Spingineering: Quantum Control in the Presence of Relaxation

by

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Submitted to the Program in Media Arts and Sciences,
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Abstract

For certain problems quantum resources can exponentially increase computing power, but these quantum resources are very fragile in practice. When a quantum system interacts with an external environment, it undergoes decoherence - the loss of quantum correlation - and relaxation - the loss of energy - and eventually all of the quantum information is lost.

Here we show a general principle of using unitary operators to suppress relaxation processes. Unitary operations do not cool a quantum system and seem an unlikely candidate for preventing irreversible thermodynamic heating processes, but surprisingly most decoherence processes can be corrected or ameliorated using open loop control with unitary controllers.

We examine the different mechanisms of decoherence and relaxation on simple spin systems and discuss when the modes can be corrected. We show experimentally the feasibility of our correction schemes using nuclear magnetic resonance. We also demonstrate control of the nuclear spins over long time scales. Finally, we discuss the applications of unitary correction to higher dimensional systems and the potential applications to quantum information processing.

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Contents

Chapter 1

Introduction

The development of quantum mechanics has revolutionized the way we think about the world and interact with it. Paradoxes of non-locality and of multiple worlds baffled scientists and philosophers alike, but experiments consistently confirmed that quantum mechanics better described microscopic phenomena than any other theory.

It is now widely accepted that quantum mechanics properly describes all physical systems, but this leaves many non-physicists asking, "Why don't I see anything quantum?" Where are the non-local effects and interference fringes? Such phenomena do not arise on a macroscopic scale because when a quantum system has enough degrees of freedom and involves many moles of particles (in excess of 10^{26} or so), it obeys the laws of thermodynamics. In essence, when there are many states for quantum systems to occupy, they look like big hot classical objects.

When quantum systems couple to macroscopic systems, their interaction tends to destroy coherent quantum correlations through a process called *decoherence*. In addition, this coupling can exchange energy or angular momentum between the system and the environment which leads to damping or *relaxation*. Decoherence and relaxation are the most daunting obstacles in modern quantum mechanical engineering. The normal approach of suppressing such processes is to isolate quantum systems from all sources of heat and disorder. This thesis presents a different approach to preserve quantum coherence in the presence of relaxation. We show that it is possible to use open-loop coherent unitary operations to preserve quantum states. In this approach, as will be shown, relaxation can actually help preserve quantum states.

Before discussing our approach in more detail, we first frame a possible situation where it would be advantageous to fight decoherence, namely quantum computation. Quantum computation is the inspiration for this work, and many of the techniques used in this thesis were developed in the context of using quantum mechanical systems as information processors.

1.1 Quantum Computation

Quantum computation was initially proposed by Paul Benioff [Ben80] and expanded upon by Richard Feynman [Fey], David Deutsch [Deu85] and others in the early 1980s, in an attempt to apply the laws of quantum mechanics to computation. At that time, the majority of the computer science community believed that any computation that could be achieved physically could be simulated by a Turing machine. By "achieved physically" they assumed that the Turing machine would only utilize the resources of classical mechanics. Instead, Feynman, Deutsch, and Benioff asked what computational power would be gained by allowing for "quantum Turing machines."

A whirlwind of activity in this field developed many surprising results. Bennett first showed any computation that could be performed on an ordinary computer could also be performed only using reversible operations on a quantum computer with only a polynomial loss in compute time [Ben89]. More strikingly, quantum computation was shown to be exponentially more powerful than classical computation in a class of oracle problems [Sim97].

The crowning achievement of this early push into quantum algorithms was Peter Shor's factoring algorithm [Sho97]. Factoring is considered so difficult that it is the backbone of most public key cryptography protocols [RSA78]. Shor showed that quantum computers could factor numbers exponentially faster than classical computers.

These theoretical discoveries were enough to begin an experimental push to build a quantum computer. Gershenfeld and Chuang [GC97] [CGK98] and Cory, Havel and Fahmy [CFH97] built the first working quantum computers using liquid state nuclear magnetic resonance. The former demonstrated the feasibility of implementing Grover's database search algorithm, an oracle problem with a square root speed up over classical computers [Gro96]. Since then, the only realized quantum computations have been in liquid NMR.

As the hype over quantum computing grew, researchers began to determine that it was

actually quite difficult to perform quantum computation. What makes quantum mechanics such a special resource for computation? No one is really quite sure, but the ability for a system to exist as a superposition of many different states appears to be essential.

As pointed out by Chuang et al [CLSZ95] and Unruh [Unr95], these superpositions are extremely fragile. Any external environment which comes in contact with the quantum systems causes a process known as decoherence. The precise superposition is quickly destroyed and one is left with a classical thermodynamic state. At this point, all of the wins in quantum computing power are lost.

To the rescue of quantum computation, Shor [Sho95] and Steane [Ste96] independently showed that quantum coherence could be maintained by implementing quantum error correction. Error correction uses redundant copies of quantum logic to battle decoherence by forcing the system to evolve in spaces where the decoherence cannot effect it. Error correction has proven to be experimentally realizable in NMR [CPM$^+$98]. Unfortunately, error correction does not provide us a short term win in the battle against decoherence. It requires chaining long redundant sequences of quantum bits together, and quantum bits are hard to come by. This sacrificing computational bits to these quantum codes is inconvenient. Furthermore, the set of operations one has to do to perform computation gets complicated quickly when one tries to work with these long encoded sequences.

1.2 Control in the Quantum Domain

Even if quantum computers never overcome these obstacles, trying to build them has brought new perspectives to our understanding of quantum mechanics. In particular, applications of ideas from information theory, communications, and computer science have transformed the way we talk about the quantum world.

Control theory is another mature discipline that is infiltrating the physics community. Loosely, control theory studies how we can engineer interactions with systems to affect what they do.

A control system consists of three parts. The *plant* is the system whose dynamics we want to control. The *sensors* (or observers) monitor outputs from the plant. The *controller* takes these observations and turns them into an appropriate interaction with the plant to create the desired output dynamics.

Consider, for example, your home. We would like to keep our plant, the living room, at a constant temperature. We can adjust the temperature using a controller, the furnace. We use a sensor, a thermostat, to measure the current temperature in the living room. If it is too hot, we tell the furnace to shut off. If it is too cold, we tell the furnace to turn on.

What are the classes of problems we might want to solve? *Controllability* is the study of which states we can make the plant reach. *Stabilization* is determining how to keep the plant in a particular state. *Observability* is the study of how much information we can gain about the state of our plant given our sensor implementation.

The application of control theory to quantum mechanics has been gaining much attention in recent years. Initial steps toward dealing with the nonlinearity of controlling such systems [RSD+95] [BK99] have led to many new research directions applying control theory to the quantum domain. Recent work has shown how quantum systems can control each other [LV00], how techniques of classical feedback can be used to regularize and cool quantum systems [DHJ+00], and how aspects of geometric control theory can be used to time optimally control quantum systems [KGB02].

1.3 Unitary controllers and the suppression of relaxation

In this thesis, we will study how to control relaxing quantum systems. This work differs from error correction in that we want to determine how to maintain quantum coherence when our controllers can strictly implement *unitary* operations. Unitary operators are easy to implement as they are the natural language of quantum systems. On the other hand, they do not change the entropy of a system and are reversible. This makes them unlikely candidates for the suppression of the irreversible process of decoherence. Surprisingly, we will show that unitary operators can prevent decoherence in a wide variety of situations.

In Chapter 2, we will begin with a review of modern quantum mechanics from the stand point of information theory. We will formalize the notion of quantum information and show how it can be passed from system to system. We will then discuss how quantum systems couple to macroscopic environments in Chapter 3 and the different ways that these couplings can disrupt quantum coherence.

Then we will focus our attention to the simplest quantum systems, known as *spins*, in Chapter 4. We will look at all of the possible modes of decoherence and relaxation and all

of the possible unitary operations on such systems.

In Chapter 5, we will show that any relaxing quantum processes on spins are correctable using unitary operations in the sense that we can prevent a manifold of states from relaxing. We will discuss the necessary and sufficient conditions for an operation to be correctable and discuss how we can stabilize quantum states for an arbitrarily long time.

In Chapter 6, we will show experimentally that these correction schemes are realizable with modern technology. We will provide new insight into old problems in pulsed NMR, and demonstrate the controllability of spin systems. We will investigate how unitary correction when combined with recursive estimation and feedback allows for a new form of NMR spectroscopy in Chapter 7.

Finally, in Chapter 8, we will discuss the prospects for extending these result s to higher dimensional systems. We will show that even in these more complicated systems, any relaxation process is correctable with unitary operations. We will discuss how unitary correction inherently preserves quantum information for an arbitrarily long time.

Chapter 2

Foundations of Quantum Mechanics

First, let us begin with a review of the modern formulation of quantum mechanics. This description will be by no means comprehensive, but it will highlight the connections between information theory and quantum mechanics.

2.1 Mathematics of Quantum Mechanics

There is a certain mathematical maturity required to understand the quantum mechanics of finite dimensional systems. We review only the basics here and this is mostly to familiarize the reader with the notation used for the remainder of this thesis.

A Hilbert space is a vector space over $\mathbb{C}$ with a complete inner product structure. By complete, we mean that all Cauchy sequences in the Hilbert space will converge to a point in the Hilbert space. For the purpose of this thesis, all Hilbert spaces will be finite dimensional and we need not worry about the many complications which arise in infinite dimensional systems.

Vectors in Hilbert space will be denoted using Dirac notation. $|\psi\rangle$ will denote an element in Hilbert space. The inner product between $|\psi\rangle$ and $|\phi\rangle$ will be $\langle\psi|\phi\rangle$ and adjoints will be denoted by Dirac bras $\langle\psi| = |\psi\rangle^\dagger$.

Linear maps will either be denoted as matrices or as products of states and adjoints

$$A|\psi\rangle = \sum_{j,k} \alpha_{jk}|j\rangle\langle k|\psi\rangle \tag{2.1}$$

When two quantum systems are combined, the resulting Hilbert space is the tensor product of the two Hilbert spaces. Tensor products will be denoted either by "$\otimes$" or by concatenated kets

$$|\psi\rangle|\phi\rangle = |\psi\rangle \otimes |\phi\rangle \tag{2.2}$$

2.2 Pure State Quantum Mechanics

To describe a physical system as an information processor, we must discuss three components. First, we must specify the quantities observable via some measurement process called *observables*. We also must determine how these observables change with time. We finally must discuss how we can interact with these systems to bias the outcomes of our observations.

In order to fully describe the observation model in quantum mechanics, we first introduce a higher level of abstraction. We model the internal states of the system as vectors in a Hilbert space. This inner product structure induces a norm on the Hilbert space as

$$\|\psi\| = \sqrt{\langle\psi|\psi\rangle} \tag{2.3}$$

We take the set of all accessible states to be the set of vectors with norm one.

The state of a quantum system evolves in time according to the Schrödinger equation

$$\frac{d|\psi\rangle}{dt} = -iH|\psi\rangle \tag{2.4}$$

where H is a Hermitian operator called the *Hamiltonian* of the system.

We can now describe the observation model. We want to describe an interaction such that when the system is in the state $|n\rangle$, our measurement apparatus is in a state $|m(n)\rangle$. We set up a large Hilbert space, $\mathcal{H}_S \otimes \mathcal{H}_A$, where $\mathcal{H}_S$ is the Hilbert space of the system we wish to observe and $\mathcal{H}_A$ is the Hilbert space of the measurement apparatus we are using to observe the system. The interaction of the system with the apparatus is given by a

Hamiltonian H_{SA}.

The dynamics are governed by the Schrödinger equation

$$\frac{d}{dt}|\psi\rangle = -iH_{SA}|\psi\rangle\,. \tag{2.5}$$

Let us suppose the system and the apparatus begin their interaction in the state

$$|\psi_S\rangle|0_A\rangle \tag{2.6}$$

where the state $|0_A\rangle$ represents the initialized state of our apparatus.

We postulate that the measurement corresponds to a set of projection operators P_k, that sum to the identity, and a projection on the apparatus Hilbert space M_k corresponding to measuring the quantity "k." In this model, we have by the Schrödinger equation that the system will be in the state

$$\sum_k \alpha_k|k_S\rangle|m(k)_A\rangle \tag{2.7}$$

which is a superposition over all measurement outcomes.

But in our classical world we'll only see one outcome and conclude at the end of the interaction, our system and apparatus must be in the state

$$|n_S\rangle|m(n)_A\rangle\,. \tag{2.8}$$

That is, our apparatus reads "the system is in state n" and our quantum system must also be in the state $|n_S\rangle$. In turn, we assign $|\alpha_k|^2$ to be the probability of measuring the state $|k\rangle$. Note that this measurement corresponds to a discontinuity in the dynamics of evolution.

2.3 The Density Matrix

While the pure state theory is fully consistent, it does not really help us to fully describe the quantum world. For example, we are unable to describe how a quantum system can interact with a macroscopic system such as a measurement apparatus. We can resolve all of these issues by remembering that our formulation only tells us how to predict measurement outcomes. The state of a quantum system is a convenient mathematical model only insofar as it predicts the results of experiments. It makes sense that the state should represent

"what we know" about a quantum system at any particular time.

In this section, we will introduce a new object called the *density matrix* to describe our knowledge of a quantum system. We will also see how the density matrix gives us a powerful tool for describing how a quantum system interacts with much larger thermal systems.

Take a state $|\psi\rangle \in \mathcal{H}$ and write the matrix

$$\rho = |\psi\rangle\langle\psi| \,. \tag{2.9}$$

This object is called the density matrix of the state $|\psi\rangle$. The density matrix is an element of $\mathcal{H} \otimes \mathcal{H}^*$. It has trace one, is positive semidefinite and is Hermitian.

The Schrödinger equation now becomes

$$\begin{aligned}
\frac{d\rho}{dt} &= \frac{d}{dt}|\psi\rangle\langle\psi| && (2.10)\\
&= \frac{d|\psi\rangle}{dt}\langle\psi| + |\psi\rangle\frac{d\langle\psi|}{dt} && (2.11)\\
&= (-iH)|\psi\rangle\langle\psi| + |\psi\rangle\langle\psi|(-iH)^\dagger && (2.12)\\
&= -(iH|\psi\rangle\langle\psi| + |\psi\rangle\langle\psi|iH) && (2.13)\\
&= -i[H,\rho] && (2.14)
\end{aligned}$$

Similarly, we can calculate the expectation values of observables with respect to the density matrix

$$\begin{aligned}
\langle A\rangle &= \langle\psi|A|\psi\rangle && (2.15)\\
&= \mathrm{Tr}(A|\psi\rangle\langle\psi|) && (2.16)\\
&= \mathrm{Tr}(A\rho) && (2.17)
\end{aligned}$$

So we can formulate quantum mechanics in terms of the density matrix instead of in terms of the state vector. This seems like too much work, as carrying matrices around for computation is more cumbersome than just using vectors, but the utility becomes clear when we allow *any* positive semidefinite Hermitian matrix with trace one to be a density matrix. Now, not only are there are more states available than we had before, but we can start to discuss the concepts of quantum ensembles and irreversible quantum processes.

2.3.1 Mixed States

Let $\mathcal{H}$ be a quantum system of dimension N with basis $\{|\psi_k\rangle\}$. Let $\{p_k\}$ be a probability distribution over these N basis vectors. Define the density matrix

$$\rho = \sum_{k=1}^{N} p_k |\psi_k\rangle\langle\psi_k| \tag{2.18}$$

then this is a classical mixture of the states ψ_k. Any measurement of this state is now biased by a classical probability distribution.

Note that if all of the p_k are equal to zero except for one, the the density matrix of the system is $|\psi\rangle\langle\psi|$ and this corresponds to a state in Hilbert space. We will call such a state a *pure state*, and note that a state is pure if and only if $\operatorname{Tr}\rho^2 = 1$. Otherwise we say that the state is *mixed*. Let's explore these two cases.

Given any density matrix ρ we can always diagonalize it into the form of equation 2.18. The p_k are the eigenvalues of ρ. Since ρ is Hermitian, the $|\psi_k\rangle$ are all orthogonal, and hence we conclude that a state is pure if and only if it has 1 as an eigenvalue. Clearly, this also means that $\rho = |\psi\rangle\langle\psi|$ for a unique $|\psi\rangle$.

