynamic signature of chaos is hypersensitivity to perturbation. For chaotic systems (both classical and quantum), the amount of information necessary to track the system state when the dynamics is interrupted by an unknown perturbation grows at an exponential rate with increasing time [70]. Other signatures of quantum chaos look at the entropy growth of chaotic systems versus regular systems [95]. In subsequent chapters we investigate another dynamic signature of quantum chaos: fidelity decay. The behavior and rate of the fidelity decay (where fidelity is defined as the overlap squared) between a wavefunction undergoing a given unitary evolution and the same wavefunction under a perturbed evolution depends on the chaoticity of the system. We examine the exact behavior of the fidelity decay in quantum chaotic systems.

We will also discuss the experimental implementation of the quantum baker’s map, the quantized version of the widely used classical baker’s map. The quantum baker’s map is another example of a complex quantum operation we use to study the controllability of our system. In addition, we provide instruction for testing certain conjectures of quantum chaos on a quantum computer.
Chapter 4

The Quantum Fourier Transform

4.1 Why the Quantum Fourier Transform?

A key subroutine of the many quantum algorithms such as factoring [75], simulations of quantum systems [2, 92, 87], and quantum chaos [3, 70, 95], is the quantum Fourier transform (QFT) [21, 28, 49], a discrete Fourier transform appropriate for qubits. Like its classical counterpart, the QFT can extract the periodicity of a function, or in the quantum case a wavefunction. The QFT can also be used to transform from position to momentum representation, making it an important component of quantum simulations. This chapter and the next discuss experiments that exhibit these characteristics of the QFT. The ability to perform these functions is an important measure of the control we have over our system. Later, we will use the QFT as the main focus of our attempts to extract experimental error information.

The QFT is defined as follows:

\[ QFT_N |x\rangle = \frac{1}{\sqrt{N}} \sum_{x'=0}^{N-1} e^{2\pi i x x'/N} |x'\rangle. \]  \hspace{1cm} (4.1)

where, \( N \) is the dimension of the system’s Hilbert space.

To understand the action of the QFT, it is instructive to look at the matrix
representing the unitary operator of the two qubit QFT,

\[ QFT_4 = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix} \]  

(4.2)

The operator separates the input states by multiples of \( \frac{\pi}{2} \), 0 degrees in the first row and column, and then by 90 degrees, 180 degrees and 270 degrees in subsequent rows and columns.

Let us now examine how this structure allows the QFT to extract periodicity.

\[ \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \]  

(4.3)

\[ \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \]  

(4.4)

Equations (4.3) and (4.4) show how the QFT acts on periodic states. The initial states in the above equations both have a periodicity of 2. However, there is a shift in that periodicity. Most algorithms requiring multiple repetitions, like Shor's factoring algorithm, will randomly output the initial state of (4.3) or the initial state of (4.4). Measurement on the state cannot determine the periodicity since it is impossible to know which state was the output. Thus the QFT is used to wash out the shift of periodicity as shown in the above equations. In general, if \( f(x) \) is a periodic wavefunction with period \( r \), then \( \hat{f}(p) \), the wavefunction after application of the QFT, will exhibit a peak at \( p = N/r \). The classical Fourier transform reveals the
periodicity in functions, the QFT reveals periodicity of wavefunctions.

4.2 The Quantum Fourier Transform on a Quantum Computer

The QFT can be constructed from two basic unitary operations [21], the Hadamard gate, $H_j$, operating on the $j$th qubit

$$H_j = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad (4.5)$$

and the conditional phase gate, $B_{jk}$, operating on the $j$th and $k$th qubits

$$B_{jk} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\theta_{jk}} \end{pmatrix}, \quad (4.6)$$

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

To implement the QFT, these gates (applied from right to left),

$$H_j B_{j,j-1} \ldots B_{j,2} B_{j,1} \quad (4.7)$$

are implemented on each bit as $j$ is indexed from 1, the most significant qubit, to $L$, the least significant qubit. In other words, each qubit is subject to a conditional phase gate between itself and all qubits more significant then it followed by a Hadamard. This process is repeated for all qubits starting with the most significant. The total number of basic operations for $n$ qubits is thus $n(n+1)/2$. A bit reversal will complete the QFT. The bit reversal can be achieved by $n/2$ swap gates or by relabeling bits.
4.3 The Quantum Fourier Transform on an NMR Quantum Information Processor

The Hadamard and conditional phase gates that make up the QFT can be realized via liquid state NMR. The pulse program is conveniently derived from an idempotent or projection operator description of the propagators. Operators $E^\pm$ 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 thus,

$$H_j = \left( \frac{\pi}{2} \right)_y^j - \left( \pi \right)_x^j. \quad (4.8)$$

The $B_{jk}$ gate, can be implemented using the coupling between qubits. In terms of projection operators the $B_{jk}$ gate is $1 - E_-^1E_-^2 + e^{i\theta}E_-^1E_-^2$, and the following pulse sequence can be derived:

$$\left( \pi \right)_\phi^j - \left( \frac{\theta_{jk}}{2\pi J_{jk}} \right)_y^j - \left( \pi \right)_\phi^j - \left( \frac{\pi}{2} \right)_y^j - \left( \frac{\theta_{jk}}{2} \right)_x^j - \left( \frac{\pi}{2} \right)_{-y}^j. \quad (4.9)$$

where $\phi$ is an arbitrary phase. The superscript $j,k$ denotes a pulse on both spins $j$ and $k$. The final three pulses effectively perform a rotation around the z-axis.

A bit reversal can be achieved by simply renaming the bits, however, in our current experiment, we implement the bit reversal so as to fully observe the extraction of periodicity by the QFT. This requires a series of swap gates. $\text{Swap}_{jk}$ gates can be done with the following pulse sequence:

$$\left( \frac{\pi}{2} \right)^{j,k}_y - \left( \frac{1}{2J_{jk}} \right)^{j,k}_y - \left( \frac{\pi}{2} \right)^{j,k}_{-y} - \left( \frac{1}{2J_{jk}} \right)^{j,k}_x - \left( \frac{\pi}{2} \right)^{j,k}_{-x}. \quad (4.10)$$

The complete gate sequence for the three qubit QFT is:

$$\text{Swap}_{13}H_3B_{23}B_{13}H_2B_{12}H_1 \quad (4.11)$$

and the complete pulse sequence is just the aggregate of the sequences described.
Figure 4-1: Circuit diagram for implementation of $U_{QFT}$ for three qubits. For each qubit $j$, starting with the most significant, a series of conditional phase gates are implemented between qubit $j$ and all qubits more significant than $j$, followed by a Hadamard on $j$. The amount of phase added is $\theta_{jk} = \pi/2^j$. A bit reversal completes the QFT. Thus, on the first, most significant, qubit just a Hadamard is applied. On the second qubit, a phase of $\theta_{12} = \pi/2$ is applied if the first qubit is a $|1\rangle$, followed by a Hadamard. On the third qubit, there are two conditional phase gates with $\theta_{13} = \pi/4$ and $\theta_{23} = \pi/2$, followed by a Hadamard. A swap gate between qubits 1 and 3 performs the bit reversal.

When possible pulses were combined without effecting 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 [16]. 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.

4.4 Experimental Results

The implemented QFT will give the correct results to any input state as will be shown more clearly in the next chapter. To demonstrate the ability of the QFT to extract periodicity, we implement the QFT on a periodic input state with periodicity $r = 2$. This state was created by performing a Hadamard on the first and second bits of the initial $|000\rangle$ pseudo-pure state. The real part of the experimental density matrix of the input state is shown in figure (4-2).
Figure 4-2: Real part of the density matrix of the periodic input state used for the QFT implementation. This state was created by applying Hadamards on the first and second qubit after all three qubits were transformed into a pseudo-pure state. The state is a superposition of the $|000\rangle + |010\rangle + |100\rangle + |110\rangle$ states. Note that this state has a periodicity of $r = 2$.

Figure (4-3) shows the density matrix after implementation of the QFT including the $\text{Swap}_{13}$ gate which performs the necessary bit reversal. Clearly, the density matrix is now periodic with a periodicity of $N/r = 4$. This shows that the QFT did, indeed, extract the periodicity of the input state.

The correlation of the QFT implementation before the swap gate is .80 and after the swap gate .62. 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. As a check to the accuracy of the results, we also performed the QFT on a thermal state (without a final swap), obtaining an correlation of .87 without the swap gate (the greater accuracy for the thermal state arises because no pseudo-pure state need be created). The fact that our algorithm gives the correct results for both a pseudo-pure and the thermal states suggests that the high accuracy obtained is not due to accidental cancellation of anomalous results.

In this chapter we have experimentally demonstrated the ability of the QFT to extract periodicity of an input wavefunction. This ability is essential for quantum
Figure 4-3: Real part of the density matrix of the state after implementation of the QFT. Notice there is now a periodicity of $N/r = 4$ in the density matrix. This shows that the QFT extracted the periodicity of the input state.

algorithms such as Shor’s factoring algorithm. In the next chapter we will use the QFT as a key element in the simulation of quantum systems, specifically in implementing the quantum baker’s map.
Chapter 5

The Quantum Baker’s Map

The QFT plays a primary role in quantum simulations. In this chapter, we discuss the experimental realization of the quantum baker’s map, a quantized phase space map used to study quantum chaos. The quantum baker’s map is constructed entirely out of QFTs and can again be used to demonstrate control of our system while implementing complex quantum operations.

5.1 Quantum Chaos on a Quantum Information Processor

Chaos is a phenomenon in which systems exhibit heightened sensitivity to small perturbations [53, 12, 13, 37, 38, 61, 62, 70]. When the chaotic system is quantum-mechanical, simulating its dynamics on a classical computer is notoriously difficult: the computational complexity of the calculation rises exponentially with the number of degrees of freedom of the simulated quantum chaotic system and with the accuracy required of the simulation [37, 30, 55]. If one can simulate quantum chaos on a quantum computer the computational complexity rises only as a small polynomial in the number of degrees of freedom and in the required accuracy [55, 15, 69]. Consequently, quantum computation represents a potentially powerful technique for investigating quantum chaos.
We implement experimentally an approach suggested by Ballentine and Zbib [4] to explore the correspondence between classical and quantum chaotic dynamics. We evolve our quantum system forward in time under the quantum baker’s map, perturb it, and evolve it backwards by the inverse map. The total evolution is \( \rho_i \rightarrow \rho_f = \sum_k QB^\dagger A_k QB \rho_i Q B \) where \( \rho \) is the density matrix of the system, \( QB \) is the unitary transformation corresponding to the quantum baker’s map, and \( A_k \) are Kraus operators which provide a perturbation whose strength can be varied. We compare the final state, \( \rho_f \), with the initial state, \( \rho_i \) for different perturbation strengths. The sensitivity of the system to the perturbations can be characterized by the overlap, \( Tr(\rho_i \rho_f) \).

We show that this approach allows for confirmation of the ideas of Zurek and Paz [95] who suggest that quantum chaotic systems, when decohered by their environment, produce information at a rate equal to their Kolomogorov-Sinai entropy. Further applications of our experimental methods could be used to test the criteria for quantum chaotic dynamics of Peres and of Schack and Caves. Peres [61, 62] noted that under quantum chaotic dynamics with a slight perturbation, a state moves apart at an exponential rate from the same state evolving under the unperturbed dynamics, a phenomenon discussed at length in later chapters. Schack and Caves [70] characterized chaotic dynamics (both classical and quantum) in terms of the exponential growth of the information required to specify a state that evolves according to an unknown perturbed version of the dynamics, a phenomenon they termed ‘hypersensitivity to perturbation.’

The quantum information processor used to simulate perturbed quantum chaotic maps is an NMR quantum information processor [22, 33]. The number of quantum bits used (three) is sufficiently small that the precision of the quantum computation can be checked on a classical computer. Of course, the small number of qubits means that the simulation could have been performed on a classical computer. The goal of the research reported here was to actually simulate quantum chaos on a quantum information processor and demonstrate how accurately a complex quantum operation such as this one can be implemented on our system. A further goal of experimental
Figure 5-1: Action of the baker's map on the unit square phase space. Phase space is first stretched to twice its length in one direction and squeezed to half its height in the other direction, keeping the total area constant. A vertical cut is made in the center, and the right half of phase space is placed on top of the left half. Two very close initial conditions on opposite sides of the cut will end up far apart. Repeated applications of the map cause chaotic dynamics throughout the phase space.

investigations is to identify practical experimental signatures of quantum chaos.

5.2 The Baker’s Map, Classical and Quantum

The classical baker’s map acts on the unit square in phase space as follows:

\[
q' = q/2, \quad p' = p/2; \quad 0 < q < 1/2
\]
\[
q' = 2q - 1, \quad p' = (p + 1)/2; \quad 1/2 \leq q < 1
\]  

(5.1)

The baker’s map first stretches phase space to twice its length, while squeezing it to half its height. Then, the map cuts phase space in half vertically and stacks the right portion on top of the left portion, similar to the way a baker kneads dough. This action is showed in figure (5-1). Because of the stretching and the cut, the baker’s map is fully chaotic and has two Lyapunov exponents, ± ln 2.

Balazs and Voros [3, 68] presented a quantized version of the baker’s map that reproduces the behavior of the classical map in the limit \( \hbar \to 0 \). The quantum baker’s map is a simple unitary operator which consists of a quantum Fourier transform (QFT) on half of the Hilbert space followed by an inverse QFT on the whole Hilbert space.

\[
QB_N = QFT_N^{-1} \begin{pmatrix} QFT_{N/2} & 0 \\ 0 & QFT_{N/2} \end{pmatrix}
\]  

(5.2)
where $N$ is the Hilbert space dimension.

The QFT, and hence, the quantum baker's map, can be expressed as a sequence of two basic unitary operations, the Hadamard gate, $H_j$, operating on spin $j$ and the conditional phase gate, $B_{jk}(\theta)$, which applies a phase of $\theta$ on spin $k$ if spin $j$ is in the state $|1\rangle$. Schack [69] utilized this decomposition to develop an algorithm for simulating the quantum baker’s map on a quantum computer. The three qubit version of the quantum baker’s map is

$$\text{Swap}_{13}H_3B_{23}^\dagger \left(\frac{\pi}{2}\right) B_{13}^\dagger \left(\frac{\pi}{4}\right) H_2B_{12}^\dagger \left(\frac{\pi}{2}\right) H_1 \times \text{Swap}_{23}H_3B_{23}^\dagger \left(\frac{\pi}{2}\right) H_2$$  \hspace{1cm} (5.3)

where $\text{Swap}_{jk}$ is a swap gate between bits $j$ and $k$. The first term of equation (5.3) implements a QFT on bits 2 and 3 and the second term implements the inverse QFT on all three bits [21]. Brun and Schack [15] introduced a simplified version of the baker’s map and simulated, on a classical computer, its implementation on a quantum information processor. For this experiment we implement the complete baker’s map defined in equation (5.3) with swap gates applied by relabeling bits.