What is a mixed state then? Its eigenvalues,$\{p_k\}$, are not all ones and zeros. In this case, ρ is a probabilistic mixture of pure states. In this way, the density matrix quantifies our knowledge of a quantum state.

The density matrix allows us to consider component parts of quantum systems. If we have a state ρ in large quantum system with Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ and we are only interested in the component in $\mathcal{H}_1$, then if we let $|e_k\rangle$ be a basis for $\mathcal{H}_2$, we can define the *partial trace* over $\mathcal{H}_2$ as

$$\begin{aligned} \rho_1 &= \sum_k (\mathbf{1} \otimes \langle e_k|)\rho(\mathbf{1} \otimes |e_k\rangle) \\ &\equiv \operatorname{Tr}_2(\rho) \end{aligned} \tag{2.19}$$

One can readily check that this definition of partial trace is invariant under choice of the $|e_k\rangle$ and that for any $|\psi\rangle$, $|\phi\rangle$ in $\mathcal{H}_1$

$$\langle\phi|\operatorname{Tr}_2(\rho)|\psi\rangle = \sum_k \langle\phi \otimes e_k|\rho|\psi \otimes e_k\rangle\,. \tag{2.20}$$

Returning to the discussion of measurement, consider a system-apparatus Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_A$. The operators, $\{A_{jk}\}$, which perform measurement on an ensemble in $\mathcal{H}_S$ form a *projection operator valued measurement* (POVM). The set of operators must satisfy $\sum_{j,k} A_{j,k}^\dagger A_{j,k} = \mathbf{1}$ and measurement corresponding to this POVM gives the result j with probability

$$p_j = \sum_{j,k} A_{jk} \rho_S A_{jk}^\dagger \tag{2.21}$$

In this case the system density matrix is in the state

$$\rho_j = (1/p_j) \sum_{j,k} A_{jk} \rho_S A_{jk}^\dagger \tag{2.22}$$

Again, we break down measurement into a set of probabilities and projection operators, but this is only a formal pair. A measurement still corresponds to the evolution of a Schrodinger equation and equation 2.22 corresponds to the state of the system after tracing out the measurement apparatus. ρ_j represents our knowledge of the system after a measurement. As we will see in Chapter 3, any interaction, when traced out, produces an evolution on $\mathcal{H}_S$ of this kind.

The ensemble representation allows us to further model measurement without projection at all. By a *weak measurement*, we mean a measurement of a quantum ensemble that only perturbs the density matrix by a small amount. If this perturbation is small enough, we can approximate the density matrix after the measurement to be identical to the density matrix before the measurement. Formally, we can consider the density matrix to describe an ensemble $\rho_S = \rho \otimes \cdots \otimes \rho$. Under a measurement, the lth system has the density matrix

$$\rho_{lj} = \mathrm{Tr}_{l' \neq l} (1/p_j) \sum_{j,k} A_{jk} \rho_S A_{jk}^\dagger \tag{2.23}$$

found by a partial trace of equation 2.22. A measurement is weak if for a small $\epsilon > 0$

$$\sum_j p_j \,\mathrm{Tr} \left(\sqrt{(\rho - \rho_{lj})^2} \right) < \epsilon \tag{2.24}$$

If an ensemble consists of many identical subsystems, then an arbitrarily small perturbation can be scaled to an arbitrarily precise measurement [LS00]. Using weak measurement, we may hence talk of observing the expectation value of any observable without effecting the

state of an ensemble. In the remainder of this thesis, all measurements will be weak unless we note otherwise.

We will now turn quantify the *information* transferred between quantum systems via measurements and interactions.

2.4 Quantum Information

2.4.1 Entropy and Information

Defining the *entropy* of a density matrix as

$$S(\rho) = -\operatorname{Tr}(\rho \log \rho) \tag{2.25}$$

it is straightforward to show that

$$\begin{aligned} S(\rho) &= -\operatorname{Tr}(\rho \log \rho) && (2.26)\\ &= -\operatorname{Tr}(\sum_k p_k |\psi_k\rangle\langle\psi_k|) \log(\sum_k p_k |\psi_k\rangle\langle\psi_k|)) && (2.27)\\ &= -\operatorname{Tr}(\sum_k p_k \log p_k |\psi_k\rangle\langle\psi_k|) && (2.28)\\ &= -\sum_k p_k \log p_k && (2.29) \end{aligned}$$

The meaning of this derivation is that quantum entropy measures the classical entropy of the probability distribution $\{p_k\}$. It should be clear from this definition that a state is pure if and only if its entropy is zero.

We can also use arguments about entropy to characterize the state of a quantum system based only on the information that we have about it. For example, suppose we have a quantum system with Hamiltonian H and we know that the total energy of the system is E. Let $|\psi_k\rangle$ be the eigenstates of H with the eigenvalues E_k. Given no other information, we can assign a state to this system by imposing the *maximum entropy principle*. This principles states that we should assign the state with the largest entropy satisfying the constraint equations for our system. That is, the quantum state we assign only represents the information that we have about the system. Such a state can be found using variational

methods [Sak94]

$$\rho_B = \frac{\sum_k \exp(-\beta E_k)|\psi_k\rangle\langle\psi_k|}{\sum_k \exp(-\beta E_k)} \tag{2.30}$$

and is called the *Boltzmann distribution*. The quantity $\beta = k_B T$ is the familiar function of temperature from thermodynamics and $\mathcal{Z} = \sum_k \exp(-\beta E_k)$ is called the partition function of the system.

Extending these definitions of quantum information, we can introduce a measure of quantum correlations called *entanglement*, which definitively distinguishes between quantum and classical distributions.

2.4.2 Entanglement

Entanglement is what makes quantum mechanics quantum. The odd behaviors and correlations that we don't typically see in the macroscopic world arise from parts of the density matrix that are not classical.

Indeed, to show that unitary correction schemes can preserve inherently quantum information, it suffices to show that entangled states can be preserved for an arbitrarily long time.

First, we can quantify the entanglement of a pure quantum system. Given two coupled quantum systems with Hilbert Space $\mathcal{H}_A \otimes \mathcal{H}_B$, we say that a state $|\psi\rangle$ is *entangled* if it cannot be expressed as a product $|\psi_1\rangle_A|\psi_2\rangle_B$.

We can measure the entanglement of identical systems as follows. First we note that any pure quantum state can be written as

$$|\psi\rangle = \sum_k \alpha_k |k\rangle_A |k\rangle_B \tag{2.31}$$

where the $|k\rangle_A$ and $|k\rangle_B$ are an orthonormal set of states for A and B respectively and the α_k, called the *Schmidt coefficients* of $|\psi\rangle$, are positive real numbers [Per95]. The Schmidt coefficients are unique for a given $|\psi\rangle$ and hence the measure

$$E(\psi) = S(\alpha_k) = -\sum \alpha_k \log(\alpha_k) \tag{2.32}$$

is well defined. It is called the *entanglement of* $|\psi\rangle$ and ranges between 0 and 1.

Now what about for mixed states? We can define the *entanglement of formation* [BDSW96]

as

$$E(\rho) = \min \sum_k p_k E(\psi_k) \tag{2.33}$$

where the minimum is taken over all ensembles of pure states satisfying $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$. It is called the entanglement of formation as it is the minimum entanglement required to produce a particular mixed state from pure states.

Whenever $E(\rho) > 0$, we can say that our density matrix describes a state which is allowed by the laws of quantum mechanics but not by the classical laws of probability.

Chapter 3

Open Quantum Systems

In this chapter, we will outline the procedure for describing quantum systems which interact with thermal environments. We will generalize the notion of unitary evolution to a new concept of *quantum dynamical semigroups* and show that these dynamics are generated by a differential equation called the Lindblad equation. This equation describes the dynamics of all decoherence processes which we will outline in detail in Chapter 5.

3.1 Kraus Operators

Let's return to the evolution of a quantum system coupled to an environment that we initially discussed in the pure state case in Chapter 2. Let the system of interest have Hilbert Space $\mathcal{H}_S$ and the environment have Hilbert Space $\mathcal{H}_E$. Their joint Hilbert space is $\mathcal{H}_S \otimes \mathcal{H}_E$.

We'll use the word "environment" as an umbrella term to describe any quantum system which interacts with $\mathcal{H}_S$, but whose dynamics are not of interest themselves. The environment could be a measurement apparatus, a thermal heat bath, or even another microscopic quantum system. Our goal will be to find the state of the quantum system after it interacts with an environment.

Assume that we begin initially uncorrelated in the state

$$\rho_S \otimes \rho_A \tag{3.1}$$

The system and environment will then evolve according to unitary dynamics

$$U_t \rho_S \otimes \rho_A U_t^\dagger \tag{3.2}$$

The resulting state of our system can be found by tracing out the environment

$$\rho(t) = \mathrm{Tr}_A(U_t \rho_S \otimes \rho_A U_t^\dagger) \tag{3.3}$$

This partial trace was discussed in the previous chapter. We'll take this a step further now. What if we want to ignore the environment altogether? If we are only interested in a particular mode of interaction and not the environment itself, can we find a class of dynamics which describes all possible interactions with all possible environments?

These questions are intentionally leading. We can, in fact, describe all physically allowable transformations on density matrices in a compact form.

The key insight is to introduce a basis $\{|e_l\rangle\}$ for the Hilbert space $\mathcal{H}_E$ such that $\rho_A = \sum_l \lambda_l |e_l\rangle\langle e_l|$ and a basis $\{|\psi_j\rangle\}$ for $\mathcal{H}_S$ such that $\rho_S = \sum_j p_j |\psi_j\rangle\langle\psi_j|$. The unitary evolution can be written in this basis as

$$U|\psi_j\rangle|e_l\rangle = \sum_{m,n} U_{jl,mn}|\psi_m\rangle|e_n\rangle \tag{3.4}$$

and acting on the state $\rho_S \otimes \rho_E$, we find

$$U\rho_S \otimes \rho_E U^\dagger = \sum_{j,l,m,n,r,s} p_j \lambda_l U_{jl,mn}|\psi_m\rangle|e_n\rangle\langle\psi_r|\langle e_s|\bar{U}_{rs,jl} \tag{3.5}$$

The partial trace can now be written by setting $r = s$ and removing the $|e_l\rangle$'s

$$\begin{aligned}
\mathrm{Tr}_E(U\rho_S \otimes \rho_E U^\dagger) &= \sum_{j,l,m,n,r} p_k \lambda_l U_{jl,mn}|\psi_m\rangle\langle\psi_r|\bar{U}_{rn,jl} && (3.6)\\
&= \sum_{l,n}\sum_j p_j \left(\sum_m \sqrt{\lambda_l} U_{jl,mn}|\psi_m\rangle\right)\left(\sum_r \langle\psi_r|\sqrt{\lambda_l}\bar{U}_{rn,jl}\right) && (3.7)\\
&\equiv \sum_k E_k \sum_j p_j |\psi_j\rangle\langle\psi_j| E_k^\dagger && (3.8)\\
&= \sum_k E_k \rho_S E_k^\dagger && (3.9)
\end{aligned}$$

where the E_k are operators on $\mathcal{H}_S$ and are defined by summing over l and n. It is straightforward to check that

$$\left(\sum_k E_k(t)^\dagger E_k(t)\right)_{rs} = \sum_{l,n,a} \lambda_l \bar{U}_{rl,an} U_{sl,an} = \sum_l \lambda_l \delta_{rs} = \delta_{rs} \tag{3.10}$$

That is, $\sum_k E_k(t)^\dagger E_k(t) = \mathbf{1}$. The operators E_k are called *Kraus operators*, named for their discoverer Karl Kraus [Kra71]. The map in equation 3.20 is called a *quantum operation*.

3.1.1 Comments on Complete Positivity

If we have a quantum operation $\mathcal{E}$ acting on a quantum system $\mathcal{H}_S$, it must not affect systems which are not coupled to $\mathcal{H}_S$. That is, the map $\rho_1 \otimes \rho_2 \mapsto \mathcal{E}(\rho_1) \otimes \rho_2$ must remain a density matrix. The class of maps which satisfy this preservation of both tensor products and the positivity of density matrices are called *completely positive*.

Definition 1 *A map, Λ, on $\mathcal{M}_n$ matrices is* positive *if it maps positive matrices to positive matrices. It is* completely positive *if $\Lambda \otimes \mathbf{1}_d : \mathcal{M}_n \otimes \mathcal{M}_d \to \mathcal{M}_n \otimes \mathcal{M}_d$ is positive for all d.*

A theorem by Kraus completely characterizes the set of completely positive maps on density matrices.

Theorem 2 *A linear map Λ is completely positive if and only if it can be written in the form*

$$\Lambda(\rho) = \sum_k E_k \rho E_k^\dagger \tag{3.11}$$

for some set of matrices E_k.

The proof of the above result can be found in [AF].

For a map to be a valid map on density matrices, the matrix $\Lambda(\rho)$ must not only be positive, but its trace must be one. Under this restriction we find

$$1 = \mathrm{Tr}(\sum_k E_k \rho E_k^\dagger) = \mathrm{Tr}((\sum_k E_k^\dagger E_k)\rho) \tag{3.12}$$

using the cyclic property of the trace. This holds for all ρ only if $\sum_k E_k^\dagger E_k = \mathbf{1}$.

Hence we have shown that any map produced by tracing out unitary dynamics is completely positive and trace preserving. What about the converse?

If we have any operators E_k satisfying $\sum_{k=1}^{N} E_k^\dagger E_k = \mathbf{1}$, then consider the map $\rho \mapsto \sum_k^N E_k \rho E_k^\dagger$ on $\mathcal{H}_1$. We can construct a Hilbert Space $\mathcal{H}_2$ with dimension N and basis $\{|e_1\rangle, \ldots |e_n\rangle\}$. Define

$$U(|\phi_S\rangle|e_1\rangle) = \sum_k (E_k|\phi_S\rangle)|e_k\rangle \tag{3.13}$$

for any $|\phi_S\rangle \in \mathcal{H}_\mathcal{S}$. It is immediate that for any $|\phi_S\rangle$,$|\psi_S\rangle$

$$\begin{aligned}
(\langle e_1|\langle\phi_S|)U^\dagger U(|\psi_S\rangle|e_1\rangle) &= \sum_{k,j} \langle\phi_S|E_j^\dagger E_k|\psi_S\rangle\langle e_j|e_k\rangle & (3.14)\\
&= \sum_k \langle\phi_S|E_k^\dagger E_k|\psi_S\rangle & (3.15)\\
&= \langle\phi_S|\psi_S\rangle & (3.16)
\end{aligned}$$

so U preserves inner products on the subspace $\mathcal{H}_\mathcal{S} \otimes |e_1\rangle$ and can thus be extended to a unitary operator on all of $\mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{E}$.

Now we just have to verify that when we trace out the environment, the reduced map is given by the Kraus operators we started with. Indeed, when the environment begins in the state $\rho_E = |e_1\rangle\langle e_1|$

$$\begin{aligned}
\mathrm{Tr}_E(U\rho_S \otimes \rho_E U^\dagger) &= \mathrm{Tr}_E(\sum_{j,k} E_j \rho_S E^\dagger |e_j\rangle\langle e_k|) & (3.17)\\
&= \sum_{j,k,l} E_j \rho_S E_k^\dagger \langle e_l|e_j\rangle\langle e_k|e_l\rangle & (3.18)\\
&= \sum_k E_k \rho_S E_k^\dagger & (3.19)
\end{aligned}$$

So we have found that the most general form of quantum dynamics is the set of all maps of the form

$$\rho \mapsto \sum_k E_k \rho E_k^\dagger \tag{3.20}$$

where $\sum_k E_k^\dagger E_k = \mathbf{1}$.

It should be clear from equation 3.13 that many different unitary processes can give rise to the same Kraus operators. Similarly, there is a large freedom in the representation of the E_k. For a detailed discussion of the representation of E_k see [NC00].

3.2 The Lindblad Equation

Let $\mathcal{E}$ be a quantum process which satisfies

$$\mathcal{E}_t \mathcal{E}_s = \mathcal{E}_{t+s} \tag{3.21}$$

That is, if the operation acts for time s and then for time t then this is equivalent to the operation acting for time $t+s$. The dynamics of such a system would be Markovian, and a map satisfying 3.21 is called a *quantum dynamical semigroup*. It is only "semi" as the inverses of the maps $\mathcal{E}_t$ are not necessarily defined. Indeed, only in the case where $\mathcal{E}_t$ is unitary is a quantum process reversible (i.e., invertible).

Just as in the case of unitary dynamics, a quantum dynamical semigroup is completely characterized by its *generator*, or its derivative at $t = 0$. This is because the maps $\mathcal{E}$ are linear, and hence there exists a linear map L satisfying $\mathcal{E}_t = \exp(Lt)$.

The generator must satisfy

$$\frac{d\mathcal{E}_t(\rho)}{dt} = L\mathcal{E}_t^\dagger(\rho) \tag{3.22}$$

and 3.22 is the *Lindblad Equation*. We can derive the form of the Lindblad equation as follows. Let F_k be a basis for $\mathcal{M}_N$ with $F_0 = \mathbf{1}$. Then

$$\begin{aligned}
\mathcal{E}_t(\rho) &= \sum_k E_k(t)\rho E_k(t) && (3.23)\\
&= \sum_{k,l,m} (r_{kl}(t)F_l)\rho(\bar{r}_{km}(t)F_m^\dagger) && (3.24)\\
&= \sum_{k,l,m} r_{kl}(t)\bar{r}_{km}(t)F_l\rho F_m^\dagger && (3.25)\\
&= \sum_{l,m} c_{lm}(t)F_l\rho F_m^\dagger && (3.26)
\end{aligned}$$

where $c_{lm}(t) = \sum_k r_{kl}(t)\bar{r}_{km}(t)$. Note that $c_{lm} = \bar{c}_{ml}$ and $c_{00}(0) = 1$ and $c_{lm}(0) = 0$ for all l,m.

The time derivative is easily evaluated:

$$
\begin{aligned}
L(\rho) &= \lim_{\epsilon\to 0}\frac{\mathcal{E}_t-\mathbf{1}}{\epsilon}(\rho) && (3.27)\\
&= \lim_{\epsilon\to 0}\frac{c_{00}(\epsilon)-1}{\epsilon}\rho+\sum_l\frac{c_{l0}}{\epsilon}F_l\rho+\sum_m\frac{\bar{c}_{m0}}{\epsilon}\rho F_m^\dagger+\sum_{l,m}\frac{c_{lm}}{\epsilon}F_l\rho F_m^\dagger && (3.28)\\
&= A\rho+\rho A^\dagger+\sum_{l,m}a_{lm}F_l\rho F_m^\dagger && (3.29)\\
& && (3.30)
\end{aligned}
$$

Bear with us for a second, we will simplify these calculations into a much more compact form. First note that the dynamics must preserve the trace of ρ and, subsequently, $\mathrm{Tr}(L(\rho))=0$. This means that for all ρ

$$\mathrm{Tr}(A\rho+\rho A^\dagger+\sum_{l,m}a_{lm}F_l\rho F_m^\dagger)=\mathrm{Tr}((A+A^\dagger+\sum_{l,m}a_{lm}F_m^\dagger F_l)\rho)=0 \tag{3.31}$$

using the cyclic property of the trace. But this in turn means that

$$A+A^\dagger=-\sum_{l,m}a_{lm}F_m^\dagger F_l \tag{3.32}$$

Performing some rearranging yields

$$
\begin{aligned}
A\rho+\rho A^\dagger &= \tfrac{1}{2}(A\rho+A\rho+\rho A-\rho A+\rho A^\dagger+\rho A^\dagger+A^\dagger\rho-A^\dagger\rho) && (3.33)\\
&= \tfrac{1}{2}(A\rho-A^\dagger\rho-\rho A+\rho A^\dagger)+\tfrac{1}{2}(A\rho+A^\dagger\rho+\rho A+\rho A^\dagger) && (3.34)\\
&= [\tfrac{1}{2}(A-A^\dagger),\rho]+\tfrac{1}{2}(A+A^\dagger)\rho+\tfrac{1}{2}\rho(A+A^\dagger) && (3.35)
\end{aligned}
$$

and for any A, $A-A^\dagger$ is skew symmetric. This means that

$$H=\frac{i}{2}(A-A^\dagger) \tag{3.36}$$

is Hermitian. Plugging the results of 3.32 and 3.33 into 3.27 gives

$$L\rho=-i[H,\rho]-\frac{1}{2}\sum_{l,m}a_{lm}(F_m^\dagger F_l\rho+\rho F_m^\dagger F_l-2F_l\rho F_m^\dagger) \tag{3.37}$$

or, breaking the second term into commutators

$$L\rho = -i[H,\rho] + \frac{1}{2}\sum_{l,m} a_{lm}([F_l\rho, F_m^\dagger] + [F_l, \rho F_m^\dagger]) \tag{3.38}$$

This fully describes all possible quantum dynamical semigroups. Once we have chosen a basis F_k, we need only specify a Hermitian matrix H and a positive semidefinite operator $\mathbf{A} = (a_{jk})$. Of course, this structure is dependent on the basis F_k, and the form of equation 3.38 is not unique.

Note that in the case $\mathbf{A} = 0$, the Lindblad equation reduces to our old friend the Schrödinger equation and our dynamics are unitary. The term $-i[H,\rho]$ is the *Hermitian part* of the Lindblad equation. On the other hand, all of the dissipative non-unitary dynamics can be found in the double commutator terms. These are called the *dissipative part* of the Lindblad equation.

Note that if we diagonalize the matrix $\mathbf{A}$, we are left with the Lindblad equation

$$L\rho = -i[H,\rho] + \frac{1}{2}\sum_{k}([L_k\rho, L_k^\dagger] + [L_k, \rho L_k^\dagger]) \tag{3.39}$$

in the form originally discovered by Lindblad [Lin76].

We can also derive the Lindblad equation from our old unitary picture. Given a system environment interaction Hamiltonian H_{int}, we can expand the unitary dynamics to second order

$$\begin{aligned}
U_t(\rho_S \otimes \rho_E)U_t^\dagger &= \exp(-iH_{int}t)(\rho_S \otimes \rho_E)\exp(iH_{int}t) && (3.40)\\
&= (\mathbf{1} - iH_{int}t + \frac{1}{2}H_{int}^2t^2)(\rho_S \otimes \rho_E)(\mathbf{1} + iH_{int}t + \frac{1}{2}H_{int}^2t^2) && (3.41)\\
&= \rho_S \otimes \rho_E - i[H_{int}, \rho_S \otimes \rho_E]t && (3.42)\\
&\quad + \left(-\frac{1}{2}H_{int}^2\rho_S \otimes \rho_E - \frac{1}{2}\rho_S \otimes \rho_E H_{int}^2 + H_{int}\rho_S H_{int}\right)t^2 && (3.43)
\end{aligned}$$

We can write H_{int} as a sum of tensored operators $\sum_k H_k^S \otimes H_k^A$. When we trace over

the environment, the first order terms become

$$\begin{aligned}
\mathrm{Tr}_2([H_k^S \otimes H_k^E, \rho_S \otimes \rho_E]) &= \mathrm{Tr}_2(H_k^S \rho_S \otimes H_k^E \rho_E - \rho_S H_k^S \otimes \rho_E H_k^E) && (3.44)\\
&= H_k^S \rho_S \,\mathrm{Tr}(H_k^E \rho_E) - \rho_S H_k^S \,\mathrm{Tr}(\rho_E H_k^E) && (3.45)\\
&= [H_k^S, \rho]\,\mathrm{Tr}(H_k^E \rho_E) && (3.46)
\end{aligned}$$

The last term follows from the cyclic property of the trace. These first order terms, called *Lamb Shifts*, are perturbations on the system Hamiltonian due to an environmental coupling. We can also trace out the environment on the second order terms to recover the full Lindblad equation.

This derivation from a unitary process is a more physically intuitive version of the Lindblad equation. If we know the specific mode of interaction between the environment and the system, then this form of the Lindblad equation is probably the better to work with. On the other hand, if we want to concoct an arbitrary quantum dynamical semigroup without mention of the coupling to an external environment, equation 3.38 is more appropriate.

3.3 Coherence Vectors

Now let F_k be a basis for $\mathfrak{su}(N)$ with $\mathrm{Tr}(F_i F_j) = \delta_{ij}$. Note that any density matrix can be written in the form

$$\rho = \frac{\mathbf{1} + \sum_{k=1}^{N^2-1} r_k F_k}{N} \tag{3.47}$$

$\vec{r} = (r_k)$ is the *coherence vector*. $\vec{r}$ is a real vector and is the analog of the Bloch vector for single spins (see Chapter 5).

Consider the *trace norm* of ρ given by

$$\begin{aligned}
\|\rho\|^2 &= \mathrm{Tr}(\rho\rho^\dagger)\\
&= \mathrm{Tr}(\frac{\mathbf{1} + \sum_k r_k F_k + \sum_{k,j} r_k r_j F_k F_j}{N^2})\\
&= \frac{1}{N^2}(N + \sum_k r_k^2)
\end{aligned} \tag{3.48}$$

Since the density matrix is positive semidefinite and has trace one, all of the eigenvalues of

ρ lie between zero and one. It follows that

$$\frac{1}{\sqrt{N}} \leq \|\rho\| \leq 1 \tag{3.49}$$

which means that

$$0 \leq \|\vec{r}\| \leq \sqrt{N^2 - N} \tag{3.50}$$

Hence any map on a quantum system cannot increase the lengths of coherence vectors. In other words, the dynamics of the coherence vector have eigenvalues with real parts strictly less than one.

Note that equation 3.50 is only a necessary, not a sufficient, condition for the length of a coherence vector. In particular it does not imply that the density matrices form a sphere! Indeed, we can define three operators on a 4-level Hilbert space as

$$M_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{3.51}$$

$$M_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{3.52}$$

$$M_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.53}$$

$$\tag{3.54}$$

These matrices are trace orthogonal and can be extended to a basis for the coherence vectors. The state $\rho = (\mathbf{1}+M_1+M_2+M_3)/4$ is a pure state and has coherence vector length $\sqrt{3}$. But the matrix $\rho_{bad} = (\mathbf{1} + 3M_1)/4)$ has eigenvalues $1/2, -1/4$ and is not positive semidefinite. So we must be careful. We can bound the length of the coherence vector, but the intrinsic geometry of density matrices does not necessarily form a nice sphere except in the special

case of $\mathfrak{su}(2)$.

Let's reformulate some of the last sections results in terms of this coherence vector. First, consider commutation with $H = \sum_k h_k F_k$:

$$\begin{aligned} -i[H,\rho] &= \frac{\mathbf{1} + \sum_{k=1}^{N^2-1} r_k [H, F_k]}{N} \\ &= \frac{\mathbf{1} + \sum_{k,l=1}^{N^2-1} r_k h_l [F_l, F_k]}{N} \\ &= \frac{\mathbf{1} + \sum_{k,l,m=1}^{N^2-1} r_k h_l g_{lkm} F_m}{N} \end{aligned} \tag{3.55}$$

where g_{lkm} are the structure constants of $\mathfrak{su}(N)$. Evidently we can define the matrix

$$C_{lm} = \sum_k g_{kml} h_k \tag{3.56}$$

and then in this representation $\vec{r} \mapsto \vec{C}\vec{r}$ under H.

Next consider the dissipative part of the Lindblad Equation of the form in equation 3.38. As shown by Lendi [AL87], we have $\vec{r} \mapsto \mathbf{A}\vec{r} + \vec{b}$ with

$$A_{mn} = -\frac{1}{4} \sum_{j,k,l} a_{jk} (z_{jln} f_{klm} + \bar{z}_{kln} f_{jlm}) \tag{3.57}$$

$$b_m = \frac{1}{N} \sum_{j,k} a_{jk} f_{jkm} \tag{3.58}$$

Here

$$z_{mnl} = f_{mnl} + i d_{mnl} \tag{3.59}$$

where f_{mnl} and d_{mnl} are the symmetric and antisymmetric structure constants of $\mathfrak{su}(N)$.

The computations involving structure constants are often difficult in practice, but the form of equation 3.57 describes all of the possible transformations on density matrices in an intuitive way. We see that the only admissible maps are a subset of the linear affine transformations of the coherence vectors. Hence the general Lindblad equation is rewritten in a much more familiar form

$$\frac{d\vec{r}}{dt} = \mathbf{A}\vec{r} + \vec{b} + \mathbf{C}\vec{r} \tag{3.60}$$

Unfortunately, we cannot impose any symmetry conditions on the matrix $\mathbf{A}$ except when $N = 2$ (see Chapter 4). But we can still analyze the properties of this ODE to determine

what it tells us about open system evolution.

Using this notation to analyze the structure of the Lindblad equation, first consider when $\mathbf{A} = 0$ and $\vec{b} = 0$. Then we are left with an ODE

$$\frac{d\vec{r}}{dt} = \mathbf{C}\vec{r} \tag{3.61}$$

where $\mathbf{C}$ is skew-symmetric. Then $\exp(\mathbf{C}t)$ is an orthogonal matrix for all t and hence the dynamics are orthogonal. It is not surprising that the coherence vector doesn't change length under these dynamics as we know the dynamics under a Schrödinger equation are unitary.

When $\mathbf{C} = 0$ and $\vec{b} = 0$. Since the dynamics of the Lindblad equation must not increase the length of coherence vectors, the real parts of the eigenvalues of A must be less than or equal to zero. Unfortunately, again we have to reiterate that this is *all we can say* about the structure of $\mathbf{A}$. Remember, that $\mathbf{A}$ is not usually diagonalizable when $N > 2$.

We will close this chapter with two definitions. A quantum operation is called *relaxing* or a *relaxation process* if $\vec{b} \neq 0$. In this case, all density matrices damp exponentially to a unique fixed point. If $\vec{b} = 0$ and $\mathbf{A}$ has negative eigenvalues, we say that the process is *dephasing*. The distinction between these two types of decoherence is essential for what follows as the main result of this document is that relaxation processes can be corrected by unitary operations while dephasing processes cannot.

Chapter 4

Spins and Spin Dynamics

As we saw in the previous chapter, it can be difficult to discuss concrete examples of open system evolution as many of the matrices involved are not diagonalizable. Since we can't diagonalize them, computing closed form expressions of arbitrary state dynamics requires a great deal of care.

On the other hand, we note that when a system is 2 dimensional, the matrices describing the dynamics are always diagonalizable. In this chapter we will restrict our attention to such 2 level systems, called *spins* or *spin-1/2 particles*. We will analyze all forms of open evolution for these systems and develop all of the machinery needed to discuss unitary suppression of decoherence.

4.1 The Bloch Sphere

The coherence vector for a two level system has an intuitive geometric form. First of all, we can introduce an orthonormal matrix set for $\mathfrak{su}(2)$ called the *Pauli Matrices*

$$X = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, Y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \text{ and } Z = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.1}$$

It is trivial to check that these matrices satisfy the trace orthogonality conditions, and that the Lie Algebra structure of $\mathfrak{su}(2)$ is given by

$$\begin{aligned} i[X,Y] &= Z \\ i[Y,Z] &= X \\ i[Z,X] &= Y \end{aligned} \tag{4.2}$$

In terms of the structure constants, we get that f_{ijk} is the anti-symmetric three pseudotensor

$$\epsilon_{ijk} = \begin{cases} 1 & \text{if i,j,k are a symmetric permutation of 1,2,3} \\ -1 & \text{if i,j,k are an antisymmetric permutation of 1,2,3} \\ 0 & \text{otherwise} \end{cases} \tag{4.3}$$

Anyone who has worked problems in electrostatics, special relativity, or even mechanics has seen this matrix before.

Defining the array of matrices $\vec{\sigma} = (X, Y, Z)$ allows any density matrix over $\mathfrak{su}(N)$ to be written as

$$\rho = \frac{\mathbf{1} + \vec{r} \cdot \vec{\sigma}}{2} \tag{4.4}$$

where $\vec{r}$ is the coherence vector. In this case we call it the *Bloch vector* in honor of Felix Bloch.

The norm of the Bloch vector ranges between 0 and $\sqrt{2}$. But we can modify our matrices by multiplying by $\sqrt{2}$ to yield new

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, Y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \text{ and } Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.5}$$

these matrices are more useful for most computations and we will use them instead of the matrices in 4.1 from here on. Under the relabeling $\sigma_1 = X$, $\sigma_2 = Y$, $\sigma_3 = Z$ in equation 4.5, we get the algebraic relations

$$[\sigma_i, \sigma_j] = i2\epsilon_{ijk}\sigma_k \tag{4.6}$$

$$\sigma_i \sigma_j = \delta_{ij}\mathbf{1} + 2\epsilon_{ijk}\sigma_k \tag{4.7}$$

The Bloch vectors are now the set of all vectors in $\mathbb{R}^3$ with norms less than or equal to one. Hence, the set of all Bloch vectors hence forms a 3-dimensional sphere with radius one. We call this sphere the Bloch Sphere.