As noted above, our experimental technique is to apply the quantum baker’s map, perturb, then apply the inverse map. We began most of our simulations in the pseudo-pure state corresponding to the state $|000\rangle$. In general, the perturbed dynamics of a single state may not be sufficient to completely characterize the behavior of a map. Here, we take advantage of the fact that the overlap $Tr(\rho_i\rho_f)$ for the $|000\rangle$ initial state approaches the average of overlaps for a complete set of orthogonal initial states in the limit of small perturbation, as shown in figure (5-3). Thus, the overlap, $Tr(\rho_i\rho_f)$ for the initial state $|000\rangle$ approaches the fidelity [81, 23] of the operation: baker’s map, rotation perturbation, inverse baker’s map. We note that a complete readout of the state of the system, as done in the present work, does not scale efficiently with the number of qubits. Methods for efficient measurement of the overlap are discussed in [72, 29].

An interesting non-unitary perturbation is the application of a magnetic field gradient dephasing the least significant (third) bit. The Hamiltonian of a gradient on
Figure 5-2: Gate sequence for the three bit position perturbation. The top line, bit one, is the most significant bit. The first gate (a controlled-controlled-NOT or Toffoli gate) flips the most significant bit only if the other two bits are |1⟩. The second gate (a controlled-NOT gate) flips the second bit only if the third bit is a |1⟩, and the final gate is a NOT on the third bit. This sequence can be extended to arbitrary number of qubits. Using geometric algebra [77], we can break down this sequence into NMR implementable operators; the Toffoli gate, $e^{i \frac{\pi}{4} (1-\sigma_1^z-\sigma_2^z-\sigma_3^z+\sigma_1^z\sigma_2^z+\sigma_1^z\sigma_3^z+\sigma_2^z\sigma_3^z-\sigma_1^z\sigma_2^z\sigma_3^z)}$, the controlled-NOT gate, $e^{i \frac{\pi}{4} (1-\sigma_2^z-\sigma_3^z)}$, and the NOT gate, $e^{i \frac{\pi}{4} (1-\sigma_2^z)}$.

spin $j$ is $H^j_y(z) = e^{i \frac{\gamma}{\hbar} \frac{d_m}{m} \int \sigma^j_y \, dz}$, where $\gamma$ is the spins gyromagnetic ratio. The gradient acts as a rotation of varying magnitude across the sample. This perturbation looks like decoherence when the signal from the entire sample is measured, effectively tracing over position, $z$.

When simulating a quantized classical map, a natural perturbation is one with a simple definition in phase space, such as a displacement in position. The quantum baker’s map, as defined by equation (5.2), associates the discretized position basis on the unit square [3] with the computational basis. The smallest possible position perturbation in a Hilbert space of dimension $N$ corresponds to the addition or subtraction of $1 \pmod{N}$ which, for example, would take the state $|000\rangle$ to $|001\rangle$ or $|111\rangle$. The gate sequence to implement this perturbation is shown in figure (5-2). Simulated data in the inset of figure (5-3) shows that, as expected, the baker’s map is very sensitive to such a perturbation.

A variation of this perturbation with a simple interpretation in Hilbert space is an $x$ rotation on one bit. A 180° rotation of the least bit on the $|000\rangle$ state gives the same output as one step of the position perturbation. The sensitivity of the baker’s map to the $\sigma_x$ perturbation may be examined experimentally by controlling the angle of the rotation.

The three bit quantum baker’s map was implemented via NMR using the three carbon-13 spins of an alanine sample. The pulse sequences for realizing the $H^j_y$ and
Figure 5-3: Sensitivity of baker’s map to unitary perturbations. Solid line shows the theoretical overlap $Tr(\rho_i \rho_f)$ versus the angle of the perturbation rotation on the third bit for the initial state $|000\rangle$. The dashed curve shows the final state overlap for the same perturbation averaged over a complete set of orthonormal initial states. These curves are calculated by numerically applying the map and perturbations to the initial state. For small perturbations the results for the initial state $|000\rangle$ are very similar to that of a complete set of initial states. Stars represent the measured overlap $Tr(\rho_i \rho_f)$ for the initial state $|000\rangle$ where $\rho_i$ is the state of the system after experimental implementation of the quantum baker’s map followed by the inverse quantum baker’s map, and $\rho_f$ is the state of the system after the experimental implementation of the quantum baker’s map, the rotation perturbation, and the inverse quantum baker’s map. The difference in overlap between the experimental and theoretical curve results from imperfections in the initial experimental state. The inset plot is the overlap versus the size of the position perturbation (add 1 through add 4). The baker’s map is much more sensitive to a position space perturbation then to a rotation perturbation on the least significant bit.
Figure 5-4: Real part of experimental density matrices. The top left hand corner shows the input $|000\rangle$ pseudo-pure state. One iteration of the baker’s map on this state leads to the center density matrix. Then the inverse map is applied (top right figure) bringing the bits back to the input $|000\rangle$ state. In the second experiment, a gradient is applied to the third, least significant, bit after the forward iteration of the map (bottom left figure) followed by the application of the inverse map (bottom right figure).

$B_{jk}$ gates and the implementation of the QFT as a sequence of these gates, has been discussed in a previous chapter[83]. The pulse sequence for the complete quantum baker’s map was compressed by relabeling bits instead of performing the swaps explicitly. Readout was done using quantum state tomography as described in [81].

The first experiment consisted of two iterations of the quantum baker’s map, a forward iteration followed by the inverse of the map, starting from the $|000\rangle$ pseudo-pure state. The attenuated correlation, $C$, of the implementation of the forward map is .76, and for the forward followed by the inverse, .56. For the forward map the unattenuated correlation is .93 and for the forward followed by the inverse, .90. Since the experiment was done on the $|000\rangle$ pseudo-pure state, we expect the final state of the system to be that same state. The density matrix of the spin system after the forward and inverse iteration is shown in figure (5-4).

Another set of experiments were done to explore the dynamics of the baker’s map
under perturbations as described above. The first perturbation experimentally tested, was a dephasing gradient on the third, least significant, qubit. The gradient can be made selective by applying a gradient which dephases all of the bits followed by a π-pulse on the first two spins, followed by a gradient pulse of the same strength. The π-pulse causes the dynamics of the first gradient pulse to be undone by the second gradient pulse. Hence, the effect of the gradient is only seen by the third bit (a second π-pulse is done on the first two spins to put them back in their original state). We measured $C = .78$ for the state after the gradient and $C = .65$ for the state after the inverse map. For these correlation values the loss of magnetization due to the gradient is taken into account in the normalization of $\rho_{\text{initial}}$. The final state (after the gradient and inverse map) shows the generation of one bit of entropy as seen by the equilibration of the $|000\rangle$ and $|001\rangle$ populations, as displayed in figure (5-4). This is consistent with the Paz-Zurek model for the effect of decoherence on a quantum chaotic map: when decohered, the map produces one bit of entropy per iteration, an amount equal to the Kolmogorov-Sinai entropy of the map.

In a final set of experiments rotational perturbations of $\pi/32$, $\pi/16$, $\pi/8$, and $\pi/4$ on the third (least significant) bit were applied between the forward and inverse iterations of the baker’s map. For these experiments $C$ ranged between .52 and .53. In figure (5-3) we plot the overlap, $Tr(\rho_i \rho_f)$, of the experimental perturbed and unperturbed density matrices and compare it to theoretical predictions.

In conclusion, we describe the implementation of a chaotic map on a quantum system, a three qubit quantum information processor. The quantum baker’s map is another example of the importance of the QFT for aspects of quantum information processing. In addition, we have explored two perturbations and examined their effects on the dynamics of the map. For small quantum systems it is more difficult to find easily implementable perturbations (one or two bit rotations) that are largely noncommuting with the map. The implemented quantum baker’s map is not sensitive to the least bit rotation perturbation. However, it is sensitive to other perturbations, such as the described position perturbation. Experiments such as these establish a foundation for further experimental investigations of quantum chaotic dynamics and
the exploration of suggested theoretical approaches. For example, the hypersensitivity to perturbation suggested by Schack and Caves, should be evident even on a small Hilbert space, with only a few iterations of a chaotic map [15]. To eventually observe a characteristic such as the Peres criterion [61] will require a much larger Hilbert space and many more iterations of the map. The experiments performed are a first step towards a more thorough experimental investigation of these questions.
Chapter 6

Pseudo-Random Maps for Quantum Information Processing

In this chapter we introduce efficient random maps or pseudo-random maps, maps that may be efficiently implemented on a quantum computer, yet, have statistical properties of randomness. These maps serve as another example of complex quantum operations. We discuss the implementation of a set of these maps and show why these maps are useful for a host of quantum information processing protocols.

6.1 Why Random Maps?

The application of random matrix models to quantum physics was instigated by Wigner[88] to describe the statistics of interacting many-body systems. Wigner demonstrated that canonical models correctly characterized the universal spectral fluctuations observed in spectroscopic studies of heavy nuclei and, later, of Rydberg atoms. The significance of the canonical random ensembles was extended when these matrix models were found to apply to models of quantum chaos[11, 14, 39, 37]. Quantum systems whose classical analogues are chaotic are well described by statistical features of the random matrix ensembles.

Our motivation for exploring a QIP implementation of random unitary matrices as an example of a complex quantum operation, derives from their relevance to quantum
information processing tasks as paradigmatic models of generic quantum transformations. For example, the generation of random quantum states\cite{37, 56} which, in the limit of large Hilbert space dimension, are known to contain asymptotically as much entanglement as the maximally entanglement states\cite{5}. Thus, by generating random states, random maps can be a practical, robust means for generating states with high entanglement\cite{10}. Indeed, we will use a measure of entanglement as a benchmark for the algorithm proposed below.

Additionally, a circuit implementation of random matrices can be applied to study properties of information loss and fidelity decay, where either the system, the environment or both may be modeled as a random unitary matrix. This approach is in line with recent theoretical studies of decoherence in small Hilbert spaces that have modeled the interactions between generic systems and complex environments with random matrices \cite{35}.

Random maps may also be used to probe the noise generators of a QIP in an unbiased fashion. A random map is guaranteed to be affected by every noise generator of the QIP. Thus, the superoperator of the random map, which is generated by quantum process tomography\cite{20, 64, 52}, will contain complete information about all noise in the QIP. Regular maps, however, may commute with one or more noise generators.

Quantum process tomography can realistically be done only for a few qubits. Nevertheless, random maps can be used to explore the strength and type of noise generators via a fidelity decay experiment as described in \cite{29}. The random map is applied forward $t$ iterations, then backwards $t$ iterations. The errors inherent in the QIP system insure that the final state is not equivalent to the initial state. The fidelity between the initial and final state is measured as a function of $t$. From the fidelity decay behavior, exponential or Gaussian, and the rate of decay, we can get information about the types and strengths of internal noise of the QIP.
6.2 Efficient Random Maps for Quantum Information Processors

Here we report on theoretical and experimental results of an algorithm that produces pseudo-random operators with certain statistical signatures approaching those typical of CUE. The algorithm makes use of gate decompositions that are conveniently realized on a QIP with only nearest neighbor interactions. Our considerations start from recalling the fundamental theorem of quantum information science that any unitary matrix may be implemented on a QIP through the successive application of one and two-qubit gates. On the one hand, Pozniak et al [63] have developed a decomposition of all unitary operators, $U(N)$, parametrized in such a way that the elements of $U(N)$ are generated uniformly with respect to the Haar measure. However, the number of gates involved in this decomposition is exponential in the number of qubits, as it must be, since a matrix $U(N)$ has $N^2$ independent parameters. On the other hand, it is possible to generate matrices with spectral statistics that are typical of CUE efficiently on a QIP by simulating dynamical quantum chaos models for which efficient gate decompositions are known [69, 34, 8]. These models generically exhibit the local spectral fluctuations and characteristic eigenvector statistics of the appropriate random matrix theory (RMT) ensemble even though the dynamics is completely determined by only a few independent parameters regardless of the Hilbert space dimension. However, chaos models are not ideal for many applications because the matrix elements actually contain complicated correlations that reflect the presence of the underlying classical structure. As a result, observables of interest, such as the fidelity decay[46] and the entropy growth rate[95], can exhibit characteristics that reflect these classical structures, rather than the characteristics implied by random matrix theory. The pseudo-random maps described here have no classical analogue, and, therefore, no classical matrix element correlations. Unlike typical CUE maps which, as mentioned, require $N^2$ independent parameters, we consider a class of pseudo-random maps that have only $\text{polylog}(N)$ independent parameters and whose implementation, therefore, require significantly less gates than typical CUE
Figure 6-1: The $i$th random gate in the algorithm for applying an $n$ qubit pseudo-random map. $(\theta_i^k, \phi_i^k, \psi_i^k)$ is the random rotation of qubit $k$ and $\alpha_i^{j,k}$ is the amount of coupling between neighboring qubits $j$ and $k$ during the $i$th iteration. The complete algorithm is composed of $m$ random gates each with independently random qubit rotations and nearest neighbor couplings. The random rotations after one coupling period and before the next can be combined into one random rotation such that each map has $m + 1$ random rotations per qubit and $m$ coupling periods.

maps. Despite this restriction, we report that these pseudo-random maps exhibit certain statistical features that are very close to those of CUE matrices.