For our purposes, it is useful to link the thermodynamics of a density matrix to the geometry of the Bloch vector. Given a density matrix

$$\rho = \begin{pmatrix} 1 + r_z & r_x + ir_y \\ r_x - ir_y & 1 - r_z \end{pmatrix} \tag{4.8}$$

It is easy to compute the characteristic polynomial

$$\begin{aligned} c_\rho(\lambda) &= \lambda^2 - \mathrm{Tr}(\rho)\lambda + \det(\rho) \\ &= \lambda^2 - \lambda + \frac{1 - r_x^2 - r_y^2 - r_z^2}{4} \\ &= \lambda^2 - \lambda + \frac{1 - \|\vec{r}\|^2}{4} \end{aligned} \tag{4.9}$$

The eigenvalues of the density matrix are then given by

$$\lambda_i = \frac{1 \pm \|\vec{r}\|}{2} \tag{4.10}$$

We recall that for any two Hermitian matrices M and N, there exists a unitary matrix U satisfying $M = UNU^\dagger$ if and only if M and N have the same eigenvalues. We see from equation 4.10 that any two Bloch vectors with the same norm have corresponding density matrices with the same eigenvalues.

Furthermore, we can compute the entropy of a density matrix

$$S(\rho) = -\lambda_1 \log(\lambda_1) - \lambda_2 \log(\lambda_2) = -\frac{1 + \|\vec{r}\|}{2} \log(\frac{1 + \|\vec{r}\|}{2}) - \frac{1 - \|\vec{r}\|}{2} \log(\frac{1 - \|\vec{r}\|}{2}) \tag{4.11}$$

showing that the entropy only depends on the length of the Bloch vector.

The geometry of the Bloch vector is simple and aesthetically pleasing because the Lie Algebras $\mathfrak{su}(2)$ and $\mathfrak{so}(3)$ are isomorphic. Thus there is a perfect correspondence between the transformations of 2×2 density matrices and the geometry of $\mathbb{R}^3$. We'll explore more consequences of this correspondence in the next two sections.

4.2 Spin-1/2 Evolution

A Hamiltonian H for a spin-1/2 system is a 2×2 Hermitian matrix. Furthermore, its trace can be zero as the trace part of the matrix only contributes to a global phase in the evolution which can be ignored (see Chapter 2). We can write $H = \omega \vec{v} \cdot \vec{\sigma}$ for some unit length 3-vector $\vec{v}$ and real number ω.

We can easily translate this into a transformation of the Bloch vector as under commutation

$$\begin{aligned} -i[H, \rho] &= -i\frac{\sum_{k,j} v_k r_j [\sigma_k, \sigma_j]}{2} \\ &= -i\frac{\sum_{k,j} v_k r_j 2i\epsilon_{kjl}\sigma_l}{2} \\ &= \sum_{k,j} \epsilon_{kjl} v_k r_j \sigma_l \end{aligned} \tag{4.12}$$

In matrix form we get

$$H = \omega \begin{pmatrix} 0 & -v_z & v_y \\ v_z & 0 & -v_x \\ -v_y & v_x & 0 \end{pmatrix} \tag{4.13}$$

and from this, the Schrödinger equation can be written in a more elegant form

$$\frac{d\vec{r}}{dt} = \omega \vec{v} \times \vec{r} \tag{4.14}$$

This equation is also familiar from classical mechanics. The dynamics are such that all vectors parallel to $\vec{v}$ are fixed, while those perpendicular to $\vec{v}$ rotate with procession frequency ω.

The dynamics of two level systems might seem quite boring, but we can make life a lot more complicated once we add dissipation.

4.3 General Spin-1/2 Evolution

In this section we will describe all possible dissipative processes on a one-spin system. We will begin by describing Kraus operators for some common processes. Then we will introduce the coherence vector formalism and show that it provides a more intuitive description and makes calculations easier.

4.3.1 Kraus Operators

Recall that an arbitrary quantum process can be written in the operator sum notation

$$\mathcal{E}(\rho) = \sum_k E_k \rho E_k^\dagger \tag{4.15}$$

This form is widely accepted as standard by the quantum information community. It will do us some good to translate our work on the Bloch vector into the operator sum language. We'll fix time and analyze the map $\rho \mapsto \mathcal{E}(t)(\rho)$ for particular examples.

First, consider the Kraus operators

$$E_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{pmatrix} \text{ and } E_1 = \begin{pmatrix} 0 & \sqrt{\gamma} \\ 0 & 0 \end{pmatrix} \tag{4.16}$$

The Bloch vector $\vec{r}$ transforms as

$$(r_x, r_y, r_z) \mapsto (\sqrt{1-\gamma} r_x, \sqrt{1-\gamma} r_y, \gamma + (1-\gamma) r_z)\,. \tag{4.17}$$

The constant E_1 determines how much the Bloch vector is pushed towards the fixed point of the operation

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \tag{4.18}$$

the spin-up state. This process is called amplitude damping [NC00]. It is a relaxation process since it has a unique fixed point.

More generally, we can damp to a mixed state with the Kraus operators

$$E_0 = \sqrt{p} \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{pmatrix}, \tag{4.19}$$

$$E_1 = \sqrt{p} \begin{pmatrix} 0 & \sqrt{\gamma} \\ 0 & 0 \end{pmatrix}, \tag{4.20}$$

$$E_2 = \sqrt{1-p} \begin{pmatrix} \sqrt{1-\gamma} & 0 \\ 0 & 1 \end{pmatrix}, \text{ and} \tag{4.21}$$

$$E_3 = \sqrt{1-p} \begin{pmatrix} 0 & 0 \\ \sqrt{\gamma} & 0 \end{pmatrix}. \tag{4.22}$$

Repeated application of these operators yield a steady state or equilibrium density matrix

$$\rho_{eq} = \begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix}, \tag{4.23}$$

which can be identified with the Boltzmann distribution from Chapter 2

$$\rho_{eq} = \begin{pmatrix} e^{-\beta E_1} & 0 \\ 0 & e^{-\beta E_2} \end{pmatrix} / \mathcal{Z}\,. \tag{4.24}$$

In the case of NMR, the temperature and procession frequency of the spins set the value of p.

In this case, we note that our Bloch vector maps as

$$(r_x, r_y, r_z) \mapsto (\sqrt{1-\gamma} r_x, \sqrt{1-\gamma} r_y, \gamma(2p-1) + (1-\gamma) r_z) \tag{4.25}$$

An example of a dephasing operation is given by the operators

$$E_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{pmatrix} \text{ and } E_1 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\gamma} \end{pmatrix} \tag{4.26}$$

and is called phase damping. These operations result in the transformation

$$(r_x, r_y, r_z) \mapsto (\sqrt{1-\gamma} r_x, \sqrt{1-\gamma} r_y, r_z) \tag{4.27}$$

on the Bloch vectors. For any initial density matrix described by a nonzero Bloch vector $\vec{r}$, the norm of the density matrix is strictly decreasing and $S(\rho) < S(\mathcal{E}(\rho))$. In the Bloch Sphere picture, the x and y components of the Bloch vector are dissipated leaving the projection of the Bloch vector on the z-axis.

As a final note, and as a precursor for the next section, we will briefly describe generalized amplitude damping where the components of the Bloch vector in the x-y-plane are damped at a different rate than the components along the z-axis. This would correspond to a

situation where $T_1 \neq T_2$. Indeed, the operators

$$E_0 = \begin{pmatrix} \sqrt{p+(1-\gamma)(1-p)} & 0 \\ 0 & \sqrt{1-\lambda}\sqrt{p(1-\gamma)+(1-p)} \end{pmatrix}, \tag{4.28}$$

$$E_1 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\lambda}\sqrt{p(1-\gamma)+(1-p)} \end{pmatrix}, \tag{4.29}$$

$$E_2 = \begin{pmatrix} 0 & 0 \\ \sqrt{(1-p)\gamma} & 0 \end{pmatrix} \text{ and} \tag{4.30}$$

$$E_3 = \begin{pmatrix} 0 & \sqrt{\gamma p} \\ 0 & 0 \end{pmatrix} \tag{4.31}$$

where

$$\lambda = 1 - \kappa(1-\beta) < 1 \tag{4.32}$$

and

$$\kappa = ((p + (1-\gamma)(1-p))(p(1-\gamma) + (1-p)))^{-1} \tag{4.33}$$

perform the desired operation

$$(r_x, r_y, r_z) \mapsto (\sqrt{1-\beta}r_x, \sqrt{1-\beta}r_y, \gamma(2p-1) + (1-\gamma)r_z) \tag{4.34}$$

this is like amplitude damping, but the rate of relaxation in the x-y-plane is faster than that in along the z-axis.

4.3.2 Coherence Vector Approach

In this section, we will derive the most general form of evolution of a spin-1/2 particle as a set of 3×3 matrices and relate them to the Kraus operators in the last section.

We start with the Lindblad equation in density matrix form and then derive the Lindblad equation for the Bloch vector. We begin with a Hermitian matrix $\mathbf{D} = (d_{jk})$ and the Lindblad operator

$$L\rho = \frac{1}{2}\sum_{j,k} d_{jk}[\sigma_j\rho, \sigma_k] + [\sigma_j, \rho\sigma_k] \tag{4.35}$$

Plugging in the identity matrix divided by 2 yields

$$\begin{aligned} L\frac{\mathbf{1}}{2} &= \frac{1}{4}\sum_{j,k} d_{j,k}[\sigma_j, \sigma_k] \\ &= \frac{1}{2}\sum_{j,k} i\epsilon_{jkl} d_{jk} \\ &= \frac{1}{2}\sum_{j<k} i\epsilon_{jkl}(d_{jk} - d_{kj}) \\ &= \sum_{j<k} \epsilon_{kjl}\mathrm{Im}(d_{jk}) \end{aligned} \tag{4.36}$$

and for σ_l

$$\begin{aligned} L\sigma_l &= \frac{1}{2}\sum_{j,k} d_{j,k}([\sigma_j\sigma_l, \sigma_k] + [\sigma_j, \sigma_l\sigma_k]) \\ &= \frac{1}{2}\sum_{j,k,m} d_{j,k} i(\epsilon_{jlm}[\sigma_m, \sigma_k] + \epsilon_{lkm}[\sigma_j, \sigma_m]) \\ &= -\sum_{j,k,m,n} d_{j,k}(\epsilon_{jlm}\epsilon_{mkn} + \epsilon_{lkm}\epsilon_{jmn})\sigma_n \\ &= -\sum_{j,k,n} d_{j,k}(\delta_{jk}\delta_{ln} - \delta_{jn}\delta_{lk} + \delta_{ln}\delta_{kj} - \delta_{lj}\delta_{kn})\sigma_n \\ &= \sum_n (-2\,\mathrm{Tr}\,\mathbf{D} + (d_{nl} + d_{ln}))\sigma_n \end{aligned} \tag{4.37}$$

We can now write the Lindblad equation for the Bloch vector as

$$\frac{d\vec{r}}{dt} = \mathbf{A}\vec{r} + \vec{b} \tag{4.38}$$

with

$$\mathbf{A} = (\mathbf{D} + \mathbf{D}^T - 2\,\mathrm{Tr}(\mathbf{D})\mathbf{1}) \text{ and } \vec{b} = (\mathrm{Im}(d_{23}), \mathrm{Im}(d_{31}), \mathrm{Im}(d_{12})) \tag{4.39}$$

Since $\mathbf{D}$ is Hermitian and positive, $\mathbf{A}$ is symmetric and $a_{kk} < 0$ for $k = 1, 2, 3$. We can also prove

Proposition 3 *A is negative semidefinite.*

Proof That A is symmetric is clear from equation 4.39. To show that $\mathbf{A}$ is negative, consider an arbitrary unit test vector $\vec{u}$. Let the eigenvalues of $\mathbf{D}$ be $\lambda_1, \lambda_2, \lambda_3$. Since D is

positive, these λ_k are all greater than zero. Then we have

$$\vec{u}^T(\mathbf{D} - \mathrm{Tr}(\mathbf{D}))\vec{u} \leq \max_k \lambda_k - \sum_k \lambda_k \leq 0 \tag{4.40}$$

and the same holds for $\mathbf{D}^T$. Therefore $A = \mathbf{D} - \mathrm{Tr}(\mathbf{D}) + \mathbf{D}^T - \mathrm{Tr}(\mathbf{D})$ must also be negative. ■

Since A is symmetric we can diagonalize it, resulting in the decoherence matrix

$$\mathbf{A} = \begin{pmatrix} -\gamma_1 & 0 & 0 \\ 0 & -\gamma_2 & 0 \\ 0 & 0 & -\gamma_3 \end{pmatrix} \tag{4.41}$$

What else can we say about the eigenvalues of $\mathbf{A}$? Firstly, since this diagonal matrix must arise from some quantum process, there exist positive real numbers d_{11}, d_{22}, d_{33} such that

$$\mathbf{A} = \begin{pmatrix} -2d_{22} - 2d_{33} & 0 & 0 \\ 0 & -2d_{11} - 2d_{33} & 0 \\ 0 & 0 & -2d_{11} - 2d_{22} \end{pmatrix} \tag{4.42}$$

This yields the inequalities

$$0 \leq \gamma_k \leq \gamma_m + \gamma_n \tag{4.43}$$

for $\{k, m, n\}$ some permutation of $\{1, 2, 3\}$. This means, in particular, that there are no quantum processes which smoosh the Bloch Sphere into a 2-dimensional pancake. However, one can smoosh the Bloch sphere onto a 1-dimensional noodle by letting $\gamma_1 = \gamma_2 > 0$ and $\gamma_3 = 0$.

We can also place restrictions on the vector $\vec{b}$

Proposition 4 *The components b_k of the affine part of the dissipation matrix satisfy*

$$4b_k^2 \leq \gamma_k^2 - (\gamma_m - \gamma_n)^2 \tag{4.44}$$

where $\{k, m, n\}$ is a permutation of $\{1, 2, 3\}$.

Proof Without loss of generality, we let $k = 3$. The other two cases follow identically.

Considering our matrix $\mathbf{D}$ and the unit test vector $\vec{u} = (u_1, u_2, 0)$, we must have $\vec{u}^\dagger \mathbf{D} \vec{u} \geq 0$ for arbitrary choices of u_1 and u_2. Hence the minor

$$\mathbf{D} = \begin{pmatrix} d_{11} & d_{12} \\ \bar{d}_{12} & d_{22} \end{pmatrix} \tag{4.45}$$

must be positive semidefinite.

In particular, the determinant $d_{11}d_{22} - |d_{12}|^2$ must be greater than zero. Recalling that $\gamma_k = d_{mm} + d_{nn}$, we get

$$4d_{11}d_{22} = (d_{11} + d_{22})^2 - (d_{11} - d_{22})^2 = \gamma_3 - (\gamma_1 - \gamma_2)^2 \tag{4.46}$$

and since $b_3 = \mathrm{Im}(d_{12})$ we have $4b_3 \leq \gamma_3 - (\gamma_1 - \gamma_2)^2$. ■

Now that we have put the dissipation matrix in an elegant diagonal form, we find that the Lindblad equation for the Bloch vector can be written in diagonal form as

$$\frac{dr_k}{dt} = -\gamma_k r_k + b_k \tag{4.47}$$

that is, as three uncoupled differential equations whose solutions are the exponential decays to an equilibrium vector. Indeed, the homogeneous solution to these equations are clearly exponential decays and plugging in the particular solution gives the general form

$$r_k(t) = \exp(-\gamma_k t)(r_k(0) - \frac{b_k}{\gamma_k}) + \frac{b_k}{\gamma_k} \tag{4.48}$$

in matrix form. Letting $\vec{r}_{eq} = (-b_k/\gamma_k)$, we get

$$\vec{r}(t) = \exp(-\mathbf{A}t)(\vec{r}(0) - \vec{r}_{eq}) + \vec{r}_{eq} \tag{4.49}$$

This matrix form is indeed the general solution to the dissipative part of the Lindblad equation in any dimension. Yet, as discussed in Chapter 3, it is only easy compute these matrix exponentials when the dimension of the system is 2.