Our algorithm for generating pseudo-random maps is composed of only operations that are directly available to a QIP with individually addressable qubits and nearest neighbor couplings. The algorithm is comprised of $m$ successive iterations of the circuit in Figure 6-1. This circuit consists of an independent random SU(2) rotation on each qubit, followed by independent random $\sigma_x^j \sigma_x^k$ coupling, between each pair of nearest neighbor qubits $j$ and $k$, followed by the inverse rotation of each qubit. The rotations effectively transform the coupling into a random basis such that the rotations and coupling can be written as $\vec{\sigma} \cdot \hat{T} \cdot \vec{\sigma}$ where $\vec{\sigma}$ is the vector of Pauli matrices and $\hat{T}$ is a second rank tensor. A random SU(2) rotation of a qubit is given by

$$
(\theta_i^k, \phi_i^k, \psi_i^k) = \begin{pmatrix}
  e^{i\phi_i^k} \cos \theta_i^k & e^{i\psi_i^k} \sin \theta_i^k \\
  -e^{-i\psi_i^k} \sin \theta_i^k & e^{-i\phi_i^k} \cos \theta_i^k 
\end{pmatrix}
$$

where the subscript $i$ refers to the $i$th iteration of the circuit and ranges from 1 to $m$, and the superscript, $k$, refers to the $k$th qubit and ranges from 1 to $n$. The angles $\theta_i^k$, $\phi_i^k$, and $\psi_i^k$ are randomly chosen for each iteration.
\( \phi_i^k \) and \( \psi_i^k \) are drawn uniformly from the intervals

\[
0 \leq \theta_i^k \leq \frac{\pi}{2} \quad 0 \leq \phi_i^k \leq 2\pi \quad 0 \leq \psi_i^k \leq 2\pi.
\] (6.2)

\( \alpha^j_i \), the coupling between qubits \( j \) and \( k \) during the \( i \)th iteration, is drawn from the interval \( 0 \) to \( 2\pi \) with a normal distribution centered around \( \pi/4 \). At infinite variance this is equivalent to drawing from a uniform distribution and at zero variance \( \alpha \) maximizes the entanglement between the nearest neighboring qubits.

Since the gates used in the above algorithm consist of a universal set, there exists a multiple \( m \) that will generate a set of unitaries that will cover \( U(N) \). However, \( U(N) \) will most likely not be sampled uniformly with respect to the Haar measure. Therefore, our problem is to determine whether the pseudo-random maps generated from our algorithm can approximate some of the useful universal statistical signatures of CUE.

### 6.3 Entanglement of Pseudo-Random States

We are particularly interested in the degree of entanglement in the states produced by applying \( m \) iterations of the algorithm of Fig. 6-1 to an initial, unentangled state. We note that by operating on an initial computational basis state, the final state vector has the same elements as a column of the applied operator. For CUE maps, each column is a random state[96]. Thus, by studying statistical properties, such as the degree of entanglement, of the output states of pseudo-random maps applied to computational basis states, we are studying statistical properties of the map itself.

The distribution of the entangling power, or the average amount of entanglement produced by a unitary operation for a fixed partition of the Hilbert space, has been explored for CUE maps [93]. Here we want to characterize the amount of entanglement over all qubit factorizations and therefore consider the multi-qubit entanglement
metric proposed by Meyer and Wallach[57]:

\[
Q = \frac{4}{n} \sum_{q}^{n} \text{Tr}[\rho_q(0)]\text{Tr}[\rho_q(1)] - \text{Tr}[\rho_q(0)\rho_q(1)]
\]  \hspace{1cm} (6.3)

where \( n \) is the number of qubits and \( \rho_q(0), \rho_q(1) \) are the density matrices corresponding to the original state after a measurement of bit \( q \) gives a 0 or 1, respectively. We note that the average value of Eq. (6.3) over the uniform measure on all pure states may be calculated directly, giving,

\[
< Q > = \frac{N - 2}{N + 1} \simeq 1 - \frac{3}{N} + \frac{3}{N^2} + O(N^{-4})
\]  \hspace{1cm} (6.4)

which, for 8 qubits, is equal to .9883 [73].

We have numerically measured the distribution of the entanglement, \( Q \), for states obtained after evolution of the 8 qubit computational basis states under pseudo-random maps with increasing \( m \). In figure 6-2 these distributions are compared to the distribution of \( Q \) for typical 8 qubit CUE maps. As a lower bound estimate for \( m \) necessary to even approach the CUE average, we note that to produce a coupling between only the first and \( n \)th qubits requires at least \( n + 1 \) iterations. As the depth of the circuit increases the distribution of \( Q \) for the states generated by the pseudo-random maps approaches that of general CUE matrices.

To determine the efficiency with which the random circuits can reproduce the exact random distribution, we have measured the rate at which the average \( Q \) of the pseudo-random circuit columns approaches the exact CUE average. As shown in the inset to figure 6-2, this rate is exponential with increasing \( m \). The exponential rate decreases slowly as the number of qubits increases, suggesting that at worst only polylog\((N)\) resources are required to attain the CUE average. We have repeated this numerical test using different sizes for the factor spaces (in defining the bipartite entanglement) and have found a similar exponential dependence on \( m \).

It is important to point out that as \( N \) increases the difference in \( Q \) between the average over all pure states and the maximally entangled state decreases exponen-
Figure 6-2: Distribution of the entanglement metric of Meyer and Wallach for the output states of eight qubit pseudo-random maps applied to all computational basis states with $m = 16$ (+), 24 (.), 32 (x), and 40 (o). All the nearest neighbor J-couplings are $\alpha = \pi/4$. As $m$ increases the distribution of $Q$ approaches the one for actual CUE matrices (solid line). The inset shows the difference between the average $Q$ for the circuits and the CUE average decreases exponentially with increasing $m$ for different number of qubits 4 (triangles), 6 (squares), 8 (asterisks), 10 (diamonds).

Initially and the distribution of $Q$ becomes sharper. This means that the ability of $Q$ to distinguish between different random states diminishes. Hence, though the distribution of $Q$ from output states of pseudo-random maps may approach that of the CUE distribution, certainly this does not guarantee that CUE is sampled in an unbiased manner by our algorithm.

### 6.4 Experimental Realization

A set of ten pseudo-random maps were implemented via NMR using the three carbon-13 spins of the alanine sample. The construction of the maps is slightly different from that described above. We randomly choose 100 operations each of which can be an $x,y$ or $z$-rotation of each qubit by a random angle or a J-coupling between two neighboring qubits. The probability of a J-coupling is smaller than that of a rotation and the number of J-coupling periods is limited to 7. Thus, the total map consists of a random rotation, $(\theta, \phi, \psi)$, on each of the 3 qubits in between each J-coupling period. The complete random gate sequence has 8 random rotations and 7 J-coupling
periods. Due to the small Hilbert space dimension, many maps must be implemented to insure meaningful statistics.

We apply each pseudo-random map to the eight pseudo-pure states $|000\rangle...|111\rangle$ [22, 33] so that the 8 output states for each map contain the elements of the first through eighth columns of the applied operator. Readout of the complete output state was done using the quantum state tomography procedure described in [81]. The average attenuated correlation [31, 79] for the 80 output states is .68, and the average unattenuated correlation which is .84.

Of course, due to decoherent and incoherent errors, the final state after implementation of the map is not a pseudo-pure state but a mixed state. We extract the closest pure state to the mixed output state by taking the eigenvector corresponding to the largest eigenvalue of the mixed state density matrix. This maximizes the fidelity $F = \langle \psi | \rho | \psi \rangle$ where $\rho$ is the mixed state, and $\psi$ is a pure state. The average largest eigenvalue amplitude for the 80 output matrices was .78, which is a measure of the purity of the output states.

Although in our numerical study of 8 qubits we calculated the amount of entanglement produced by the pseudo-random map, for the 3 qubit experiment the most significant statistical test is the distribution of matrix elements. The squared modulus of the matrix elements, $\eta$, of a CUE map follow the $\chi^2_2[39]$ distribution

$$P_{CUE}(y) = (N - 1)(1 - \frac{y}{N})^{N-2}$$  \hspace{1cm} (6.5)

where $y = N\eta$.

The distribution of elements of the purified output states compared to the $\chi^2_2$ distribution of 8 dimensional Hilbert space CUE maps is shown in figure 6-3 (d). The agreement is good ($\chi^2 \simeq 1.7$) given the limited statistics, and comparable to the agreement expected for the corresponding theoretical pseudo-random circuits ($\chi^2 \simeq 1.6$) shown in figure 6-3 (c). In addition, we show that the desired maps exhibit other statistics typical of CUE; the nearest neighbor level spacing distribution, $s$, figure 6-3 (a) and the distribution of the magnitude of the elements of the maps eigenvectors,
Figure 6-3: (a) The distribution of nearest neighbor energy level spacings, \( s = l_i - l_{i+1} \), where \( l_i \) is the systems \( i \)th ordered energy level for the set of ten 3 qubit pseudo-random maps compared to the expected CUE distribution. (b) The distribution of the magnitude of eigenvector elements, \( y = N \eta \) for the set of ten 3 qubit pseudo-random maps compared to the expected \( \chi^2 \) distribution [39]. Though we do not determine the level spacings or eigenvector statistics experimentally, these distributions show that the pseudo-random maps we have constructed exhibit statistics close to that of typical CUE. The lower plots show the ideal (c) and experimental distributions (d) of the operator matrix elements compared to the \( \chi^2 \) prediction with \( N = 8 \). For the experimental distribution, the operator matrix elements are the elements of the purified final state vectors.

Figure 6-3 (b), both closely approximate the expected statistics for CUE maps.

As mentioned above, quantum systems with classically chaotic counterparts share many features of random matrices, including the distribution of operator elements. Thus, the above experimental procedure can be used to determine whether an applied operator is the quantized version of a classically chaotic system. Specifically, the operator to be tested is applied to each of the computational states \(|0 \ldots 0\rangle\) to \(|1 \ldots 1\rangle\). The output states correspond to the columns of the applied operator. The distribution of the elements of these states are then compared to the distribution expected for random matrices.

In conclusion, we have introduced pseudo-random maps which, with only a polynomial number of gates, have selected statistical distributions similar to those of typical CUE. The algorithm is comprised of random rotations and nearest neighbor couplings and can be implemented on any QIP with nearest neighbor couplings. Nu-
Numerical simulations show that the created maps have eigenvalue distributions, nearest neighbor level spacings, and operator element distributions, similar to maps typical of CUE. In addition, the amount of entanglement produced by applying these maps to an unentangled state approaches that of CUE as a function of the number of iterations. We expect this to be important for the creation of random states. However, we leave as an open question how well a pseudo-random map produced by a polynomial number random gates actually approaches typical CUE distributions or samples CUE. This question is dependent upon what distribution is used to determine the random rotations and couplings. Examples of random gate sequence are experimentally implemented on an NMR QIP. The distribution of the matrix elements of the implemented maps are shown to be in good agreement with the distribution of the elements of typical CUE matrices.
Chapter 7

The Quantum Fourier Transform Superoperator

In the previous chapter we discussed the implementation of the quantum Fourier transform on a three-qubit NMR system. The experiment demonstrated the ability of the QFT to extract the periodicity of an initial state. In addition, we provided the fidelity as a measure of accuracy with which the QFT was performed. However, the fidelity provides little useful information regarding what errors occurred during implementation or how these errors can be corrected.

In this chapter, experimental data from quantum process tomography (QPT) is used to provide a detailed description of the evolution of the same three qubit NMR QIP implementing the QFT. We explore methods of extracting information about the errors that occur during implementation through various representations of the experimental data. Distinct signatures are identified for coherent, incoherent, and decoherent errors. To aid our analysis, we make use of simulations of the experiment where only some of these errors are present. The choice of the QFT reflects its essential role in the simulation of quantum systems and in many quantum algorithms as described in the previous chapter.
7.1 Quantum Process Tomography

Quantifying the extent of control is an essential element of quantum information processing. Generally, this information is reported as a single number, the fidelity of the operation. Such numbers provide the experimentalist with little useful information on what went wrong or how to improve the control over the quantum system. Quantum process tomography (QPT)[20] may be the next step. The data collected from QPT, the mapping of a complete set of operators under the dynamics, provides some additional details as to what went wrong. QPT still does not provide unique information on how things went wrong or how to fix them, however, with a model of the control process, the mapping recorded by QPT permits checks for consistency and can be used to find the means of designing sequences with improved fidelities. Here we explore the QFT in some detail to understand what information may be gleaned by QPT.

The dynamics of an isolated quantum system is fully described by the Schroedinger equation which gives rise to an $N \times N$ unitary operator, where $N = 2^n$ is the system Hilbert space dimension and $n$ is the number of qubits that would span this space. Open quantum systems, however, interact with an inaccessible environment and are thus subject to decoherence. Furthermore, if the system is an ensemble of many quantum systems, such as in NMR, each element of the ensemble may undergo a slightly different evolution, what we refer to as an incoherent processes. QPT allows the determination of the superoperator of an open quantum system. The superoperator (or an equivalent operator sum representation) contains all of the information available for measurement at one time point. In quantum information processing QPT is used to compare the desired gate or algorithm with an implementation to determine such measures of success as the superoperator fidelity, entanglement fidelity and quantum channel capacity. The experimental superoperator includes the results of all implementation errors. The identification and extraction of these errors is the major goal of the present work.

An experimental implementation of QPT has been done on the controlled-NOT
$\rho_{eq} \rightarrow \{\rho_{\text{initial}}\} \rightarrow \{\rho_{\text{final}}\} \rightarrow \{\rho_{\text{obs}}\}$

Figure 7-1: A schematic of how to implement QPT is shown. The system always starts out in its equilibrium state, $\rho_{eq}$. A series of operations are performed to this state to create a complete set of input states, $\{\rho_{\text{initial}}\}$. The gate on which QPT is to be performed, in this case the QFT, is applied to each of these states giving a complete set of output states, $\{\rho_{\text{final}}\}$. To readout the complete state of each $\rho_{\text{final}}$ requires repetition of the experiment with appropriate readout sequences from the set $\{U_{\text{tomo}}\}$. This gives a set of density matrices, $\{\rho_{\text{obs}}\}$ which allow for the reconstruction of each $\rho_{\text{final}}$.

gate of a two-qubit nuclear magnetic resonance (NMR) quantum information processor (QIP) [19]. In that work, data from QPT was used to assess certain decoherence models. Here, QPT is carried out with the goal of identifying the type and strength of errors that occur during implementation. Specifically, we would like to distinguish between coherent, incoherent, and decoherent errors, provide as complete a description as possible of each type of error, and determine how the relevant information about each type of error is manifest in the various representations of our QPT data. In the case of coherent and incoherent errors we would like to use this information to develop improved quantum gates.

There are several methods of performing QPT outlined in the literature. Some of these methods [64, 52], require increasing the Hilbert space size beyond that of the system whose dynamics is to be studied. This is unappealing for current experimental studies of quantum information processing where qubits are at a premium. The method used in this work is most similar to that of [24], which requires implementation of the desired gate on a complete set of $N^2$ fully known input states and full knowledge of the resulting output states.