Now, let's revisit the maps on density matrices from section 4.3.1. Note that all of the maps were in the form of equation 4.49. So to find a generator to produce the appropriate transformation, we need only set the diagonal entries of the matrix $\mathbf{A}$ and then fix the

equilibrium matrix $\vec{b} = -\mathbf{A}^{-1}\vec{r}_{eq}$. No further work is required to determine the coefficients.

Having analyzed all possible evolutions, we can now move on to describing our central result - correcting relaxation via unitary operations.

Chapter 5

Unitary Correction of Single-Spin Relaxation

In this chapter, we show how spin 1/2 systems contain submanifolds of states which can be stabilized for an arbitrarily long time from the effects of relaxation. In general, these spaces are ellipsoids in the Bloch Sphere.

5.1 Correction with strobed untiaries

We'll first operate under the assumption that these dissipative processes are unwanted. What can we do to prevent the Bloch vector from relaxing to the equilibrium state?

Consider the following situation for one spin. We have a system which evolves under a Hamiltonian H and Lindblad operator L. We have a method for applying an arbitrary unitary operator to this system at arbitrary times. This situation is the common model for a quantum computer and is physically realizable in NMR as we will discuss in Chapter 6

Consider how one might attempt to keep a quantum system in a state for an arbitrarily long time. If quantum process acts for time t, then we can try to push the spin system back to where it started (see figure 5-1). If our pushes are unitary then we cannot change the length of the Bloch vector. Though in general quantum processes are free to change the Bloch vector length, but there is no reason why they must do so. We can correct the quantum process with a unitary operation only when *the Bloch vector hasn't changed length* under its evolution. We formulate this as

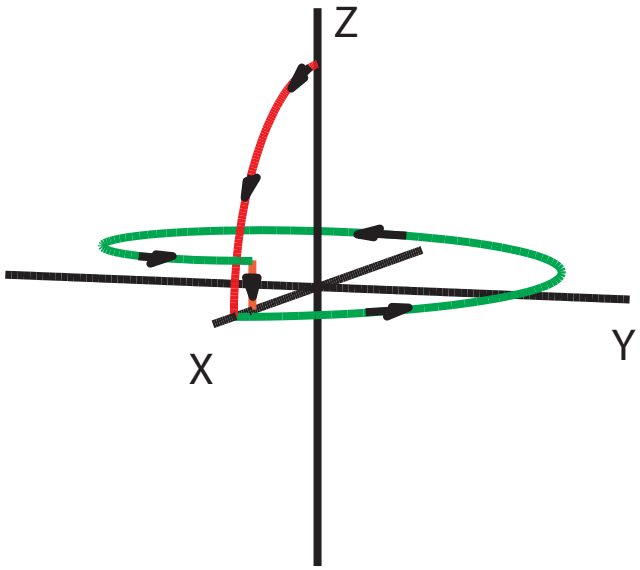

Figure 5-1: The idea behind unitary correction. Suppose we want to keep the Bloch vector in the x-y-plane. We first rotate the vector into the x-y-plane (the red path). The vector spins about the z-axis and relaxes (the green path). Then we try to push it back into the x-y-plane (the orange path). Such a procedure will result in a steady state Bloch vector.

Definition 5 *A quantum state is stabilizable under a quantum process $\mathcal{E}_t$ if there is a unitary operation U such that*

$$\epsilon_t(\rho) = U\rho U^\dagger \tag{5.1}$$

and it follows immediately that

Theorem 6 *A quantum state is stabilizable under $\mathcal{E}_t$ if and only if the corresponding Bloch vector at time t has the same norm as at time 0.*

For certain processes, like pure phase damping, the z-axis is fixed by the quantum process, and in these cases doing nothing stabilizes any Bloch vector along the z-axis. In the above definition, this can be interpreted as the identity operator correcting the quantum process. On the other hand, any state with a nonzero component in the x-y-plane is not stabilizable at all as the vector's length is necessarily strictly decreasing under phase damping.

Unitary stabilization is uninteresting in this class of processes. We can either stabilize states that are initially unaffected by the quantum process by doing nothing, or we can try in vain to stabilize states which decohere.

To avoid such dead ends, we'll concern ourselves with processes that admit a manifold of stabilizable states of dimension greater than or equal to the space of pure states. For single spins this means

Definition 7 *A quantum operation $\mathcal{E}$ can be corrected by unitary operations if the manifold of stabilizable states has dimension* 2.

5.1.1 Example: Amplitude Damping

Consider the amplitude damping to zero temperature outlined in the last section. Recall the Bloch vector maps as

$$(x, y, z) \mapsto (E_2 x, E_2 y, 1 + E_1(z - 1)) \tag{5.2}$$

A state is stabilizable under this process if and only if

$$x^2 + y^2 + z^2 = E_2^2 x^2 + E_2^2 y^2 + (1 + E_1(z - 1))^2 \tag{5.3}$$

Rearranging this equation shows that the set of stabilizable states satisfy

$$\frac{1 - E_2^2}{1 - E_1^2}(x^2 + y^2) + (z - \frac{E_1}{1 + E_1})^2 = \frac{1}{(1 + E_1)^2} \tag{5.4}$$

Note that this is an ellipse. It is no coincidence. The norm is a quadratic form on $\mathbb{R}^3$ and hence the solution had to be a conic section. The decoherence rate in the x-y-plane determines the minor axis and the relaxation rate along the z-axis determines the major axis.

How can we correct a point on our stabilizable ellipse? If the Bloch vector is initially on the ellipse at $\vec{r}$, it will relax towards the equilibrium state to $\mathcal{E}(\vec{r})$. Hence, we find the plane containing both $\vec{r}$ and $\mathcal{E}(\vec{r})$ and then apply a rotation by the angle between these vectors about an axis perpendicular to the plane. The angle between the vectors can be found by

taking a dot product

$$\cos(\theta_c) = \frac{\langle \vec{r}, \mathcal{E}(\vec{r}) \rangle}{\|r\|^2} \tag{5.5}$$

A picture of the x components resulting from such a correction scheme is shown in figure 5-2

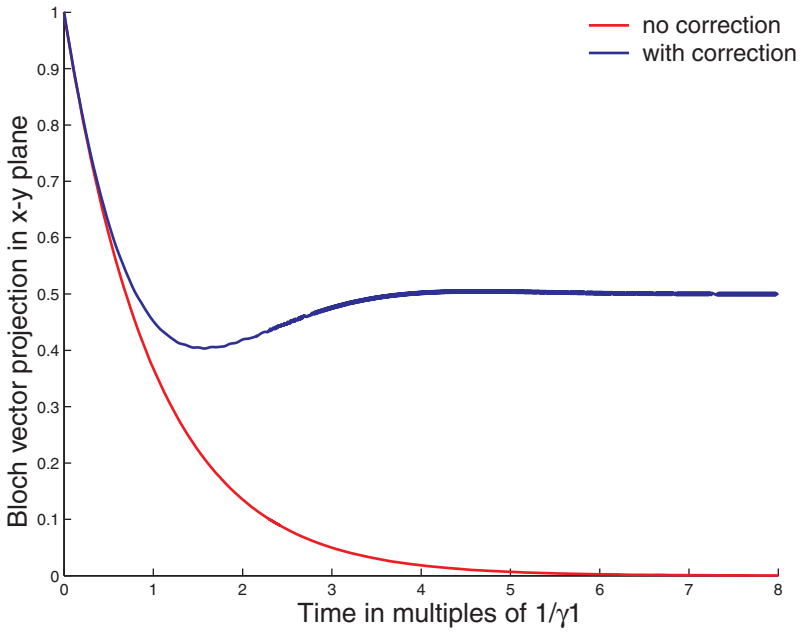

Figure 5-2: The x-component of the Bloch vector when we perform y-rotations to correct amplitude damping.

5.1.2 Stabilizable States

In general, the previous technique will map out the set of unitarily stabilizable states for an arbitrary quantum process.

Given an operation on a Bloch vector, we can solve the equation

$$\|\mathcal{E}(\vec{r})\| = \|\vec{r}\| \tag{5.6}$$

This will necessarily result in a conic section as the inner product is a quadratic form.

Similarly, to find the correction angle for a particular state, we solve the equation

$$\cos(\theta_c) = \frac{\langle \vec{r}, \mathcal{E}(\vec{r}) \rangle}{\|r\|^2} \tag{5.7}$$

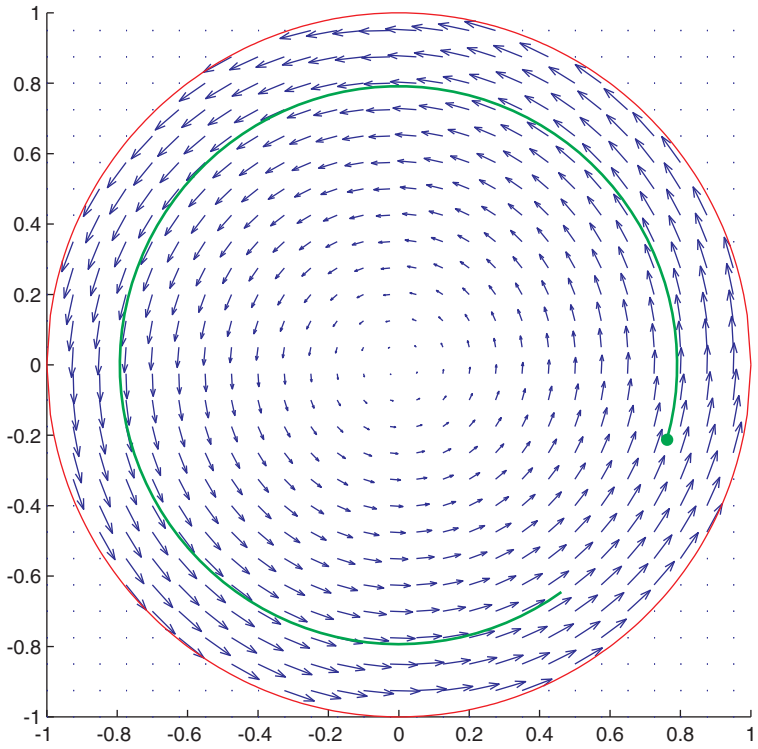

Figure 5-3: In our Bloch sphere picture, unitary operators rotate the Bloch vector about some axis. Here we take a cross section representing the x-z-plane. The vertical axis is z and the horizontal axis is x. This labeling also holds for figures /reffig:fielddec, /reffig:fieldad, and /reffig:fieldra. The green dot represents a starting Bloch vector and its trajectory is also plotted in green.

5.2 Entropy Production and Stabilizability

The length of the Bloch vector is in one to one correspondence with the entropy of the density matrix. If the entropy is strictly increasing (e.g., when we have a dephasing process), then unitary correction is impossible because the trajectories of the quantum process never return the Bloch vector to the appropriate length for a correction step.

The inability to perform unitary correction related to the H-theorem of statistical mechanics. A system obeys an H theorem if its entropy is increasing. We conclude

Theorem 8 *Any system which obeys an H-theorem is not correctable.*

Proof Assume that for all ρ, $S(\mathcal{E}(\rho)) \geq S(\rho)$. As we saw above, this means that the Bloch vector has the property that $\|\mathcal{E}(\vec{r})\| \leq \|\vec{r}\|$. Furthermore, the maximally mixed state is fixed. This implies that the affine part of the dissipative process $\vec{b}$ is zero and we have a dephasing process.

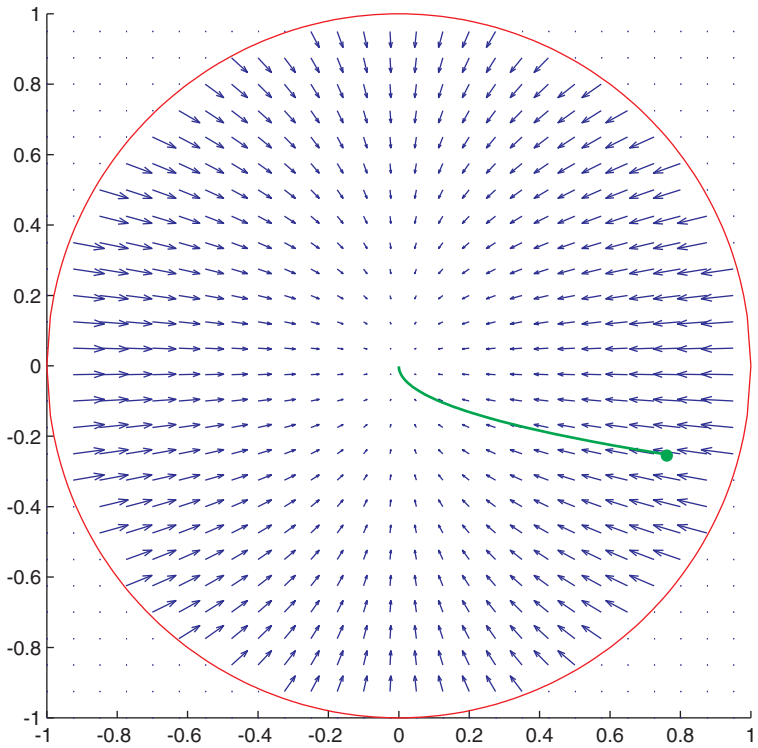

Figure 5-4: Here is an example of a process which cannot be corrected using unitary operations again in the x-z-plane. The vector field maps all points to the central mixed state and hence the entropy is strictly increasing.

The real parts of the eigenvalues of the dissipation matrix must be less than or equal to zero. If all of the eigenvalues are zero, then the process is unitary and we can correct the process with unitary operations. But if any eigenvalues are less than zero, then at least two eigenvalues have real parts less than zero and this process collapses onto one axis or onto the maximally mixed state and is not correctable. ■

While the proof of this corollary was trivial, the result is important for unitary correction. There must be a cooling component to the quantum process in order for it to be correctable. That is, only relaxation processes can be corrected.

Consider, for example, the above case of amplitude damping. In figure 5-7, we plot the entropy of a density matrix initialized to the pure state $\vec{r} = (1, 0, 0)$. The entropy increases as the spin begins its relaxation, but as it approaches the equilibrium state its entropy decreases.

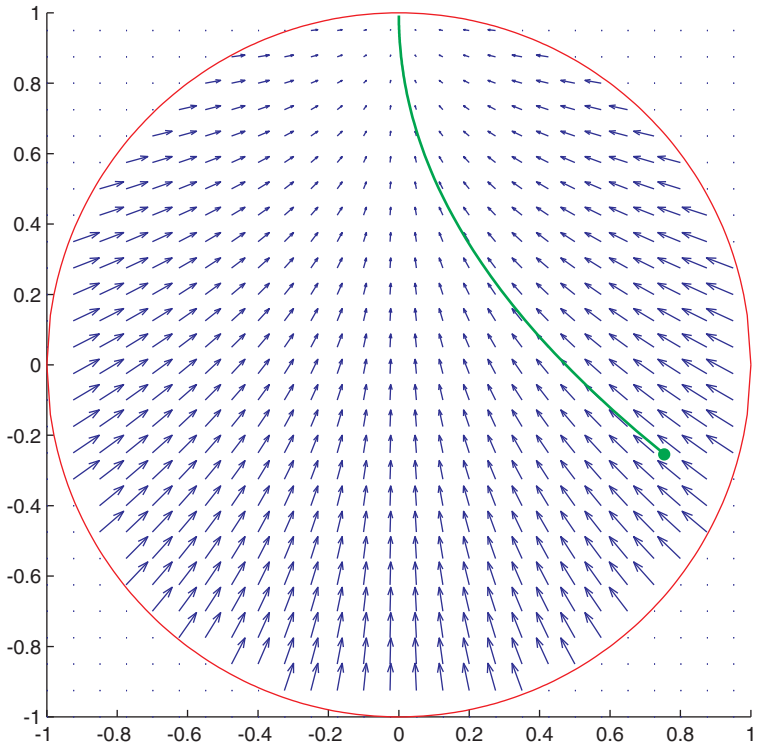

Figure 5-5: This is a vector field representing amplitude damping.