Our analysis utilizes two different representations of the open quantum system dynamics, superoperator representation and the Kraus operator sum representation.
The superoperator, \( S \), is an \( N^2 \times N^2 \) matrix operating on the density matrix

\[
\text{col}(\rho_f) = S\text{col}(\rho_i)
\]  
(7.1)

where \( \rho_i \) and \( \rho_f \) are the initial and final system density matrices and the \( \text{col} \) operation stacks the columns of the density matrices on top of one another, such that the leftmost column is on top. This results in an \( N \times N \) matrix becoming an \( N^2 \times 1 \) vector. An element of \( S \) is simply the amplitude of going from one element of the density matrix to another. \( S \) preserves hermiticity and trace, and is completely positive.

The open quantum system equation of motion is given by the Liouville-Von Neumann equation

\[
\text{col}(\dot{\rho}) = -L\text{col}(\rho)
\]  
(7.2)

where the \( L \), the Liouvillian or supergenerator, is a matrix of dimensions \( N^2 \) by \( N^2 \). The superoperator \( S \) is related to the Liouvillian \( S = e^{-lt} \), where \( t \) is time.

We will primarily work in two different basis, the computational or Zeeman basis, where the rows and columns of the density matrix are labeled from \( |0\ldots0\rangle \) to \( |1\ldots1\rangle \) and the product operator basis. The product operator basis is related to the structure of the NMR Hamiltonian and rows and columns of the superoperator in this basis are labeled as \( I_2 \otimes \ldots \otimes I_2, I_2 \otimes \ldots \otimes I_2 \otimes \sigma_x \), to \( \sigma_x \otimes \ldots \otimes \sigma_x \), where “\( \otimes \)” represents tensor multiplication, \( I_2 \) represents the two dimensional identity matrix and each term has \( n \) components.

The information contained in the superoperator can also be expressed as a Kraus operator sum representation. This representation is comprised of a set of up to \( N^2 \) matrices, \( A_k \) such that

\[
\rho_f = \sum_{k}^{N^2} A_k \rho_i A_k^\dagger
\]  
(7.3)

and

\[
\sum_{k}^{N^2} A_k^\dagger A_k = 1.
\]  
(7.4)

If the dynamics is purely unitary there is only one Kraus operator, the unitary operator of the system. Just as the with the superoperator, \( S \), the Kraus operators sum

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must preserve hermiticity, trace and be completely positive.

There are an infinite number of equivalent Kraus operator representations. The method of extracting Kraus operators described below is advantageous in that it finds the Kraus operator with the largest amplitude. This process can be repeated to extract an ordered set of Kraus operators.

One can convert from the superoperator in the computational, or Zeeman, basis into a Kraus operator sum representation by constructing the Choi matrix [40]:

\[
T = \sum_{ij=0}^{N-1} (E_{ij} \otimes I_N) S(I_N \otimes E_{ij})
\]  

(7.5)

where \(I_N\) is the \(N \times N\) identity matrix and \(E_{ij}\) is a matrix of all zeros except for a 1 in the \(i\)th, \(j\)th element. The Kraus operators, \(A_k\), are just the eigenvectors, \(v_k\), of the Choi matrix unstacked such that the \(N^2 \times 1\) vector becomes an \(N \times N\) matrix (in the opposite sense of the \textit{col} operator defined above), times the square root of the corresponding eigenvalue, \(\lambda_k\). We can order the Kraus operators in terms of weight by defining the amplitude of the Kraus operator \(m_k = \sqrt{\lambda_k / N}\).

In general, we are interested in extracting information concerning three types of errors; coherent, or unitary, errors, incoherent errors, due to inhomogeneity of the total Hamiltonian, and decoherent errors, non-unitary errors due to interactions with the environment. One of the main goals of this work is to identify the part of the overall error in our experimental implementation is coherent, what part is incoherent and what part is decoherent. In particular, the unitary and incoherent errors are in principle correctable. Of course, the superoperator itself does not contain sufficient information to clearly separate incoherent and decoherent errors, but, given a model of the incoherence, we can still make some progress.

That the method used here, and all other known QPT procedures, is inefficient. The inefficiency comes from the exponentially more experiments needed for every additional qubit. Therefore, QPT can practically be carried out only on small Hilbert spaces. Nevertheless, a complete analysis of a complex dynamics will provide insight and understanding that will be necessary in the identification of errors and the control
of larger systems.

7.2 The Experiment

The gate on which we perform QPT is the quantum Fourier transform (QFT). The QFT is a key subroutine in many quantum algorithms [75, 49] and in simulations of quantum dynamics [92, 69] and has been discussed in detail in the previous chapter.

The experiments were implemented on a three qubit NMR quantum information processor [22, 33]. The three qubits used were the three carbon-13 spins of an alanine sample.

The goal of the work in the previous chapter [83] was to demonstrate the ability of the QFT to extract periodicity of a given input state. In this chapter we would like to study the ability of our system to accurately perform the QFT. Nevertheless, the method of implementation is the same. The pulse sequences for the Hadamard and conditional phase gates are derived from an idempotent or projection operator description of the propagators [77]. We note that in the previous chapter the bit reversal was implemented experimentally. Here the bit reversal is achieved by simply renaming the bits.

We stress that the various building blocks of the QFT implementation, the individual pulses and evolution periods, remain unchanged during all experiments. After creation of the initial state a set sequence is applied which is completely independent of the initial state.

The initial states used were the 64 product operator states $I_8$, the identity, and states such as $\sigma_x^1, \sigma_z^3, \sigma_y^2\sigma_x^3$ where the superscript represents the qubit number. These states were chosen because they are easy to create on a liquid state NMR system. We order the states ‘alphabetically’ starting with the $N = 8$ identity, $I_8 = I_2 \otimes I_2 \otimes I_2$, followed by $\sigma_x^3 = I_2 \otimes I_2 \otimes \sigma_x$, $\sigma_y^3 = I_2 \otimes I_2 \otimes \sigma_y$, and so on until $\sigma_z^1\sigma_z^2\sigma_z^3 = \sigma_z \otimes \sigma_z \otimes \sigma_z$. The QFT gate sequence described above is applied to each of the 64 states. Readout of the complete input and output states is done via quantum state tomography as described in [31].
Complete QPT was done twice using different types of RF pulses. The first set of pulses are of the type described in [31] which compensate for internal Hamiltonian evolution of the system during the pulse. The second set of pulses compensates for evolution of the internal Hamiltonian during the pulse and accounts for RF inhomogeneity over the length of the sample [65]. All of the analysis in this work uses the data from the second implementation. We mention both sets of data here to show the improvement made with the next generation pulses as seen in Figure 7-2.

To measure the accuracy with which the initial state was created we calculated the projection [31],

$$P(\rho_{th}, \rho_{in}) = \frac{Tr(\rho_{th}\rho_{in})}{\sqrt{Tr(\rho_{th}^2)Tr(\rho_{in}^2)}} \quad (7.6)$$

where $\rho_{th}$ is the desired input state and $\rho_{in}$ is the experimental input state. The projection quantifies the similarity of ‘direction’ between the desired and actual state. The projection for each of the input states is shown in figure 7-2 (squares). The average of all input state projections is .96.

For the output states, an appropriate measure of implementation accuracy requires a term to account for loss in total magnetization, caused by non-unitary evolution, during the experiment. The attenuated correlation [31] is defined as

$$C(\rho_{th}, \rho_{out}) = P(\rho_{th}, \rho_{out}) \sqrt{\frac{Tr(\rho_{out}^2)}{Tr(\rho_{in}^2)}} \quad (7.7)$$

where $\rho_{th}$ is now the desired output state, $\rho_{in}$ is the experimental input state, and $\rho_{out}$ is the experimental output state. The average attenuated correlation for a complete set of input states is equal to the gate fidelity, $F$. For our experimental implementation of the QFT we find a gate fidelity of .64. The attenuated correlation of each output state is shown in figure 7-2 (x).

To estimate the accuracy of an experimental implementation without considering the losses due to decoherence one can use the the projection of the output states. For our QFT implementation the average projection of the 64 output states is .82. The projection for each of the 64 output states is shown in figure 7-2 (o).
Figure 7-2: The initial state projection (squares), final state projections (o) and final state attenuated correlations (x) for the 64 initial states and 64 final states for the first (left) and second (right) set of QPT data. For the first QPT data the average initial state projection is .93, the average final state projection is .64 and the average attenuated correlation, which is equal to the gate fidelity, is .37. For the second QPT data set, the average initial state projection is .96, the average final state projection is .82, and the gate fidelity .64. The 64 states are ordered alphabetically as described in the text.

We note that the average projection and correlation can be calculated directly from the theoretical and experimental superoperators. The average final state projection is equal to \( T\text{r}(S_{th})T\text{r}(S_{exp})/\sqrt{T\text{r}(S_{th}^2)T\text{r}(S_{exp}^2)} \) and the gate fidelity or average final state correlation is equal to \( T\text{r}(S_{th})T\text{r}(S_{exp})/T\text{r}(S_{th}^2) \).

Once all of the experimental input and output states have been completely determined, the experimental superoperator can be calculated as

\[
S_{exp} = R_{out} \ast R^{-1}_{in}
\]  

(7.8)

where \( R_{in} \) and \( R_{out} \) are \( N^2 \times N^2 \) matrices whose columns are the experimental input and output states \( \text{col}(\rho_{in}) \) and \( \text{col}(\rho_{out}) \), respectively. Though there are errors in the input states, the determination of the superoperator requires only a complete set of states such that \( R_{in} \) has a rank of \( N^2 \). The rank of the experimental \( R_{in} \) is not changed by the small errors of our implementation.

Another possible metric of accuracy for the experimental implementation, is the
Figure 7-3: The theoretical (left) and completely positive experimental (right) superoperator matrices, $S_{th}^{QFT}$ and $S_{exp}^{QFT}$, in the computational or Zeeman basis. The theoretical superoperator is calculated from the unitary operator $S_{th}^{QFT} = U_{QFT} \otimes \overline{U}_{QFT}$, where the over-line represents complex (non-Hermitian) conjugate. The figure shows the amplitudes of real part of each element of the superoperators. These elements form a distinct pattern due to the structure of the QFT unitary operator. Note the strong similarity between the matrix elements of the theoretical and experimental superoperators. However, it is not at all obvious from this vantage point what errors have occurred during implementation or how they can be corrected.

worst possible output correlation. Using a minimization search, we find a pure states with output correlations of just .45 with the desired output state for the experimental superoperators.

A final interesting metric to explore is the correlation of QFT stationary points, states that do not evolve under the theoretical QFT evolution. Three of these states are easily seen from the QFT superoperator in the product operator basis. They are the identity, $\sigma_x^1 \sigma_z^3$ and $(\sigma_x^1 + \sigma_z^3)/2$. These terms can be easily seen in the product operator basis (figure 7-4). Linear combinations of these states are also stationary points. The correlations between the experimental and desired output states of these points are 1, .91, and .93, respectively.

While the QPT data cast as a superoperator in the computational basis allows for the calculation of various measures of accuracy, it does not shed light on what errors
Figure 7-4: Amplitudes of the real part of the theoretical (left) and completely positive experimental (right) superoperator matrices, $S_{th}^{QFT}$ and $S_{exp}^{QFT}$, in the product operator basis. In the theoretical superoperator, the first and twentieth elements along the diagonal have amplitudes of 1, corresponding to the identity and $\sigma_z^1\sigma_z^3$ stationary points. In addition, elements (17,4) and (4,17) have an amplitude of 1 showing that $\sigma_z^1$ transforms into $\sigma_z^3$ under QFT evolution. The sum $(\sigma_z^1 + \sigma_z^3)/2$ is thus another stationary point. These elements remain fairly stable under the experimental implementation.

occurred during the experimental implementation or how to correct such errors in future implementations. In addition, the experimental superoperator is not completely positive as required for any physical evolution. We will explore these issues in the coming sections.

7.3 Completely Positive

A significant percentage of the experimental superoperator is not completely positive, as evidenced by the presence of Kraus operators with imaginary amplitudes (corresponding to negative Choi matrix eigenvalues). This phenomenon is not due to the experiments per se, but is an artifact of the QPT process. Perhaps the most important cause of incomplete positivity in QPT is incoherence. In an NMR system, the source of incoherence is the inhomogeneity of the RF over the finite sample. Thus, different parts of the sample undergo different unitary evolution as shown in figure 7-5.

Let us assume that we can divide the sample into $k$ sections each undergoing
Complete Superoperator:

$$S = (U_1 \otimes U_2 \otimes \ldots \otimes U_k) \otimes (U_1 \otimes U_2 \otimes \ldots \otimes U_j)$$

Reduced Superoperator:

$$S' = \sum_j p_j \bar{U}_j \otimes U_j$$

Figure 7-5: Pictorial representation of information loss when describing an NMR system with incoherence. A full description would encompass a Hilbert space of dimension $N^k \times N^k$ which includes the spatial degrees of freedom. The complete evolution could then be described by $U_{total} = U_1 \otimes U_2 \otimes \ldots \otimes U_k$ as shown in the figure above. We describe the evolution on a $N \times N$ Hilbert space accounting for the incoherence by including a probability factor based on how much of the ensemble undergoes a particular unitary operation. When no quantum coherences exist between sections of the sample (as in our experiments) the two descriptions are equivalent. However, when the sample undergoes further evolution, the spatial information lost by going from the first representation to the second causes incomplete positivity in the superoperator.

slightly different unitary evolution due to the inhomogeneity of RF power. For a complete description of the ensemble evolution the spatial coordinate should be taken into account. The complete unitary evolution resides in a Hilbert space of dimension $N^k \times N^k$ where $N = 2^n$ is the Hilbert space dimension of one sample section (based on the number of qubits),

$$U_{total} = U_1 \otimes U_2 \otimes \ldots \otimes U_k$$

and the superoperator is then

$$S_c = \overline{U}_{total} \otimes U_{total}.$$

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In the experiments performed there are no quantum correlations between the different sections of the sample. Therefore, we can trace over the spatial degrees of freedom without loss of information and write

$$S_r = \sum_{i}^{k} p_i U_i \otimes U_i,$$

(7.11)

where $p_i$ is the percentage of the ensemble undergoing the evolution described by $U_i$. In this section, we will refer to this as the reduced superoperator. In our experiments we do not readout the spatial degrees of freedom, thus, we must use the reduced superoperator description of the evolution.

Describing the evolution of the ensemble system by tracing out spatial degrees of freedom works well when describing one operation. However, when a second operation is to appended to the first, we suffer a loss of information. This is easily seen by analyzing the action of a gradient. A gradient is an incoherent operation since its action depends on a spatial coordinate. The Hamiltonian for a gradient on qubit $j$ is $H_j(z) = e^{i \gamma \frac{\partial H_j}{\partial z} - \frac{z^2}{2}}$. When applied to magnetization in the transverse plane, the gradient winds up the magnetization into a helix across the sample which integrates to identity. We can describe this process via a reduced superoperator. If we then applied an inverse gradient of the same power and duration the to the system, the magnetization would unwind causing an echo. This echo is not properly described by a second reduced superoperator acting after the first since the second superoperator cannot differentiate between identity and magnetization that has been wound up by a gradient. We can state this condition simply by observing

$$Tr_z(S_1 S_2) \neq Tr_z(S_1) Tr_z(S_2)$$

(7.12)

A simulated example of the lack of correspondence between the two descriptions is shown in figure 7-6.

QPT as done in this work requires creation of a complete set of input and output states. The input state experiments start from $\rho_{eq}$, create the necessary input states, and read out the state via state tomography. Similarly, the output states are created
Figure 7-6: Eigenvalues of simulated superoperators on the complex plane. The simulation is done on an alanine sample to demonstrate the effects of incoherence. Eigenvalues of the product of superoperators describing the evolution of a 90 degree pulse on spin 1 about the negative y-axis followed by a 180 degree pulse on spins 1 and 2 about the x-axis, $S_{180x}^{1,2} \times S_{90y}^{1}$ (o) are compared to the superoperator eigenvalues for the evolution of the two pulses(x). Due to the presence of incoherence the eigenvalues are not the same. This simulation includes unitary errors due to imperfect pulses and incoherent errors due to the inhomogeneous RF power across the sample.

starting from $\rho_{eq}$ creating the input state, applying the QFT, and performing state tomography. The superoperator is then constructed from the input and output states. However, we have just explained that, due to incoherence, the reduced superoperator does not correctly describe two evolutions applied one after the other. Thus, the reconstructed superoperator is not physical as evidenced by the fact that it is not completely positive.

Another source of the not completely positive pat of the superoperator is the state tomography. In order to measure all of the terms in the density matrix each experiment must be repeated a number of times, each time appending a different readout pulse. The readout pulses serve to rotate different density matrix elements into terms that are observable in an NMR spectrum. Enough readout pulses are done such that every term is observed in at least one of the repetitions.

To reconstruct the density matrix the unitary part of the readout pulse is numerically reversed, including any coherent pulse errors, and the different terms are put together to get the density matrix. Terms that are read out more then once, and each
has a slightly different outcome, are simply averaged together.

The above process leads to other sources of not completely positive parts of the superoperator. The set of readout pulses is the same for every state, but the readout pulses themselves vary in time and RF-power. However, when reconstructing the density matrix, incoherent errors during the different readout pulses are not taken into account. This again leads to not completely positive parts of the reduced superoperator as explained above. Additionally, unitary errors in readout pulses cause terms that are read out more then once to have slightly different values. These values are averaged but can cause the density matrix to be non-physical. Finally, decoherence during the readout pulses can also cause incomplete positivity. The readout pulses are of different lengths and RF powers. The decoherent evolution depends on the external Hamiltonian and these effects are not taken into account when reconstructing the input or output density matrices. Therefore, decoherence contribute to the non-physicality of the reconstructed density matrix.

To show that this lack of a completely positive superoperator is not an experimental effect, we have simulated the experimental procedure, including readout pulses, on our simulator. This simulation uses the same pulses as in the experiment and includes incoherent, but not decoherent, errors. The simulation creates a full set of input and output states but makes use only of the terms observable on an NMR spectrum. A series of readout pulses is thus required to completely reconstruct the state. The readout pulses are the same used in the actual experiments. The resulting superoperator, reconstructed in the same way as the experimental superoperator, is not completely positive. We quantify the amount incomplete positivity by the sum of the magnitude of the negative Choi matrix eigenvalues divided by the sum of the positive Choi matrix eigenvalues. For the simulations 22.5% of the superoperator is not completely positive, while for the experiment 39.5% is not completely positive. The difference is most likely due to decoherence effects which are not included in the simulation, and imperfect readouts in the experiments due to noisy spectra.

The experimental superoperator can be made completely positive by keeping only those Kraus operators with non-imaginary amplitudes and appropriately renormaliz-
Figure 7-7: $S_{th}^{QFT}$ (left) and $S_{exp}^{QFT}$ (right) in the phase space basis. Since phase space is a natural basis for a Fourier transform, the QFT superoperator has a very simple form and the errors are clearly seen. However, phase space is a description in terms of position and momentum while our systems internal and external Hamiltonians are more easily written in terms of SU(8) rotations. Therefore, while this description is natural for the QFT, it is not helpful in identifying errors that occurred during implementation or for finding means to correct these errors.

ing the superoperator such that its Choi matrix eigenvalues sum to $N$. From here on in we work with the completely positive experimental superoperator, unless otherwise noted.

### 7.4 The QFT Superoperator in Phase Space

A Fourier transform, be it classical or quantum, transforms between reciprocal position and momentum basis. Hence, a Fourier transform has a very simple interpretation on phase space. Classically, a Fourier transform rotates phase space by 90 degrees. Quantum mechanically, we would expect the QFT superoperator to have a simple representation on a quantum phase space [58]. The QFT superoperator on a quantum phase space, is shown in figure 7-7, has only one element in each row and column populated. The populated elements all have a magnitude of 1.

From the above figure one can clearly recognize that there are errors in the QFT implementation. However, these errors are formulated in terms of position and mo-
Figure 7-8: The amplitudes, $m_k$, of experimental QFT Kraus operators (x). There is one dominant Kraus operator, $m_1 = .86$, which we expect to be similar to $U_{QFT}$. The second Kraus operator, $m_2 = .34$, is the largest error operator and the remaining continuum of Kraus operators are less significant errors. Also shown (o) are the amplitudes of the Kraus operators taken from the experimental superoperator after being made completely positive and renormalizing the Choi matrix. There is still one dominant Kraus operator $m_1 = .67$, a large error operator $m_2 = .27$ and a continuum of smaller error operators.

mentum while the internal and external Hamiltonians of our system are in terms of SU(8) rotations. So, although the phase space representation is the natural one to see the action of the QFT, it has not proven helpful to us in studying the errors.

### 7.5 The Kraus Operator Sum Representation

As mentioned above, the deconstruction of the superoperator into a Kraus operator sum yields a set of Kraus operators, $A_k$, each with an associated amplitude, $m_k$. For experiments that are close to ideal, one would expect that the Kraus operator with the highest amplitude, $A_1$, would be similar to the ideal unitary operator. From our experimental results and from many simulations, we observe that there is usually a second Kraus operator, $A_2$, that has a higher amplitude then the rest, and represents the largest error operator. Finally, there is a continuum of remaining Kraus operators. The spectrum of Kraus operators for the experimental QFT is shown in figure 7-8 (7-8).
Simply by looking at the spectrum of the Kraus operators one can approximate
the accuracy of the experiment with respect to incoherent and decoherent errors.
Were the errors purely unitary the Kraus sum would still yield a lone Kraus operator
with an amplitude of 1. Thus, the amplitude of the $A_1$, the first order Kraus operator,
with respect to the others is a measure of the unitarity of the implementation. In our
experiments, $A_1$ accounts for .90 of the squared Frobenius norm of the superoperator.
The non-completely positive experimental superoperator has a squared Frobenius
norm that is only .62 of its theoretical value. Thus, we can view this as saying that
a random molecule from the pseudo-pure NMR ensemble has a 38% chance of being
completely depolarized, and $.62 \times .90 = 55\%$ chance of undergoing unitary evolution
closest to $A_1$.

The projection between $A_1^{exp}$ and $U_1^{exp}$, the unitary operator that minimizes the
sum of the square of the elements $A_1 - U_1$, is $.997$ and the attenuation factor (ratio
of norms) is $.86$. This means that $A_1$ is very nearly a scaled down unitary operator.
We note that the unitary operator from this minimization is the same as the unitary
part of a polar decomposition. $U_1$ can be compared to the desired unitary operator
by means of the fidelity, the average correlation between a complete set of output
states for the two evolution operators [31]. The fidelity between $U_1$ and the $U_{QFT}$ is
$.86$, which is the same as the average experimental output state projection. This is
a strong indication that all of the action of the QFT is contained in the first Kraus
operator.

The action of the first Kraus operator can be removed from the superoperator by
forming a superoperator from the $A_1$ dynamics, and subtracting it from the experi-
mental superoperator. Upon renormalization, we can take another set of Kraus oper-
ators, the largest of which accounts for .023 of the squared norm of the experimental
superoperator and has a projection of .97 with its closest unitary approximation.
7.6 Identifying Errors

We now present methods for identifying the various types of errors that occur during experimental implementation. This will serve as our recipe for the analysis of the experimental results which will be done in the next section. We start by identifying coherent errors.

The Kraus operators form an orthogonal set. Thus, assuming that the dynamics of the open quantum system is close to the desired evolution, $A_1$ should be similar to the desired unitary operator but it should also include all coherent errors. These errors can be identified in the following way: extract the unitary part, $U_1$, of $A_1$ through a polar decomposition. The error operator $E_1$ is the multiplication of $U_1$ by the Hermitian conjugate of the desired dynamics, $E_1 = U_1 U_{QPT}^\dagger$. $E_1$ can now be decomposed into SU(8) rotations of the type we can directly control via the internal and external Hamiltonians of liquid state NMR.

Another method for identifying the coherent implementation errors is by looking at the superoperator in a basis reflecting our methods of control, the product operator basis. We can pinpoint the coherent errors by transforming from the computational basis to the product operator basis and multiplying by the Hermitian conjugate of the desired superoperator, $S_{error} = S_{exp} S_{th}^\dagger$. We will demonstrate both of these methods using our experimental data.

Coherent errors can also be detected, though not identified, by looking at the superoperator eigenvalues. Coherent errors will cause a rotation of eigenvalues on the complex plane. However, unlike incoherent and decoherent errors, coherent errors leave the superoperator unitary and the eigenvalues will all have amplitudes of one.

Purely decoherent errors can be identified from the overall reduction of magnetization during the experiments. This can be seen from the superoperator eigenvalues as a reduction in amplitude without rotation on the complex plane. This effect can also be seen from an overall reduction in the amplitudes of the superoperator matrix elements.

Incoherent errors can also be identified from their effect on the superoperator
eigenvalues. The eigenvalues tend to spread out under incoherent evolution. First order perturbation theory tells us that the further the eigenvalue rotates from its original position, the higher loss of amplitude [65]. This is seen in the simulations below.

For future reference, we note that the QFT superoperator has 4 degenerate eigenvalues: 1, -1, $i$, and $-i$. For the three qubit QFT superoperator the eigenvalue 1 is 18 times degenerate, -1 is 16 times degenerate, and $i$ and $-i$, are both 15 times degenerate.

7.7 Discussion

We will now go through the process of identifying the coherent, incoherent, and decoherent errors found in our experimental implementation of the QFT. To assist in this process, we will make use of a four sets of numerical simulations. Each set of simulations is meant to isolate an error type or to distinguish the results of certain error combinations.

The first simulation includes only coherent errors. As mentioned above, the pulses used in the experiment are the type described in [31] which refocus all unwanted internal Hamiltonian evolution during the pulse and are robust against RF inhomogeneity. These pulses, however, are not perfect due to incomplete refocusing of unwanted internal Hamiltonian evolution and inexact performance of the desired rotations. Our first simulation includes these pulse errors but no incoherent or decoherent errors. Thus, the simulated dynamics is unitary, $U_{coh}$ with superoperator $S_{coh} = U_{coh} \otimes U_{coh}$.

The fidelity between the simulated QFT with coherent errors and the ideal QFT evolution is .95. Since these pulses are used in our experimental implementation, this is the maximum experimental gate fidelity we can expect even if there was no incoherence or decoherence effecting our system. All of the other simulations include the same coherent errors plus other types of errors. Therefore, when trying to isolate the effects of incoherent and decoherent errors in our simulations, we will refer back to $U_{coh}$ as the ‘ideal’ evolution.
The second simulation includes coherent and decoherent errors. The simulation uses the experimentally determined relaxation supergenerator, $L_{\text{relax}}$, for the alanine sample. The supergenerator is made completely positive by keeping only Linblad operators corresponding to positive eigenvalues of the projected Choi matrix. Linblad operators are constructed by projecting its Choi matrix $-P \times \text{Choi}(L_{\text{relax}}) \times P$, where $P = I_N \otimes I_N - \text{col}(I_N) \times \text{col}(I_N)^\dagger/N$, and unstacking the eigenvectors of this matrix [40]. We also assume that the relaxation superoperator does not depend on the presence or strength of an applied external Hamiltonian.

The effect of the relaxation can be analyzed by looking at the superoperator eigenvalues. Figure (7-9) compares the superoperator eigenvalues of the purely unitary simulation (only coherent errors) with the eigenvalues of the simulation with coherent and decoherent errors (the eigenvalues of the unitary simulation all have a magnitude of 1 but are multiplied by a constant in the figure to show highlight the comparison). This figure highlights that, to a remarkable degree, the effect of the decoherence on the QFT is simply to uniformly decrease the magnitude of the eigenvectors. There are no unitary errors, which would simply move the eigenvalues, or incoherent errors, which would spread and dissipate the eigenvalues.

Further corroboration that the decoherent errors can be cleanly separated from the coherent errors is seen from the Kraus operators of the relaxation simulation, $A_k^R$. The first order Kraus operator, $A_1^R$, has an amplitude of .91. We take the unitary part, $U_1^R$, of $A_1^R$ via polar decomposition and compare it to $U_{\text{coh}}$, the unitary operator corresponding to the QFT simulation with just coherent errors. The fidelity between the two $F(U_{\text{coh}}, U_1^R)$ is $1 - 10^{-5}$. This is because $A_1^R$ is almost exactly $U_{\text{coh}}$ multiplied by a constant. The high fidelity between these two operators and the eigenvalue distribution shown in figure 7-9 demonstrate that, to a great degree, the relaxation applied causes a uniform reduction in the overall magnetization during the experiment. The relaxation does not cause any coherent evolution.