5.3 Stabilizable States in Hamiltonian Approach

In the previous section we studied the set of states stabilizable under unitary operations and found that they formed an ellipse. The ellipse was based on a coarse graining of time where we perform the operations

$$\ldots \mathcal{U}\mathcal{E}_t\mathcal{U}\mathcal{E}_t\mathcal{U}\mathcal{E}_t \ldots \tag{5.8}$$

where $\mathcal{U}(\rho) = U\rho U^\dagger$. Consequently, the ellipse was a function of the time between unitary pulses.

Now recall that if we have two matrices A and B then

$$\exp((A+B)t) = \lim_{n\to\infty} (\exp(A\frac{t}{n})\exp(B\frac{t}{n}))^n \tag{5.9}$$

We can think of our correction scheme as performing a coarse grained approximation to equation 5.9, using the matrices H_c and L as the generators of the unitary correction and dissipative parts of the dynamics respectively. Under this identification we are approxi-

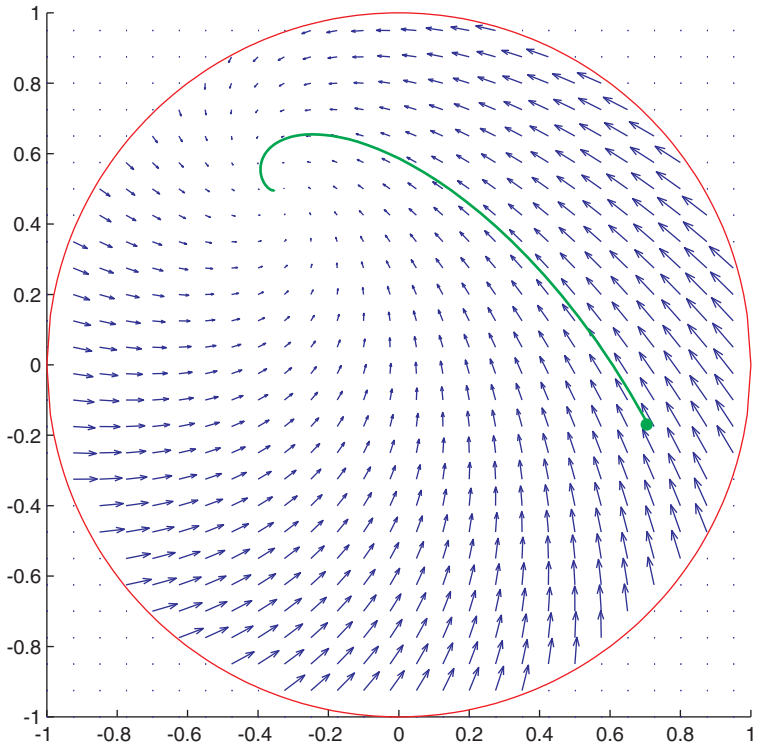

Figure 5-6: Combining figures 5-3 and 5-5 we see that the trajectory of our Bloch vector now converges to a point which is not the north pole. Indeed the points which we can reach are fixed by the damping process we begin with.

mately evolving the quantum dynamical semigroup corresponding to the Lindblad equation

$$\frac{d\rho}{dt} = -i[H_c, \rho] + L(\rho) \tag{5.10}$$

Consider again the case of amplitude damping. With controls we get the Lindblad equation

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} -\gamma_2 & u_z & u_y \\ -u_z & -\gamma_2 & u_x \\ -u_y & -u_x & -\gamma_1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \gamma_1 \end{pmatrix} \tag{5.11}$$

The set of stabilizable points is where $d\vec{r}/dt = 0$. We need not consider the u_z control as it commutes with the relaxation operator. Setting equation 5.11 to zero, we can solve to find

$$\frac{1}{4} = (z - \frac{1}{2})^2 + \frac{x^2 + y^2}{\theta_r} \tag{5.12}$$

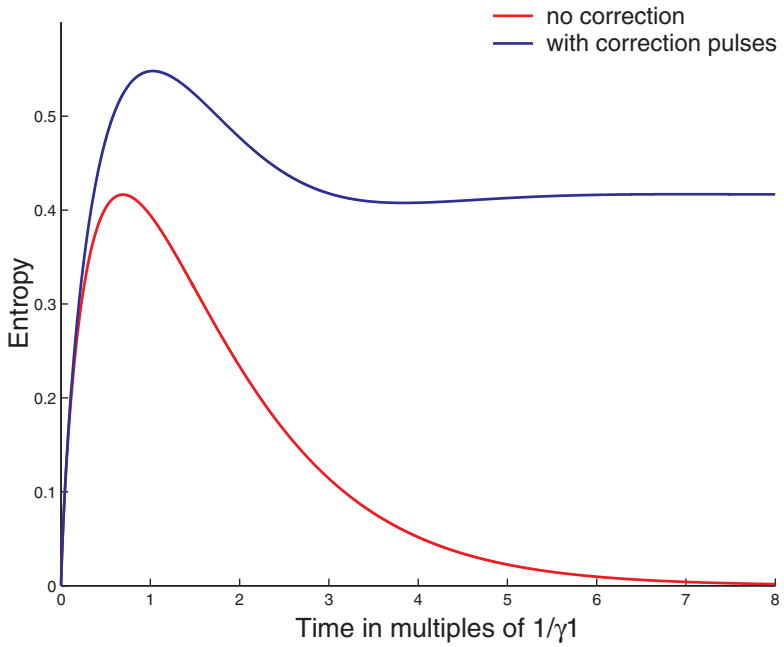

Figure 5-7: Entropy production in a correction scheme. The red curve marks no correction, and the state begins and ends with zero entropy. When we apply correction, we sit at a state of higher entropy and do not relax back to the ground state.

where $\theta_r = \frac{\gamma_1}{\gamma_2}$. To get to a steady-state point $\vec{r}_{ss} = (x_{ss}, y_{ss}, z_{ss})$, we apply the control

$$u_x = \gamma_2 \frac{x_{ss}}{z_{ss}} \tag{5.13}$$

$$u_y = -\gamma_z \frac{y_{ss}}{z_{ss}} \tag{5.14}$$

5.4 Open Loop Control of Spin Envelopes

In the last section, we saw that we could quickly reach steady state points by a sequence of particular rotations. In this section, we examine the controllability of the Bloch vector on the finite time horizon. Given arbitrary unitary operators as our controls, we wish to control the expectation of the observable X, the first Pauli matrix. This corresponds to controlling the first component of the Bloch vector.

Assume that we can continuously observe the x-component of the Bloch vector. This corresponds to a continuous measurement of the expectation value of X. Our goal will be to set the inclination of the Bloch vector to the appropriate angle to produce a desired

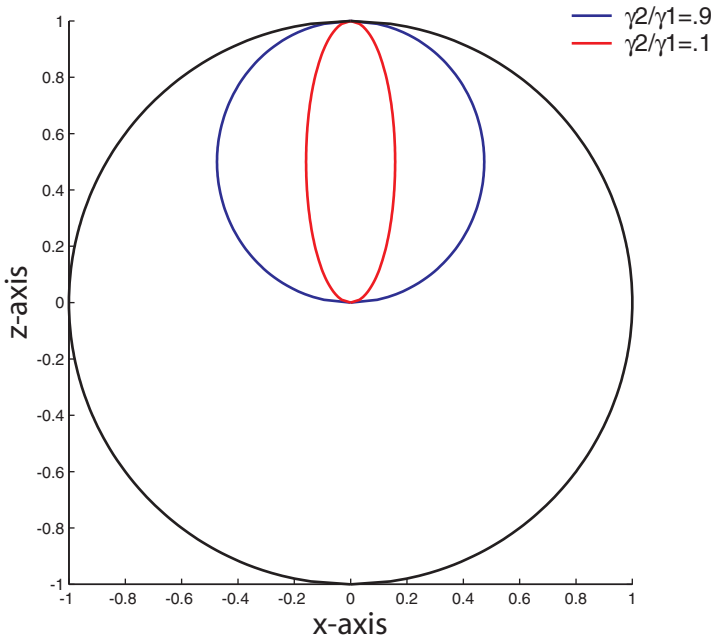

Figure 5-8: The set of stabilizable states under amplitude damping. The two ellipses represent different ratios between the transverse and longitudinal relaxation rates.

observation. Indeed, this can be done by calculating the angle of inclination with respect to the x-y-plane where the Bloch vector currently is, then calculating the angle of the target inclination, and finally applying a y-rotation by the difference of these two angles.

But how can we be sure that under relaxation the vector does not become too short to reach the desired rotation angle? The solution is illustrated in figure 5-9. If we set a maximum amplitude which we want to attain, we can draw a sphere inside the Bloch sphere at this amplitude. As shown in figure 5-5, the flow of amplitude damping is towards the north pole. Hence, if we always remain above the line tangent to the point on the sphere of maximum amplitude, we can perform this scheme of open loop envelope control for an arbitrarily long time.

Now we must compromise. We want to find the sphere with the largest radius that also provides the largest projection into the x-y-plane. This corresponds to trying to both maximize the radius of the red sphere and to the z of the blue dashed line in figure 5-9.

If the sphere has radius greater than $1/2$, then the blue line will be at less than $1/2$. Similarly, if the blue line is greater than $1/2$ then the red sphere will have radius $1/2$. Clearly our maximization occurs when $r = 1/2$.

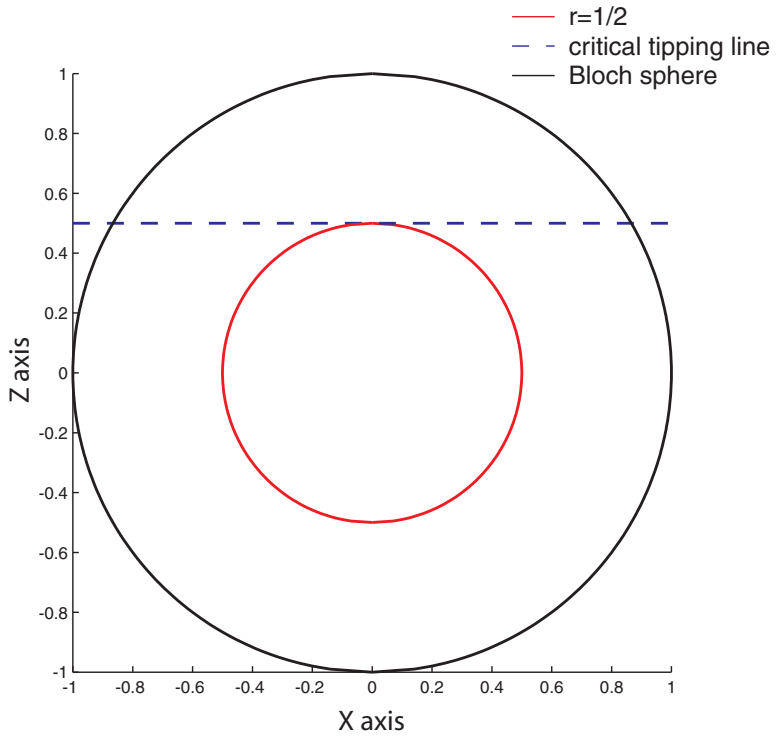

Figure 5-9: A diagram of the feasibility of spin control. The red circle denotes the radius of maximum amplitude in the x-y-plane we wish to attain. If we stay above the blue line, then since all flow under amplitude damping is towards the north pole, we never enter the red sphere.

In the next chapter, we will show an example of such open loop control in an NMR system.

Chapter 6

Applications in Nuclear Magnetic Resonance

Nuclear magnetic resonance (NMR) studies the evolution of the spin states of atomic nuclei in the presence of a static magnetic field. External fields perpendicular to the static field can control the states of the nuclei, but the nuclei also undergo relaxation to a finite temperature.

Our goal is not to present a from scratch derivation of nuclear magnetic resonance here. Such a description can be found in a variety of excellent sources (for example, see classic texts by Slichter [Sli90] or Ernst [EBW87]). Instead, we are going to describe how to formulate the principles of NMR on single spins in the language we develop throughout this thesis. Then we will discuss experimental realizations of the previous chapter's developments.

In our language, NMR system will be described as follows. We have an ensemble of nuclear spins in a static magnetic field whose state is described by a two level density matrix. We pulse the spins with alternating magnetic fields in a direction perpendicular to the static field corresponding to x or y rotations. We measure the x and y components of the density matrix by an induction signal in a pickup coil from the spins processing about the magnetic field axis. Our primary modes of relaxation will be a "spin-lattice" relaxation and a "spin-spin" decoherence mode. We will model these relaxation modes in a purely phenomenological sense as generalized amplitude damping.

The simplest instance of an NMR system is an ensemble of spin-1/2 particles with the Hamiltonian

$$H = \frac{1}{2}\hbar\omega Z \tag{6.1}$$

where Z is the Pauli matrix discussed in Chapter 4 and ω is proportional to the static magnetic field. We can phase lock our NMR apparatus so that our observation is synchronous with the procession around the z-axis. This allows us to approximate the system Hamiltonian as 0.

The spins in this simple system undergo amplitude damping to finite temperature, which we recall is modeled by the map

$$(x, y, z) \mapsto (E_2 x, E_2 y, E_1(z - p) + p) \tag{6.2}$$

on the Bloch vector. $E_2 = \exp -t/T_2$ is the "spin-spin" relaxation and $E_1 = \exp(-t/T_1)$ is the "spin-lattice" relaxation. The term p is the equilibrium polarization found from the identification

$$\rho_e q = \frac{\exp(-\beta Z)}{\mathcal{Z}} = \begin{pmatrix} \frac{1+p}{2} & 0 \\ 0 & \frac{1-p}{2} \end{pmatrix} \tag{6.3}$$

where $\beta = k_B T$ and T is the temperature of the ensemble. Note that at room temperature, even in the presence of a 12 Tesla field, this mixture has a polarization of less that 10^{-5}. Nonetheless, the geometry of the spins behaves identically for a Bloch sphere of radius 10^{-5} as it does for a sphere of radius 1.

Finally, we can introduce control terms to the Hamiltonian. In the rotating frame, we model our RF pulses by Hamiltonian terms

$$H_c = \frac{1}{2}(r_x X + r_y Y) \tag{6.4}$$

If we apply this H_c over a short window of time, one can easily check that the Bloch vector is rotated about the axis (r_x, r_y). Hence, we can talk about the *angle* of a pulse as the amount of rotation that a Bloch vector undergoes after the application of H_c.

6.1 Experimental demonstration of Unitary Correction

NMR proved to be a perfect experimental context for our coherence schemes, with the ability to prepare a quantum system undergoing amplitude damping and the application of strobed unitaries.

To implement our experiment, we needed a sample with T_1 roughly equal to T_2. Under

this condition, our steady state magnetization would be dramatically large. We prepared a solution of copper sulfate in water following the prescription in [VFL+00] to reduce the T_1 time of the proton relaxation. We were able to produce a system with $T_1 = 3.9 \pm 0.5 \times 10^{-2}$ s and $T_2 = 3.232 \pm 0.005 \times 10^{-2}$ s. A π pulse was measured to be 16.1 ms.

In our Varian 500 MHz spectrometer, we prepared the following pulse sequence

- Apply a 90 degree pulse about the x-axis
- Acquire signal off the pickup coil for a time Δt and then apply a pulse of size α about the x-axis
- Repeat the previous step 511 times
- Acquire the decay for time $64\Delta t$

The numbers in this experiment were chosen to be compatible with the spectrometer hardware. We were unable to repeat the procedure for any longer due to hardware limitations.

In any event, it should be easy to see that this procedure is our strobed unitary correction scheme. During the Δt acquisition times, the system relaxes. It is then pushed back towards to the x-axis by an α-pulse.

α can be calculated from equation 5.7. The acquisition from such a scheme is plotted in Figure 6-1.