Our next simulation includes coherent and incoherent errors. These errors arise
Figure 7-9: Comparison of superoperator eigenvalues for simulations with only coherent errors (o) and with coherent and decoherent (relaxation) errors (x). The eigenvalues are plotted on the complex plane. The magnitudes of the eigenvalues for the unitary simulation all have a magnitude of 1. In the figure, each of these eigenvalues has been multiplied by .82 to show that the effect of relaxation is almost completely a simple uniform decrease in eigenvalue amplitude. There is almost no coherent or incoherent errors due to the decoherence.

from an uneven radio frequency profile over the sample. The RF profile can be measured experimentally and is shown in figure 7-10. This simulation includes the incoherent errors arising from this profile.

One way to study the effect of incoherence on the system dynamics is to look at the eigenvalue spectrum. As shown in figure (7-11), the effect of incoherent errors is to spread the eigenvalues and lower their amplitude. The loss in eigenvalue amplitude is not uniform. It is seen that the further the eigenvalues deviate from there correct unitary placement, the lower the eigenvalues magnitude. This is consistent with first-order perturbation theory prediction mentioned above and has been observed in superoperator eigenvalues of less complicated desired evolution [65].

The first Kraus operator of the RF inhomogeneity simulation, $A_1^{RFI}$, has an amplitude of .96. Due to the spread of eigenvalues, the polar decomposition of this
Figure 7-10: Not every part of the NMR sample sees the same RF power. The 33 point RF profile shows how much of the sample sees what fraction of the desired power (hence, 1 is the desired power). This profile has been measured experimentally via a spin nutation experiment [65] and is used for the simulations.

Figure 7-11: Comparison of superoperator eigenvalues for simulations with only coherent errors (o) and with coherent and incoherent errors (x). The eigenvalues are plotted on the complex plane. The effect of the incoherent errors is mainly to spread out the eigenvalues. The further the eigenvalues spread the lower the amplitude of the eigenvalue.
Figure 7-12: Comparison of superoperator eigenvalues for simulations with coherent and incoherent errors (o) and with coherent, incoherent, and decoherent errors (squares). The eigenvalues are plotted on the complex plane with the eigenvalues of the superoperator with just coherent and incoherent errors multiplied by .82 to highlight the comparison between the sets of eigenvalues. Again we see that the effect of the decoherence is simply to lower the amplitude of the eigenvalues without rotating them in the complex plane.

Kraus operator is not equivalent to $U^{coh}$. The fidelity between them is .97. Thus, we can identify incoherent errors by pointing to a spread of eigenvalues accompanied by a decrease of eigenvalue amplitude dependent on the spread. This is opposed to decoherent errors which do not cause a spread of the eigenvalues but instead decrease the eigenvalue amplitude uniformly.

Our final simulation includes coherent, incoherent, and decoherent errors. This is necessary to see if the error types can be assumed to act independently or whether there is a coupling between them. Figure (7-12) compares the eigenvalues of the simulation with all three types of errors compared to the eigenvalues of the simulation with only RF inhomogeneity. Again we see that the action of the decoherence is simply to lower the amplitude of all the eigenvalues with no additional rotation of eigenvalues.

The first Kraus operator of this simulation, $A_1^{RR}$, has an amplitude of .87. Given the eigenvalue distribution, it is not surprising that the fidelity between the unitary part of $A_1^{RR}$ and the unitary part of $A_1^{RF I}$, is essentially 1. This allows for a clear
identification of decoherent errors, uniform reduction of amplitude not accompanied by rotation of eigenvalues in the complex plane, and strongly suggests that the decoherent and incoherent errors can be treated independently.

With this background we are now ready to analyze our experimental QFT superoperator. We will start by trying to identify coherent errors using the two methods described above. The first experimental Kraus operator, $A_1^{exp}$, is shown in figure 7-13 compared to the desired operator.

Following the procedure outlined in section 6, we take the unitary part of the first Kraus operator, $U_1^{exp}$, via a polar decomposition construct. The error operator $E_1^{exp} = U_1^{exp} U_{QFT}^{\dagger}$. Decomposing this into its product operators allows for the identification of the largest coherent errors and gives there strength. The largest errors are a $z$-rotation on the third spin, $exp(-i \times (.44) \times I_z^3)$, and a $z$-rotation on the second spin, $exp(i \times (.30) \times I_z^2)$.

We emphasize that an extra $z$-rotation on spins 2 and 3 did not necessarily occur during the experimental implementation. Instead, these rotation errors are the coherent part of the conglomeration of all errors, coherent and incoherent, that occur
Figure 7-14: Real parts of elements of the experimental QFT superoperator multiplied by the Hermitian conjugate of the theoretical QFT superoperator in the product operator minus .64 times the identity corresponding to the similarity between the two superoperators. The terms are ordered alphabetically as described in section 3. The elements are shaded so as to highlight the largest coherent error. The repeated pattern shows an error in which terms containing $\sigma^3_z$ are converted to terms containing $\sigma^3_y$. Thus, the largest coherent error is a $z$ rotation of the third spin.

during the experiment. Thus, rather then identify what went wrong with the implementation, this analysis provides a method to improve our QFT implementation; apply the original experimental QFT and append the inverse of the above errors. However, from this alone, we cannot pinpoint where or why the coherent part of the sum of all errors gives these specific operators. For example, we cannot say that this error occurred because a certain pulse was imperfect or there was extra chemical shift evolution at some point during the implementation. We can only identify these $z$ rotations as the coherent part of the sum of all errors in our experiment.

The other method of identifying coherent errors is to look at the superoperator in the product operator basis. Starting with our experimental superoperator (non-completely positive) $S_{\text{exp}}^{QFT}$, we extract the ideal action of the QFT by multiplying the Hermitian conjugate of the ideal QFT superoperator giving us an error superoperator $S_{\text{error}} = S_{\text{exp}}^{QFT} S_{\text{th}}^{QFT}$. This will give a large identity term whose size depends on the correlation between experimental and ideal superoperators. In order to highlight the errors, we subtract this large identity term. The results are shown in figure 7-14.
Figure 7-15: Real parts of elements of the experimental QFT superoperator multiplied by the Hermitian conjugate of the theoretical QFT superoperator and the superoperator corresponding to a z rotation of 25 degrees on the third spin minus .67 times the identity corresponding to the similarity between the ideal superoperator and the experimental superoperator multiplied by the third spin z-rotation. The superoperators are in the product operator basis with the terms ordered alphabetically as described in section 3. The elements are shaded so as to highlight the second largest coherent error. The dominant pattern shows terms containing $\sigma^2_z$ converted to terms containing $\sigma^2_y$, a z rotation on the second bit.

A pattern is easily discernible. Terms such as $\sigma^3_x$ have less than expected amplitude, while terms such as $\sigma^3_y$ have a corresponding higher than expected amplitude. Thus, we appear to have an extra z rotation on the third spin.

We can correct for this error by multiplying the experimental QFT superoperator by the superoperator corresponding to an inverse z-rotation of 25 degrees of the third spin. This allows for the identification of the second level coherent error as shown in figure (7-15). This process can be continued for six or seven steps, each time identifying a coherent error and then ‘fixing’ that error by multiplying the experimental QFT by the inverse operation. Each step will raise the gate fidelity of the QFT plus corrected errors and will give a formula to implement a better QFT.

To identify incoherent and decoherent errors we can look at the eigenvalues of the (completely positive) experimental superoperator. Let us compare these eigenvalues to the eigenvalues of the experimental QFT superoperator with the coherent errors of the experimental implementation removed. The coherent error operator is $E_1 = U_{QFT}^\dagger * U_{1}^{exp}$, where $U_{1}^{exp}$ is the unitary part of the most dominant experimental Kraus
Figure 7-16: Experimental superoperator eigenvalues (x) compared to experimental eigenvalues after removal of coherent errors (o). The error operator is $E_1 = U_{QFT}^\dagger U_1^{exp}$, where $U_1^{exp}$ is the unitary part of the most dominant experimental Kraus operator. Note that the eigenvalues are clustered around the theoretical eigenvalues.

operator, $A_1^{exp}$. This gives an idea of how the eigenvalues would look if there was no coherent experimental errors and serves to help identify the incoherent and decoherent errors of our implementation.

From our analysis of the various simulations, we would expect most of the decrease of eigenvalue amplitude to be a sign of decoherent errors. The extra spread in eigenvalues beyond what is expected from coherent errors and the dissipation of eigenvalues seen from the non-uniform amplitude of eigenvalues is due to incoherent errors. There are, however, some features of the eigenvalues that are not explained by first order perturbation theory nor have they been seen in the simulations. These include the eigenvalues in the right half plane that, though they do not seem to have rotated much from the theoretical complex angle, have a large decrease in amplitude. In addition, two of the eight eigenvalues that until this point have had no imaginary part have become complex conjugates (the scale of the figure is too large to see this). These phenomena may be due to inaccurate assumptions and simplifications made for the simulations. First of all, the simulations assume a relaxation superoperator independent of the external Hamiltonian. This is not so as evidenced by phenomeno
such as spin locking. Second, the simulations do not take into account nuclear Over-
hauser effect (NOE) from proton spins in the alanine molecule. These phenomenon
play a role in our experiments, leaving some ambiguity in the signatures of incoherent
versus decoherent errors.

We have implemented quantum process tomography of the quantum Fourier trans-
form on a three qubit NMR QIP. From the data, we can identify means of improving
future implementations of the QFT and account for the actions of other errors. The
implementation of QPT also demonstrates our ability to control the NMR system and
highlights the accuracy of recent advances in creating RF pulses. While full QPT on
larger quantum systems becomes exponentially hard the analysis done here gives the
basic guidelines of how information about certain error operations can be extracted.
Chapter 8

Fidelity Decay as an Indicator of Quantum Chaos

8.1 Fidelity Decay

A number of times in this work we have mentioned that quantum systems cannot show the extreme sensitivity to initial conditions that characterizes classical chaos. However, an analogous characterization, sensitivity to small changes in the governing Hamiltonian of the system, applies to quantum systems as well as classical systems. Peres [60] was the first to conjecture that the decay rate of fidelity due to a slight perturbation of the system Hamiltonian may depend on whether or not a quantum systems is chaotic.

The fidelity compares the output of an initial state evolved under perturbed and unperturbed dynamics

$$F(n) = |\langle \psi_0 | (U^\dagger)^n (U_\delta)^n | \psi_0 \rangle|^2$$

(8.1)

where $U$ is the unperturbed evolution, and $U_\delta = U_p U$ where $U_p = exp(-i\delta V)$ is the perturbation operator of strength $\delta$. $\psi_0$ is the initial state of the system. The fidelity decay behavior depends not only on whether the map is classically chaotic, but also on the initial state of the system and the strength of the perturbation.

There are two important regimes of perturbation strength. The first is where the
perturbations are weak enough to allow for description under first-order perturbation theory. Thus, the eigenstates of $U_d$ can be approximated by those of $U$ and the fidelity can be written simply as

\[ F(n) \simeq \left| \sum_m |c_m|^2 \exp(-i\delta V_{mn} n) \right|^2, \tag{8.2} \]

where we have written the initial state $|\psi_0\rangle$ in terms of the eigenstates of the unperturbed operator $|\psi_0\rangle = \sum_m c_m |v_m\rangle$. The matrix element $V_{mn}$ refers to the $(m, n)th$ element of the perturbation operator, $V$, written in the ordered eigenbasis of $U$ (units are such that $\hbar = 1$). For short times $F(n)$ is independent of the system Hamiltonian and depends only on the perturbation Hamiltonian, $V$. This is seen by expanding $F(n)$ as a power series: $F(n) \simeq 1 - \delta^2(\Delta V)^2 n^2 + O(\delta^4(\Delta V)^4 n^4)$, where $(\Delta V)^2 = \sum_m |c_m|^2(V_{mm})^2 - (\sum |c_m|^2 V_{mm})^2$. The time scale for this parabolic decay is $(\delta \Delta V n)^2 \ll 1$. For longer times the behavior of $F(n)$ depends on the number of $c_m$ that are populated. The $c_m$ of regular systems satisfy selection rules and most of them vanish. Therefore, $F(n)$ will simply oscillate around $\sum_m |c_m|^4$. The $c_m$ of chaotic systems, however, are randomly distributed leading to a Gaussian fidelity decay much longer than the initial parabolic decay[60, 18].

First order perturbation theory is applicable as long as $\sigma$, a typical off-diagonal matrix element of the perturbation Hamiltonian expressed in the ordered eigenbasis of the system Hamiltonian, is less than the average system level spacing, $\Delta$. Stronger perturbations, $\sigma > \Delta$, are said to be in the Fermi Golden Rule (FGR) regime [43] and the fidelity decay behavior (after the initial parabolic decay) of chaotic system is exponential. It has been shown that for some perturbations the rate of the exponential decay increases as $\delta^2$. For quantum systems and perturbation operators amenable to a semi-classical analysis, the increase in the exponential decay rate can saturate at the classical Lyapunov [46, 43, 7], or the bandwidth of the system Hamiltonian [43]. The exponential fidelity decay rate continues for a time $\log(N)/\Gamma$, where $\Gamma$ is the rate of the exponential. At this point the fidelity saturates at $F(n) \simeq 1/N$.

Following Jacquod[44], we derive the FGR regime behavior using random matrix
theory (RMT) techniques (see [67] for a derivation using time correlation functions). RMT is applicable to quantum chaotic systems because many quantum chaotic systems have statistical properties similar to those of random matrices. Let us define eigenvectors and eigenangles for the unperturbed operator $U|v_j\rangle = \exp(-i\phi_j)|v_j\rangle$, and the perturbed operator $U_\delta|v'_j\rangle = \exp(-i\phi'_k)|v'_k\rangle$. Then, for an initial random state, $|\psi_0\rangle = \sum_j c_j|v_j\rangle$, the fidelity can be written as

$$F(n) = \sum_{ij} c_i^*c_j \langle v_j|U_\delta^n|v_i\rangle e^{-i\phi_i n} \times \sum_{kl} c_k^*c_l \langle v_l|(U_\delta^n)^\dagger|v_k\rangle e^{i\phi_k n}.$$  

(8.3)

We are interested in characterizing the fidelity averaged over all random states. To this aim, we divide the above equation into three parts. $F_A(n)$ includes the terms $\delta_{ij}\delta_{kl}$ with $i \neq k$, and half of the term $\delta_{ij}\delta_{kl}\delta_{ik}$. This term leads to the initial exponential fidelity decay for chaotic systems in the FGR regime. $F_B$, consists of terms where $\delta_{il}\delta_{jk}$ and half of the term $\delta_{ij}\delta_{kl}\delta_{ik}$. As we will see in the next chapter, this term leads to the $\simeq 1/N$ saturation level for random states. The remaining terms in equation (8.3) will vanish when averaged over all random states [44].