6.1.1 Steady State NMR and the Ernst Angle

In a seminal paper, Ernst and Anderson described the foundations of pulsed NMR, effectively standardizing their method for spectroscopy [EA66]. As a method of maximizing their signal to noise in multiple experiments, they described a procedure for pulsed NMR. In the limit where $T_2 \ll T_1$, one could prepare experiments without waiting for full relaxation using the *Ernst angle*. Instead of tipping the system by 90 degrees, one could apply a pulse given by

$$\cos(\theta) = \exp(-t/T_1) \tag{6.5}$$

where t is the time between experiments. Note that this expression is completely independent of T_2. When T_1 and T_2 are commensurate, a significantly larger signal is obtained

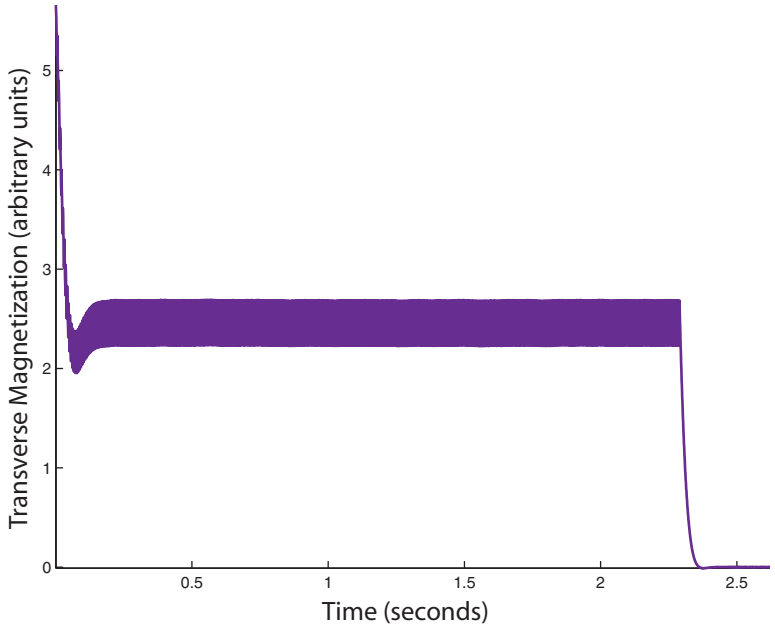

Figure 6-1: Acquisition of a steady state signal using NMR. Note that the time scale here is over 60 T_1 cycles long

from our unitary correction schemes. Figures 6-2 and 6-3 compare the Ernst angle to the *Recht angle*, the tipping angle calculated with our unitary correction methods.

Ray Freeman first analyzed the behavior of an NMR system in the steady state limit. He observed that the Bloch equations gave steady state amplitudes in the limit of fast repetition time and small angles [FH71]. We have analyzed these concepts more deeply here, but have not yet discussed a practical limitation of NMR spectrometers. Freeman realized that in any NMR implementation the phase of the transmitter and receiver could have a precession lag between them. Letting θ be this relative phase, the steady state transverse magnetization is found to be

$$M_T = \frac{p(1-E_1)(1-E_2\cos(\theta))\sin(\alpha)}{(1-E_1\cos(\alpha))(1-E_2\cos(\theta)) - (E1-cos(\alpha))(E_2-\cos(\theta))E_2} \tag{6.6}$$

Note that at the Ernst angle,

$$M_T = \frac{p\sin\alpha}{1+E_1} \tag{6.7}$$

the dependence on θ disappears. So the Ernst angle is indeed useful for spectroscopy, as any stochastic behavior in the phase of the transmitter does not effect the steady state

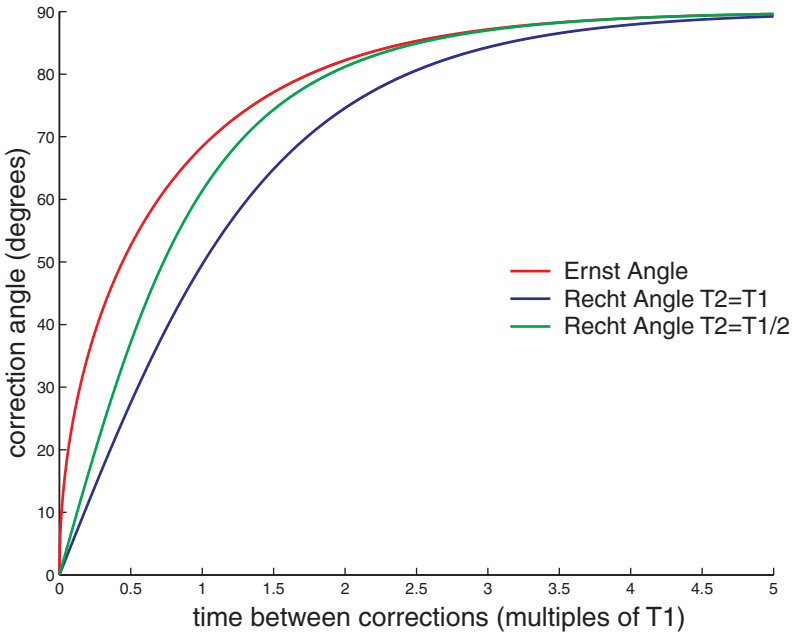

Figure 6-2: A comparison of the tipping angles for repeatable experiments. Note that our calculated angle is always less than the Ernst angle even when T_2 is considerably less than T_1.

magnetization.

Even our state-of-the-art NMR spectrometer has a nonzero precession angle. We plotted our relative steady state magnetizations in figure 6-4. The black plot is the theoretical Freeman curve with $\theta = .25$ radians and the red curve is set with the error in our parameters discussed above and an error in θ of ± 0.05. The data agreed with no fits for when $\theta = 0$. Note that the Recht angle still yields a higher steady state signal, but it is shifted off the peak of this plot as θ is not considered in our discussion.

6.2 Experimental Open Loop Control

We also experimentally demonstrated open loop control in our water with copper sulfate system. As described in Chapter 5, by calculating the difference in angle between the target magnetization and the current magnetization, we can tip the vector to the appropriate inclination with respect to the x-y-plane.

As is the tradition here at the Media Lab, we always try to write our name first. We

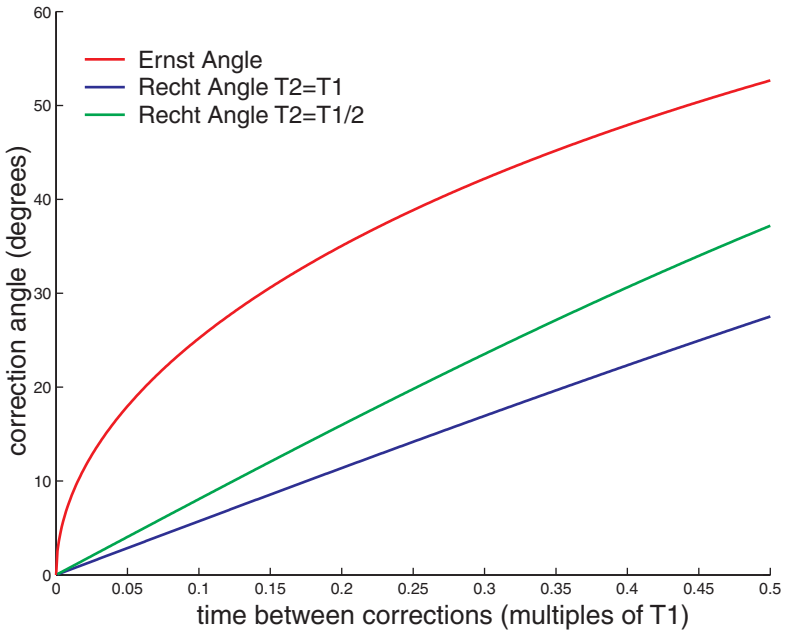

Figure 6-3: This figure magnifies figure 6-2 for small tipping angles.

wrote a Matlab script to calculate the appropriate pulses given our goal of writing the letters "ML" on the spin envelope. Using a reprate of 94 Hz (eight pulses per T_1), we acquired 8 points per tip and plot the results in 6-5.

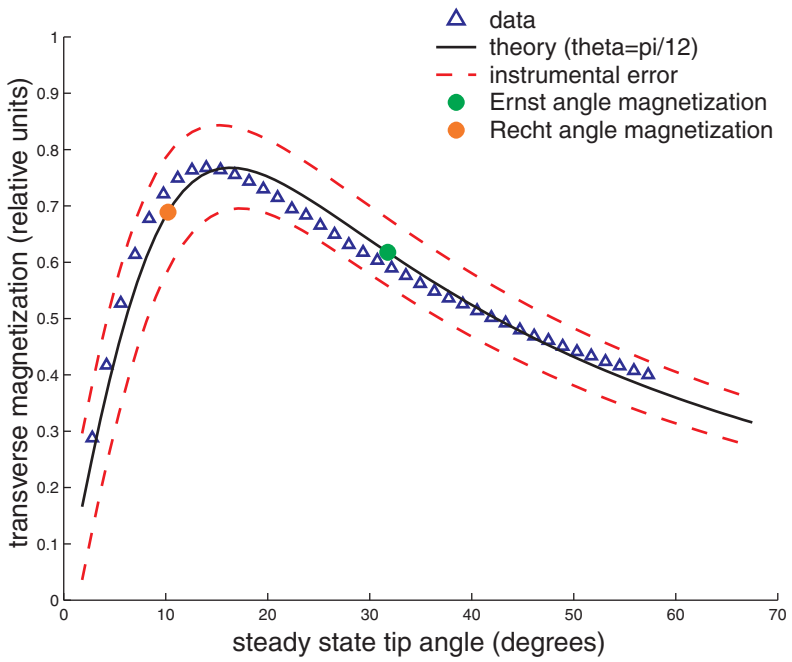

Figure 6-4: Plot of experimental steady state amplitudes as a function of pulse angle. The data falls within the theoretical error bars. Note that even when the procession angle is small but nonzero, the Recht angle still yields a larger steady state signal than the Ernst angle

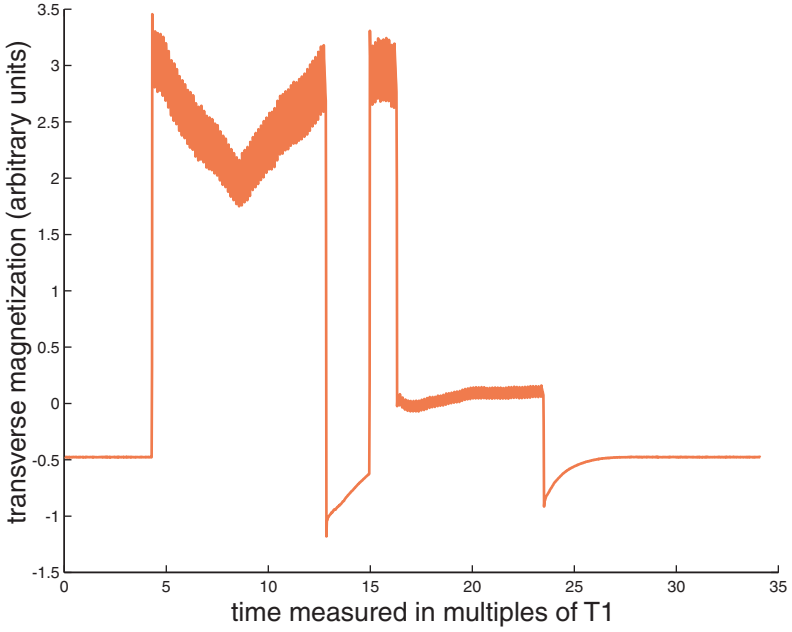

Figure 6-5: Spelling out the letters "ML" in the envelope of the spins. This takes place over many T1 and shows how controllability is successful when the maximum X target is kept less than or equal to 1/2

Chapter 7

Feedback and System Identification in NMR

Given a single spin system, some of the most important quantities to determine experimentally are the intrinsic decay rates T_1 and T_2. For example, these constants determine how quickly polarization can be transferred between different subsystems. The T_1 and T_2 rates determine how quickly we can extract information from a spin system, and are important for many spectroscopic experiments.

The standard methods for determining these quantities are called "inversion-recovery" for T_1 and a CPMG (Carr-Purcell-Meiboom-Gill) sequence for T_2. To perform an inversion-recovery one first rotates the spins by 180 degrees, then waits a time t, and then tips by 90 degrees and acquires a spectrum. The height of the spectrum as a function of t can be fit to an exponential with decay constant T_1. For a CPMG sequence, first perform a 90 degree pulse and wait a time τ. Then repeatedly apply 180 degree pulses spaced by times 2τ. This sequence produces a series of "spin-echoes" and has well defined peaks spaced by 2τ [EBW87]. These peaks can be fit to an exponential curve with decay constant T_2

Both of these sequences require "hard pulses" that require an expensive power amplifier to generate such that the large tipping angles can be implemented. On the other hand, the techniques developed in this thesis give a new method for finding these constants using very small pulses and fast repetition times, and in principle these small pulses could be implemented as "soft pulses" without the costly amplifier. Given an NMR system with

unknown decoherence constants T_1, T_2, we can apply a train of ϕ pulses spaced by Δt to land us in a steady state x_{ss} as in equation 5.13. For sufficiently small Δt, we have

$$\begin{pmatrix} z_{ss} \\ x_{ss} \end{pmatrix} = - \begin{pmatrix} \frac{-1}{T_1} & u \\ -u & \frac{-1}{T_2} \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{T_1} \\ 0 \end{pmatrix} \tag{7.1}$$

Expanding this matrix product and looking at the x term gives the relation

$$\frac{1}{T_2} + \frac{\phi^2}{\Delta t^2} T_1 = \frac{\phi}{\Delta t x_{ss}} \tag{7.2}$$

If we choose two different ϕ's then, we can determine T_1 and T_2 from the observations of x. However, we do generally have noise on our observable, so we need to determine a method for moving to a steady state point which is measurable and gives us maximal information about the decoherence times. We will accomplish this task by using a closed loop estimation process, tying in further the links between quantum information theory and control.

7.1 The Extended Kalman Filter

Such a scenario becomes possible via extended Kalman Filtering. The extended Kalman filter is a linearized version of the classic linear Kalman Filter which optimally solves the state space estimation problem for

$$\frac{d\vec{x}}{dt} = \mathbf{A}\vec{x} + v[t]\vec{y} = \mathbf{B}\vec{x} + w[t] \tag{7.3}$$

where the v and w are independent white gaussian processes, $\vec{x}$ is the internal state of the system we are trying to estimate and $\vec{y}$ is the observation vector of our equation [Ger99].

We do not go into the details of such a filter, but note that it is a recursive estimator in the sense that our update of our estimator $\hat{x}$ for our internal state $\hat{y}$ is always given by

$$\hat{x}_{new} = \hat{x}_{old} + \mathbf{K}(\vec{y} - \vec{y}_p) \tag{7.4}$$

where $\vec{y}_p$ is our predicted measurement. This is called *recursive estimation*. In the case of the linear Kalman filter, this method will produce an optimal estimator, but for a nonlinear

system, we cannot prove such optimality. Surprisingly, however, such an estimator will converge for nonlinear systems. This is due to a phenomenon called *entrainment* which leads to synchronizations in dynamical systems when the two systems are coupled. In our case, our two systems are the estimator and the state we are trying to estimate, and the coupling is through the measurement.

A large body of work has developed to determine when systems synchronize through entrainment. It is know that a necessary condition is that the the largest Lyapunov exponent associated with the coupling be negative [PCJ+97], but determining these exponents is a difficult task. Nonetheless, entrainment occurs surprisingly often, and indeed can be used for parameter estimation in NMR.

7.2 A Recursive Estimation Procedure for System Identification

Our procedure for recursive estimation is relatively simple

- decohere for a time t
- rotate about the y axis by $\theta = \sqrt{\frac{2}{T1T2}}\Delta t$
- decohere for a time Δt
- rotate about the x axis by $\theta = \sqrt{\frac{2}{T1T2}}\Delta t$
- measure x and y
- update our estimators
- repeat the procedure

The scheme is displayed graphically in figure 7-1.

Before we discuss the estimation process, let's describe what is occurring. First we tip about the y axis. As the spins relax back, we get a spread in the x-z plane distinguishing between errors in T_1 and T_2 estimates. But since we cannot measure the spread in z, we need to tip this signal into the y axis via an x-rotation. These two rotations give us a composite x-y rotation.

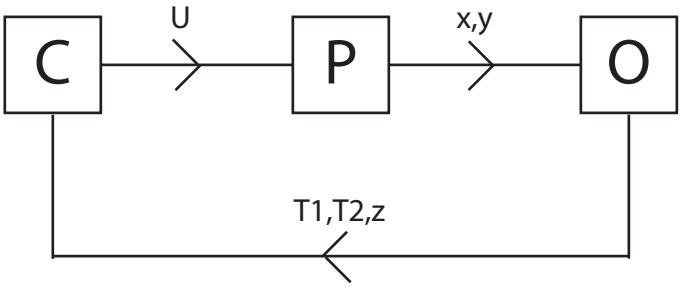

Figure 7-1: A control flow diagram for our estimation/control procedure. The plant "P" is our NMR system. Our observations "O" measure the x and y components of the Bloch vector. We update the unknown parameters T_1, T_2, and z and pass them to the controller "C" which constructs a unitary operator U for sustaining the maximal steady state signal given our knowledge of T_1 and T_2.