We can write $F_A(n)$ as follows:

$$F_A(n) = \sum_{ik, i \neq k} |c_i|^2|c_k|^2\langle v_i|U_\delta^n|v_k\rangle \langle v_k|(U_\delta^n)^\dagger|v_k\rangle e^{i(\phi_k - \phi_i) n} + \frac{1}{2} \sum_i |c_i|^4\langle v_i|U_\delta^n|v_i\rangle^2.$$  

(8.4)

We note that averaging over all pure states

$$\langle |c_i|^2|c_j|^2 \rangle = \frac{2}{N(N+1)} \simeq \frac{2}{N^2} \quad i = j$$

$$\frac{1}{N(N+1)} \simeq \frac{1}{N^2} \quad i \neq j.$$  

(8.5)

Thus, by replacing $U_\delta$ with $\sum_q e^{i\phi_q} |v'_q\rangle \langle v'_q|$ the initial fidelity decay for chaotic systems can be written as [44]

$$\langle F_A(n) \rangle \simeq \frac{1}{N^2} \sum_{iq} |\langle v_q|v'_q\rangle|^2 e^{i(\phi'_q - \phi_q) n}^2.$$  

(8.6)

Equation (8.6) is recognized as the Fourier transform of the local density of states
(LDOS). The LDOS is the spectral density of the original system under transition rules given by the perturbation. Hence, it is a measure of the overlap between perturbed and unperturbed eigenstates separated by an angle \((\phi_j - \phi'_k)\)

\[
\eta(\phi_j - \phi'_k) = |\langle v_j | v'_k \rangle|^2. \tag{8.7}
\]

The connection between the LDOS and the fidelity decay was first pointed out by Jacquod and coworkers in [43].

Previous studies suggest that the LDOS of a complex system in the regime of strong perturbation is Lorentzian[88, 32, 42, 89]

\[
\eta(\phi_j - \phi'_k) \propto \frac{\Gamma}{(\phi_j - \phi'_k)^2 + (\Gamma/2)^2} \tag{8.8}
\]

with a width of \(\Gamma = 2\pi\sigma^2/\Delta\). As before, \(\sigma\) is a typical off diagonal element of the perturbation operator and \(\Delta\) is the average system level spacing. Thus, using the Fourier transform relation, the initial fidelity decay is exponential with a rate \(\Gamma\)

\[
\langle F_A(n) \rangle \simeq \exp(-\Gamma n). \tag{8.9}
\]

The shape of the LDOS depends on the choice of perturbation and the chaotic system. An exponential fidelity decay and an exponential rate saturation at the Lyapunov exponent can be observed even with a non-Lorentzian LDOS [90].

Regular, non-chaotic, systems have a Gaussian decay in the FGR regime [67]. The Gaussian decay is faster than the exponential decay of chaotic states. This result has been explained using correlation functions and may be understood as follows: a perturbation to a chaotic system is quickly spread out to the entire Hilbert space of the system. Repetition of the same perturbation does not lead to a compounded error (the correlation time is short). Regular systems, however, do not have a mechanism which allows the perturbation to spread. Thus, the error is compounded (there is a long correlation time) leading to a faster fidelity decay. For an average over many coherent states of a regular system, each with a different rate of Gaussian decay, the
fidelity decays as a power-law [45].

8.2 Determination of the FGR Decay Rate

We now calculate the decay rate, \( \Gamma \) as a function of the perturbation Hamiltonian \( V \) and the perturbation strength \( \delta \). First we note that the eigenstates of quantum systems with chaotic classical analogues have been found to exhibit the statistics of random states when in the basis of the system coordinates [41]. Since the components of such random eigenstates are distributed uniformly over the basis states and uncorrelated with the eigenvalues of the system, the second moment of the matrix elements \( V_{mn} \) may be evaluated,

\[
\overline{V_{mn}^2} = \frac{\lambda^2}{N}
\]  

(8.10)

where \( \overline{\lambda} = N^{-1} \sum_{i=1}^{N} \lambda_i^2 \) is the variance of the eigenvalues of \( V \) and we have assumed \( \overline{\lambda} = 0 \). The fidelity decay rate for a quantum chaotic system in the FGR regime, \( \Gamma \), can now be determined by evaluating a typical off-diagonal element of the perturbation operator, \( \sigma^2 = \delta^2 \overline{V_{mn}^2} \), and the average level spacing \( \Delta = 2\pi/N \).

\[
\Gamma = \delta^2 \overline{\lambda^2}.
\]  

(8.11)

We will refer to this result as the FGR/RMT (Fermi golden rule/ random matrix theory) prediction.

To numerically test the above results, we consider a map \( U = U_{\text{CUE}} \) selected from the circular unitary ensemble (CUE). This ensemble consists of random unitary matrices, where random means drawn uniformly with respect to the invariant (Haar) measure [37]. A random map is chosen in order to avoid any possible bias that may be introduced from a map with a classical analog. CUE matrices can be generated using the gate decomposition devised in [96] or directly from the eigenvectors of a random Hermitian matrix. For numerical convenience we adopt the latter approach.

Our choice of perturbation is motivated by quantum information processing hard-
ware. Specifically, we consider

\[ U_p = \Pi_{j=1}^{n_q} \exp(-i\delta \sigma_z^j/2), \]  

(8.12)

where \( \sigma_z \) is the Pauli spin matrix. This corresponds to a collective SU(2) rotation of all the qubits through an angle \( \delta \). This choice of perturbation is also relevant to quantum control studies, in which case (8.12) is a model of coherent far-field errors [81]. For this perturbation the variance of the eigenvalue spectrum can be calculated as,

\[ \overline{\lambda^2} = \frac{1}{N} \sum_{k=0}^{n_q} \left( \frac{2k - 10}{4} \right)^2 C_k^{n_q}, \]  

(8.13)

where \( C_k^{n_q} \) are binomial coefficients.

Eigenstates of a CUE map are random by construction, thus the second moment of the perturbation operator matrix elements may be determined using (8.10). For the collective qubit rotation (8.12) with 10 qubits, \( n_q = 10 \), the rate of the exponential decay is given by,

\[ \Gamma = 2.50 \delta^2 \]  

(8.14)

where we have used (8.13).

Since computational basis states are easy to prepare in the QIP setting, we consider the fidelity decay for initial computational basis states. The behavior of the fidelity decay for a matrix typical of CUE is displayed in figure 8-1. The three perturbation values displayed in the figure are chosen near the onset of the FGR regime (\( \delta > .1 \)) and it is evident that the fidelity decay even for individual computational basis states exhibit exponential decay (8.9) with the appropriate rate.

### 8.3 Relation Between Fidelity Decay and Other Quantum Chaos Conjectures

We now explore the relationship between fidelity decay and other conjectures of quantum chaos. Specifically, we would like to know whether systems that show exponential
Figure 8-1: Fidelity decay for $U_{CUE}$ averaged over 50 computational basis states. The fidelity decay is in excellent agreement with the expected exponential golden rule decay (8.9) and the rate given by equation (8.14) (dashed lines). The three perturbation strengths shown are $\delta = (.1, .2, .3)$. Chain lines show the fidelity decay for two typical computational basis states in the case $\delta = .1$. Even these individual states are in good agreement with the FGR exponential decay and the rate determined by random matrix theory. The inset shows the LDOS for $\delta = (1, 2, 3)$ (bottom to top). As expected these are very well fit by a Lorentzian of the width $\Gamma$.

Fidelity decay in the FGR perturbation regime also satisfy the criteria of chaoticity set out by conjectures such as nearest neighbor level spacings and eigenvector statistics. To this aim we consider the fidelity decay for the Gaussian unitary ensemble (GUE). The GUE contains Hermitian matrices with independent elements drawn randomly with respect to the unique unitarily-invariant measure [37]. We examine the sensitivity to perturbations for the GUE by constructing the unitary operator $U_{GUE} = \exp(-iH_{GUE}\tau)$, where $\tau$ is a time delay between perturbations. We consider the same perturbation as in the CUE case, a collective rotation of qubits. For sufficiently small $\tau$, the propagator approaches identity and the fidelity decay is dominated by the perturbation operator,

$$F(n) = |\langle \exp(-i\delta V) \rangle|^2 + O(\delta^2 \tau^2 n^2). \quad (8.15)$$

This behavior is demonstrated in figure 8-2 for $\tau = .001$ and $\tau = .01$ and $\delta = .3$. For larger values of $\tau$ the fidelity decay under $U_{GUE}$ is exponential, as expected for the FGR regime, with the RMT rate given by equation (8.14).
Figure 8-2: Left figure: Fidelity decay for $U_{GUE}$ averaged over 50 computational basis states using the collective bit rotation perturbation with $\delta = .3$. For small $\tau$ values $\tau = .001$ (dashed line) and $\tau = .01$ (chained line), the propagator approaches identity and the fidelity decay is dominated by the perturbation operator. For larger $\tau$ values $\tau = .1$ (circles) and $\tau = 100$ (squares), the fidelity decay rate is exponential with the rate predicted by equation (8.14). Right figure: Spacing distribution of $U_{GUE}$ for $\tau = .001$ (a), $\tau = .01$ (b), $\tau = .1$ (c), $\tau = 100$ (d), compared to Poissonian and Wigner-Dyson distributions. Only the $\tau = .1$ case does the distribution approach the Wigner-Dyson distribution expected for random maps. For the $\tau = 100$ case, even though the spacing distribution is characteristic of classically integrable systems, the fidelity decay follows the exponential expected from quantum chaotic systems. This implies that it is the randomness of the eigenvectors that leads to the exponential fidelity decay behavior in the FGR regime.
It is important to note that for sufficiently large $\tau$ the eigenphases of $U_{GUE}$ become spread pseudo-randomly in the interval $[0, 2\pi)$. Under these conditions the eigenphases of the map $U_{GUE}$ exhibit the Poissonian spectral fluctuations that are characteristic of classically integrable systems [37]. In fact, the nearest-neighbor spacing distribution of $U_{GUE}$ for $\tau = 100$ are in excellent agreement with the Poissonian distribution $P(s) \propto \exp(-s)$ as shown in the inset to figure (8-2).

The occurrence of the exponential FGR decay for $\tau = 100$ with the RMT rate (8.14), despite the Poissonian nearest neighbor distribution, demonstrates an inconsistency between conjectured indicators of quantum chaos. Nevertheless, the FGR decay is consistent with the theoretical arguments leading to equation (8.10). This is because these arguments were based only on the RMT statistics of the eigenvectors (rather than the eigenvalues) of $U$. The eigenvectors of $U_{GUE}$ are, of course, random (by construction) and independent of $\tau$. From these observations it is clear that the presence of Wigner-Dyson spectral fluctuations in the implemented $U$, which comprises perhaps the most established criterion of quantum chaos, is not necessary for the exponential (FGR) fidelity decay at the rate (8.11).

We next consider the fidelity decay for a quantized classically chaotic system, the quantum kicked top (QKT). The QKT is an exemplary model of quantum chaos [38, 37] and is used extensively in many previous studies of fidelity decay. The kicked top is a unitary map $U_{QKT} = \exp(-i\pi J_y/2) \exp(-ikJ_z^2/j)$ acting on the Hilbert space of dimension $N = 2j + 1$, where $\vec{J}$ is the operator associated with the irreducible representation of angular momentum. In light of our earlier observations, we explore the relationship between the eigenbasis of the qubit perturbation (8.12) and that of the QKT itself. We first map the perturbation eigenbasis (i.e. the computational basis states $|m_N\rangle$ where $m_N = \{0, \ldots, N - 1\}$) onto the $|m_j\rangle$ eigenstates of the kicked top coordinate $J_z$ (where $m_j = \{j, \ldots, -j\}$). In figure 8-3 we compare the fidelity decay for the chaotic and regular regimes of the kicked top for averages over 50 initial computational basis states. The fidelity decay for the chaotic QKT is in good agreement with the FGR prediction (8.9) and the RMT rate (8.14) whereas the regular QKT decays at a much slower rate. If we map the qubit eigenbasis onto the
Figure 8-3: Fidelity decay for the quantum kicked top in the chaotic regime \( (k = 12) \) when the perturbation eigenbasis has been mapped to \( J_z \) (dash lines) and \( J_y \) (chain lines) compared to the FGR decay (solid lines) at the RMT rate (8.14). Each fidelity decay is an average over 50 computational basis states and \( \delta = (0.1, 0.3) \) (top to bottom). Also shown is the fidelity decay for the quantum kicked top in the regular regime \( (k = 1) \) with the perturbation eigenbasis mapped to the \( J_z \) (lines with circles) and \( J_y \) (lines with squares) coordinate bases (for \( \delta = 0.1 \)). The fidelity decay does not follow the exponential prescribed for chaotic systems. Inset: Average fidelity decay for regular kicked top \( (k = 1) \), when the qubit perturbation with \( \delta = (0.1, 0.3) \) (dashed lines), is transformed into a random eigenbasis (8.16). This is compared to the FGR/RMT rate (solid lines). Note that because the perturbation is random with respect to the system, the fidelity decay follows that of a chaotic system even though the system is the quantized version of a classically non-chaotic system. This further corroborates that it is the randomness of the perturbation eigenvectors that give rise to the exponential FGR fidelity decay.
$J_y$ basis of the kicked top, the fidelity decay for the chaotic top remains in agreement with the RMT rate but the regular top again exhibits non-FGR decay, in this case with a faster decay rate than the FGR/RMT prediction (8.14).

Finally, we demonstrate that FGR decay at the RMT rate can arise even for quantized classically regular systems (with a Poissonian eigenspectrum) when the qubit perturbation (8.12) is transformed to a random basis with respect to the eigenbasis of $U$. Specifically, we set

$$U_p = T \left[ \prod_j \exp(-i \delta \sigma^j_z/2) \right] T^{-1},$$

(8.16)

where $T$ is drawn from CUE. As demonstrated in the inset of figure 8-3, the fidelity decay of the regular QKT under this random perturbation is indistinguishable from that of the chaotic QKT and is very accurately described by the FGR at the RMT rate (8.14). This result provides further confirmation that the crucial feature of quantum systems which leads to the FGR decay is the randomness of the eigenvectors in the basis of the perturbation, and not the spectral fluctuations of the unperturbed map $U$.

In summary, we have demonstrated that the fidelity decay under qubit perturbations for random unitary and Hermitian matrices and the chaotic kicked top follows the FGR prediction with a rate determined by the variance of the perturbation’s eigenspectrum. This characteristic decay is not dependent on the presence of Wigner-Dyson fluctuations in the unperturbed spectrum, but does depend sensitively on the statistics of the system eigenvectors in the eigenbasis of the perturbation.
Chapter 9

Fidelity Decay Saturation Level

9.1 Theoretical Analysis

In the previous chapter we derived the initial exponential fidelity decay behavior for quantum chaotic systems. Eventually, this behavior saturates and the fidelity will fluctuate about a saturation level. In this chapter we focus on the characteristics of the saturation level [85] by studying

\[ F_{\infty} = \lim_{T \to \infty} \frac{1}{T} \sum_{n=1}^{T} F(n). \]  

(9.1)

The saturation level comes only from the \( F_B \) term of equation (8.3). This is because, assuming that the eigenvalues of \( U \) are non-degenerate, the terms of \( F_A \), equation (8.4), are all of the form \( C e^{i\phi_n} \), where \( C \) is positive constant. Hence, each term has a time average equal to zero.

\( F_B \) includes the \( \delta_i \delta_{jk} \) term and the other half of the term \( \delta_i \delta_{jk} \delta_{ij} \) in equation (8.3). It can be written as

\[ F_B(n) = \sum_{ij, i \neq j} |c_i|^2 |c_j|^2 \langle v_j | U^*_\delta | v_i \rangle \langle v_i | (U^\delta)^\dagger | v_j \rangle + \frac{1}{2} \sum_i |c_i|^4 \langle v_i | U^\delta | v_i \rangle^2. \]

(9.2)
Using equation (8.5) we can take the average over all pure states and write

$$
\langle F_B \rangle = \frac{1}{N^2} \sum_{ij} \langle v_j | U_\delta^n | v_i \rangle \langle v_i | (U_\delta^n)^\dagger | v_j \rangle.
$$

(9.3)

Replacing $U_\delta$ with $\sum_q e^{-i\phi_q} |v'_q\rangle \langle v'_q|$ and averaging over time (denoted by an overline) yields

$$
\overline{\langle F_B \rangle} = \frac{1}{N^2} \sum_{ij} |a_{iq}|^2 |a_{jq}|^2 = \frac{1}{N^2} \sum_{iq} |a_{iq}|^4 + \frac{1}{N^2} \sum_{i,q,i\neq j} |a_{iq}|^2 |a_{jq}|^2
$$

(9.4)

where $a_{iq} = \langle v_i | v'_q \rangle$ is the overlap between a perturbed and unperturbed operator eigenvectors. Clearly, the $|a_{iq}|^2$ depend on perturbation strength. In the limit of strong perturbation, the overlap between an unperturbed eigenvector and the perturbed eigenvectors $|a_{iq}|^2$ has the same statistics as a random state, equation (8.5).

Hence, $\langle |a_{iq}|^2 |a_{jq}|^2 \rangle = 1/(N^2)$ for $i \neq j$, and $\langle |a_{iq}|^4 \rangle = 2/(N^2)$. Thus, we can write

$$
\langle F_\infty \rangle = 1/N + O(1/N^2).
$$

(9.5)

In the limit of weak perturbation, $a_{iq}$ is simply a $\delta$-function and $\langle F_\infty \rangle = 2/N$ [67].

The above derivation is applicable to the fidelity decay of initial random states. For initial system eigenstates the saturation level can be much larger and, unlike initial random states, depends strongly on the perturbation strength, $\delta$. The study of initial eigenstate fidelity decay is of particular interest because it is equivalent to the survival probability of a system eigenstate under the influence of a perturbation. Below we provide theoretical arguments leading to a region where $\{F_\infty\}$ (where the curly brackets denote average over eigenstates) depends quadratically on the perturbation strength. We test this prediction numerically on quantum chaotic maps.

Prosen [67] has noted that for initial eigenstates $\{F_\infty\} \rightarrow 1$ in the limit of weak perturbation and $\{F_\infty\} \rightarrow (4 - \beta)/N$ in the limit of strong perturbation where $\beta$ depends on the universality class of the system. For maps typical of circular orthogonal ensemble (COE), $\beta = 1$ while for maps typical of circular unitary ensemble (CUE) $\beta = 2$. Here, we consider $F_\infty$ for intermediate perturbation strengths and provide a theoretical argument and numerical evidence for the quadratic behavior for $F_\infty$ versus
perturbation strength.

To evaluate the dependence of the saturation level on the perturbation strength we express the fidelity for an initial eigenstate, \( |\psi_o\rangle = |v_m\rangle \), as

\[
F(n) = |\langle v_m | \sum_l a_{lm} e^{-in(\phi'_l - \phi_m)} |v_m\rangle|^2
\]

(9.6)

where once again \( a_{lm} = \langle v'_l | v_m \rangle \). The above equation can be separated into a time independent term plus a time dependent term

\[
F(n) = \sum_l |a_{lm}|^4 + \sum_{lk} |a_{lm}|^2 |a_{km}|^2 \cos[(\phi'_l - \phi'_k)n].
\]

(9.7)

The time average of the second term goes to zero while the first term casts \( F_\infty \) as the inverse participation ratio of the overlap between perturbed and unperturbed eigenvectors[67]. In other words, the fidelity saturation level is simply the sum of the squared elements of the LDOS, equation (8.7).

The number of contributing perturbed operator eigenvectors \( |v'_l\rangle \) to the initial eigenstate, \( |v_m\rangle \) can be estimated by the width of the LDOS. We make the assumption that the Lorentzian shaped LDOS can be replaced by a top-hat of width \( \Gamma \). The \( \Gamma/\Delta \) contributing \( |a_{lm}|^2 \) terms within the width \( \Gamma \) of this simplified LDOS each have weight \( 1/\Gamma \). With this approximation,

\[
\{F_\infty\} \propto 2\pi/(\Gamma N)
\]

(9.8)

where \( 2\pi/N \leq \Gamma \leq 2\pi \). A similar result is mentioned in [89].

\{ \( F_\infty \) \} for initial eigenstates can now be related to the perturbation strength. From equation (8.11) \( \Gamma = \delta^2A^2 \) and thus \( \{F_\infty\} \) is expected to have a quadratic dependence on perturbation strength in the FGR regime

\[
\{F_\infty\} \propto 2\pi/(\Gamma N) = 1/(\delta^2A^2 N).
\]

(9.9)
9.2 Numerical Simulations

The above predictions were first tested on random circular unitary ensemble (CUE) maps as done in the previous chapter. Once again, we assume that our system is composed of a collection of two-level subsystems or qubits. The perturbation used is a $z$-rotation of all of these qubits through an angle $\delta$.

Figure (9-1) shows $\{F_\infty\}$ for initial eigenstates of the CUE matrix versus perturbation strength. For perturbations weaker than the FGR perturbation regime there is very little decay, while in the limit of strong perturbation $\{F_\infty\} = 2/N$ as expected for CUE maps. Between these extremes exists a power law decrease of $\{F_\infty\}$ with increased perturbation strength. The data is compared to $\{F_\infty\} = C_{CUE}/(\delta^2 N^2)$, where the proportionality constant, $C_{CUE} = 3.6$ is chosen to best fit the data. The actual slope of the data is between 1.8 and 1.9. This discrepancy is due to the approximation made by replacing the Lorentzian LDOS with a top-hat of width $\Gamma$.

A similar analysis was carried out for random maps with statistics of the circular orthogonal ensemble (COE). COE matrices can be created from CUE matrices, $\text{COE} = \text{CUE} \times \text{transpose}(\text{CUE})$ [37]. Like the CUE maps, the COE maps have no classical analog and we use them here as models for the behavior of quantized systems with COE eigenvector statistics and energy level spacings. We note that for COE statistics $\langle |c_i|^4 \rangle = 3/(N^2 + 2N)$. Figure 9-2 shows $\{F_\infty\}$ versus perturbation strength for COE maps. Again, an approximate quadratic relationship emerges but with a proportionality coefficient, $C_{COE} = 5.4$.

In the limit of strong perturbation the ratio $\{F_{\infty}^{COE}\}/\{F_{\infty}^{CUE}\}$ is equal to $3/2$ [67] as follows from the discussion leading up to equation (9.5). Numerically we find that the proportionality remains fixed for perturbations in the FGR regime. The calculated numerical average of $\{F_{\infty}^{COE}\}/\{F_{\infty}^{CUE}\}$ in the FGR regime for the three Hilbert space dimensions explored is 1.48. This can be explained by assuming that the only $\Gamma/\Delta$ of the perturbed eigenstates contribute to a given unperturbed eigenstate, and those that contribute do so in a random fashion, with an average amplitude of $1/\Gamma$. This is to say, that $|a_{iq}|^2 = 1/\Gamma$ for $\Gamma/\Delta$ of the perturbed eigenstates and $|a_{iq}|^2 = 0$ for
Figure 9-1: Saturation level versus perturbation strength for initial eigenstates of a random CUE map of dimensions 256 (circles), 512 (stars), and 1024 (x). For weak perturbations, below the FGR regime, the fidelity barely decays. In the limit of strong perturbation \( \{F_\infty\} \) saturates at \( 2/N \) (solid line). For intermediate values of \( \delta \), \( \{F_\infty\} \) is well approximated by equation (9.9) with the proportionality constant \( C_{CUE} = 3.6 \). \( \{F_\infty\} \) is obtained by averaging over 2000 map iterations starting at iteration \( n = 2000 \), which is well after the initial exponential decay. This is averaged over all \( N \) initial eigenstates. The lower inset shows the initial exponential fidelity decay of the CUE map with \( N = 1024 \) averaged over all 1024 system eigenstates. The fidelity decay is plotted versus \( \delta^2 n \) so that the exponential decay rates overlap and the saturation level is easily seen. The perturbation strengths used are \( \delta = .1, .2, .3, .4 \) (top to bottom). The upper inset shows a semi-log plot of the local density of states for a CUE map perturbed by a collective bit \( z \)-rotation, \( \delta = .1, .2, .3, .4 \) (bottom to top). The solid line is a Lorentzian of width \( \Gamma = \frac{V_{mn}^2}{\Delta} \) with \( V_{mn}^2 \) determined numerically from the CUE map. Note that the LDOS approximates the Lorentzian of equation (8.8) extremely well.
Figure 9-2: $\{F_\infty\}$ versus perturbation strength for initial eigenstates of a random COE map (x) and the QKT with $k = 12$ (circles) of dimensions 256, 512, and 1024 (from top to bottom). For weak perturbations, below the FGR regime, the fidelity barely decays. In the limit of strong perturbation $\{F_\infty\}$ saturates at $3/N$ (solid line). For intermediate values of $\delta$, $\{F_\infty\}$ is well approximated by the estimate of equation (9.9) with the proportionality constant $C_{COE} = 5.4$. The numerical value of $\{F_\infty\}$ is determined in the same manner as for the CUE maps. As expected, the QKT has almost the exact same saturation levels as the typical COE map.

the remaining states. This argument is equivalent to the approximation of the LDOS by a top-hat discussed above. With this assumption we can analytically determine $\{F_{\infty}^{COE}\}/\{F_{\infty}^{CUE}\} = 3/2 \approx 1.48$ for perturbation strengths in the FGR regime.

We next study $\{F_\infty\}$ for a quantum system with a well defined classical analog, the quantum kicked top (QKT)[37, 38], which has been defined previously. Since the QKT shows anti-unitary symmetry, it is part of the COE class. And, indeed, the QKT has COE-like nearest neighbor level spacings [37] and eigenvector statistics [39]. The same perturbation, the collective $z$-rotation, is used.

The saturation level for the QKT and COE map are very similar. This is expected since quantum chaotic systems have statistical [14, 39] and dynamical features [29] similar to those of the canonical random matrix theory ensembles.
9.3 The Effect of Invariant Subspaces on Fidelity Decay Saturation Level

The QKT is a system with a classical analog and thus has symmetries not found in random matrices. It is interesting to see whether \( F_\infty \) for just one of these subspaces behaves differently from that of the full QKT. To do this, \( F_\infty \) is calculated for the oe subspace (odd under 180° rotations around the y-axis [60]) of the QKT. We note that while for the kicked top \( N = 2J+1 \) the oe subspace has Hilbert space dimension which has dimension \( N = J \). The results of \( F_\infty \) versus perturbation strength are shown in figure (9-3) and again demonstrates an approximate quadratic decrease of \( F_\infty \) with increased perturbation strength. However, while the saturation level at the limit of strong perturbation does reach the expected \( 3/N \) at the same perturbation strength as for the full QKT, the intermediate perturbation strengths lead to a saturation level that is higher then for the full QKT. In other words, the coefficient \( C_\infty \) is significantly higher than that of the CUE or COE maps.
In conclusion, we have given a theoretical argument estimating the dependence of the fidelity decay saturation level, \( \{ F_\infty \} \), on perturbation strength for initial states that are eigenstates of the system and perturbation strengths within the FGR regime. Numerical simulations for systems with and without classical analogs support these predictions. Interestingly, the full QKT with its invariant subspaces behaves as expected in that if follows the behavior of a typical map from the COE ensemble. However, the behavior of a map which consists of only one of these subspaces deviates from the predicted fidelity decay saturation level.
Chapter 10

Conclusions

In this work I have examined our control over a quantum system while implementing complex quantum operations. These operations include the QFT which was experimentally examined while extracting the periodicity of a wavefunction and as part of a quantum simulation. I also implement a set of pseudo-random maps and examine the accuracy of implementation including the purity of the output state. I also discuss the importance of pseudo-random states for many quantum computing tasks.

Quantum process tomography on the QFT allows for a much more careful evaluation of our control. I provide recipes to extract important error information from the QPT data. Specifically, I concentrate on coherent, incoherent, and decoherent errors and make use of the superoperator and Kraus operator representations of the QPT data.

Finally, I discussed some theoretical aspects of quantum chaos, concentrating on the fidelity decay as a signature of quantum chaos. Random matrices are used as paradigmatic ‘quantum chaotic’ operators and I provide analytical predictions for the fidelity decay rate and saturation level. These predictions are also tested on quantized chaotic systems.
Bibliography


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