On the other hand, from the point of view of the spins, the angles of rotation provide the maximum steady state magnetization, when T_1 and T_2 are accurately estimated and Δt is very small.

So given a proper estimation procedure, the above filter should simultaneously discover T_1 and T_2 and steer the system to a stable steady state with maximum transverse magnetization.

Now how do we estimate? The idea is to use the magic of entrainment. Our update rules are particularly simple. By design, the x signal measures our error in our T_2 estimate and the y signal measures the error in the T_1 estimate. The most naive update rules are then

$$\hat{z} = \hat{z} + \epsilon_1(x_p - x_m) + \epsilon_2(y_p - y_m) \tag{7.5}$$

$$\hat{T_1} = \hat{T_1} + \epsilon_3(y_p - y_m) \tag{7.6}$$

$$\hat{T_2} = \hat{T_2} + \epsilon_4(x_p - x_m) \tag{7.7}$$

We wrote a Matlab script to test the performance of this estimator. We set $T_1 = 1$, $T_2 = .15$, $\Delta t = 5 \times 10^{-3}$ and all of the ϵ's to 5 and a noise floor of 10^{-4} times the maximum x signal. Starting with a random estimate for T_1 and T_2, this filter converges most of the time. Such convergence is plotted in figure 7-2. On average, the filter takes on the order of $50T_1$ to converge, and the estimates are within .01 percent of their actual values. These

limitations are due to the instability of our nonlinear Kalman filter.

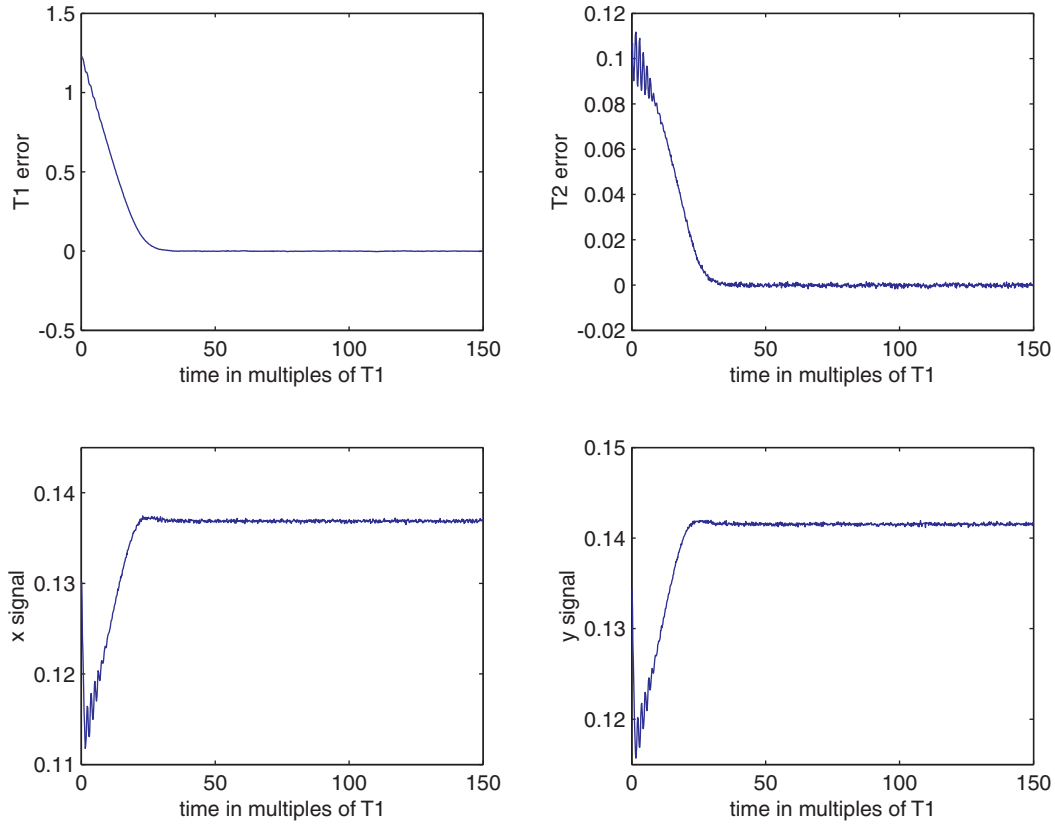

Figure 7-2: The performance of our estimator. Here $T_2/T_1 = .15$ The estimates converge to their actual values and the Bloch vector is pushed to the maximum steady state magnitude $\frac{\sqrt{T2/T1}}{2} = .19$

This is only a glimpse of the potential of such feedback algorithms and many questions are left open for future work. Among them, we need to determine how to make the convergence time faster and to make the estimator arbitrarily precise. With standard techniques, the accuracy scales as the square root of the number of measurements, and in order for our technique to be useful, we need an estimator who's accuracy goes to zero as time goes to infinity. We also want to investigate linearizing our system so that we can talk about optimality. This would involve a different control procedure than the one presented, and determining this procedure is left open. Finally, this scheme uses very small tipping angles and could possibly be implemented with "soft pulses" without a power amplifier. Our

model still uses hard pulses, but investigating how to implement a feedback scheme with soft pulses could change the face of NMR spectroscopic instrumentation.

Chapter 8

Correction of Relaxation in Higher Dimensional Systems

While the results on one-spin are surprising, all of the differential equations can actually describe classical systems. The outstanding question is what impact unitary correction has on higher dimensional quantum systems. Remarkably, many of our results readily generalize to larger systems. We will need more mathematical care to discuss such situations. We will first show that any quantum system which does not fix the maximally mixed state has a stabilizable submanifold *with higher dimension than the set of pure states*.

Characterizing the set of stabilizable states proves daunting since we are working in the context of a semigroup. The lack of symmetry in the matrix differential equation of the coherence vector described in Chapter 3 takes away any nice conclusions about the topology of the stabilized manifold. An investigation into how to control and map out this space is left as a challenging and deep open problem.

8.1 General Picture of Unitary Correction

Let's first begin with a general Hilbert space $\mathcal{H}$ of dimension N evolving under a system Hamiltonian H and undergoing a quantum process. Suppose that we can apply any unitary operation to this system arbitrarily quickly. The Lindblad equation for this system is then

$$\dot{\rho} = -i[H + H_c, \rho] + \frac{1}{2}\sum_k [L_k\rho, L_k^\dagger] + [L_k, \rho L_k^\dagger] \tag{8.1}$$

or in the coherence vector language

$$\frac{d\vec{r}}{dt} = \mathbf{A}\vec{r} + \vec{b} + (\tilde{\mathbf{H}} + \tilde{\mathbf{H}}_c)\vec{r} \tag{8.2}$$

If we allow ourselves to perform any unitary operation, then $\mathbf{H}_c$ is also arbitrary and we can hence reduce this last equation to

$$\frac{d\vec{r}}{dt} = \mathbf{A}\vec{r} + \vec{b} + \mathbf{C}\vec{r} \tag{8.3}$$

where $\mathbf{C} = \tilde{\mathbf{H}} + \tilde{\mathbf{H}}_c$ ranges over all of $\mathfrak{su}(N)$.

Our definitions in Chapter 5 can be applied to this higher dimensional case. We say that a density matrix is stabilizable if there exists a choice of $\mathbf{C}$ such that $\dot{\rho} = 0$. Again, we say that a quantum operation is correctable by unitary transformations if the set of all stabilizable density matrices has larger dimension than the set of pure states.

When is a state stabilizable by a unitary operation? If we have a quantum process $\mathcal{E} = e^{Lt}$ then $\mathcal{E}(\rho) = U\rho U^\dagger$ for some unitary if and only if the eigenvalues of $\mathcal{E}(\rho)$ are identical to the eigenvalues of ρ. This gives a good strategy for finding the stabilizable states. Given a fixed point, we will take a perturbation about the fixed point and determine the dimension of the space where the eigenvalues aren't changed. Note that here we must return to the language of quantum operations and not strictly focus on their generators.

We will find that whenever $\vec{b} \neq 0$, that there exists a submanifold of stabilizable states.

Let's proceed with our main

Theorem 9 *If a quantum operation converges to a state with nonmaximal entropy and non-degenerate eigenvalues then it is correctable by unitary operations.*

Proof First let $\mathbf{C} = 0$ and let $\mathcal{E}$ be the quantum process obtained from exponentiating the Lindblad operator. Let $\rho_{eq} = \lim_{t\to\infty} \mathcal{E}_t(\rho)$ be the fixed point of dissipative process. Since the maximally mixed state is not fixed, this ρ_{eq} is unique, and in the coherence vector representation, ρ_{eq} corresponds to the vector $\vec{r}_{eq} = -\mathbf{A}^{-1}\vec{b}$.

Consider a small perturbation $\rho_{eq} \mapsto \rho_{eq} + \delta\rho$ about the fixed point. Then $\vec{r}_{eq} \mapsto \vec{r}_{eq} + \delta\vec{r}$

and we find that

$$\begin{aligned}\mathcal{E}(\rho_{eq}+\delta\rho) &= \mathcal{E}(\frac{\mathbf{1}+(\vec{r}+\delta\vec{r})\cdot\vec{\sigma}}{N}) \\ &= \frac{\mathbf{1}+(A\vec{r}+A\delta\vec{r}+\vec{b})\cdot\vec{\sigma}}{N} \\ &= \rho_{eq}+\frac{A\delta\vec{r}\cdot\vec{\sigma}}{N}\end{aligned} \tag{8.4}$$

and we see that $\mathcal{E}(\rho_{eq}+\delta\rho)$ is also a perturbation about ρ_{eq}.

Let $|\psi_n\rangle$ be an orthonormal eigenbasis for ρ_{eq} with corresponding eigenvalues $p_1 > \ldots > p_N$. We want to show that in a neighborhood of the fixed point there is a manifold structure of dimension N^2-N in which the eigenvalues of density matrices are not changed by $\mathcal{E}$. Indeed we can calculate the change in the eigenvalues of a perturbation to first order

$$\begin{aligned}\Delta\lambda_n &= \langle\psi_n|\rho_{eq}+\delta\rho-\mathcal{E}(\rho_{eq}+\delta\rho)|\psi_n\rangle \\ &\approx \langle\psi_n|(\frac{A\delta\vec{r}}{N})\cdot\vec{\sigma}|\psi_n\rangle \\ &= \langle n|V(\frac{A\delta\vec{r}}{N})\cdot\vec{\sigma}V^\dagger|n\rangle\end{aligned} \tag{8.5}$$

where $|n\rangle$ denote the canonical basis and V is a unitary.

Now the set of matrices

$$\{M\in su(N)\mid\langle n|M|n\rangle=0\} \tag{8.6}$$

has dimension precisely N^2-N as $\langle n|M|n\rangle = m_{nn} =$ is the satisfied by all Hermitian matrices with zeros on the diagonal.

Since all of the eigenvalues of A are strictly less than zero, A is nonsingular, and hence there are N^2-N directions about the fixed point where the eigenvalues are fixed by $\mathcal{E}$. By the implicit function theorem, the set of all matrices with eigenvalues fixed by $\mathcal{E}$ is an N^2-N manifold.

Note that the set of pure states has dimension $2N-2$ in an N-dimensional system. We shall see shortly that given the ability to implement arbitrary Hamiltonians allows the stabilization of a submanifold of dimension N^2-N. For $N>2$, the set of stabilizable states is hence always strictly larger than the set of pure states completing the proof. ■

In the situation where a controller only has a subspace $\mathcal{C}$ of Hamiltonians of dimension k

that can be enacted on a time scale faster than the decoherence, the set of stabilizable states is smaller than when the entire algebra $\mathfrak{su}(N)$ can be implemented as controllers. We can say with certainty that in order for a quantum process to be correctable $\dim(\mathcal{C}) > 2N - 2$. Since the Hamiltonian is skew symmetric, we certainly have that each available control stabilizes some state. But we may have the case that the state stabilized by H_1 is the same as the one stabilized by H_2.

Proposition 10 *H_1 and H_2 stabilize the same state if and only if*

$$\det(\mathbf{1} - (A + H_1)(A + H_2)^{-1}) = 0 \tag{8.7}$$

Proof The state stabilized by any H is given by $-(A-H)^{-1}\vec{b}$. Hence H_1 and H_2 stabilize the same states if $-(A - H_1)^{-1}\vec{b} = -(A - H_2)^{-1}\vec{b}$. This can only occur if $\det((A + H_1)^{-1} - (A + H_2)^{-1}) = 0$. Multiplying through by $A + H_1$ proves this proposition. ■

While this fully characterizes the situation of degenerate stable points, it does not provide much intuition as to when two Hamiltonians will stabilize the same state.

8.1.1 Open loop control

Just as in the 2 dimensional case, we move from any state on the stabilizable states to any other state via open loop control in infinite time. Indeed, if ρ_1 and ρ_2 are stabilizable under a quantum operation, then there exists an open loop control scheme to map ρ_1 to ρ_2. If H_k stabilizes ρ_k, then switching the control from H_1 to H_2 will map ρ_1 to ρ_2.

Furthermore, since the decays are exponential in the case of strobed unitaries, we will end up orbiting around the state ρ_2 in a time characteristic of the largest eigenvalue of the decay process.

Here we say nothing about time optimality. In fact this would be a much harder problem depending on the form of the matrix $\mathbf{A}$ and would need to be analyzed on a case to case basis. Such issues are beyond the scope of this thesis.

8.2 But is it quantum?

One of the problems of this thesis is that even though all of the techniques implemented in Chapters 5 and 6 were quantum mechanical, the dynamics of one spin can be described in

a purely classical manner. On the other hand, we have shown in this chapter that higher dimensional quantum systems can also be preserved with unitary correction.

How can we show that the unitary correction can preserve quantum states? The immediate answer is to show that we can preserve states with nonzero entanglement.

There is a simple toy problem which we can construct to convince the reader that quantum mechanics is in action. Consider a two-spin system with an entangled ground state. This seems quite bizarre as we know that NMR systems at have unentangled ground states. But there are many physical examples. For instance, consider the electrons in a Helium atom. Their ground state must populate the s-orbital and have net magnetic moment zero. This leaves the choices $|\uparrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$, but by the Pauli exclusion principle, this state must switch signs under swapping particles, so we are left with a singlet state $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$. This state is maximally entangled.

Any suitable perturbation about this ground state must also be entangled. Hence in a neighborhood of this state we can preserve a 12 dimensional manifold of entangled states for an arbitrarily long time. The volume of this manifold will depend on the characteristics of the quantum process, but note that the dimension of the manifold will always be larger than the set of the pure states. This means, in particular, that unitary correction can indeed preserve quantum information.

Chapter 9

Conclusion

We have shown that unitary correction is a powerful tool in preventing the effects of relaxation. By applying a rapid succession of unitary operations, we have shown how to stop quantum systems from returning to equilibrium and how to map out which states can be stabilized. We have exhaustively described how to apply these techniques to simple one-spin systems and have demonstrated the experimental feasibility of such one-spin schemes. We have also discussed how we can apply unitary correction techniques to arbitrarily large systems.

Even still, we have only scratched the surface of the applications of unitary correction, and there are numerous extensions of beyond this thesis. In this conclusion, we will discuss a few examples of future work to be investigated. We will first describe a proposal of how to create and store quantum information using systems with unentangled ground states. Then we will discuss applications of unitary correction and feedback to nuclear magnetic resonance spectroscopy.

9.1 Entanglement

As discussed in Chapter 8, using only local operations we may be able to preserve entangled quantum states and hence preserve information that is inherently quantum for an arbitrarily long time.

Consider the standard case of amplitude damping on a system of N spins. The equilibrium state of this system is where all of the spins point in the same direction and has zero entanglement. Allowing ourselves the ability to apply unitary operations to each spin

individually, can we preserve quantum information?

The answer is clearly no unless there is some coupling between the spins. We saw very early in Chapter 2 that quantum information arises from couplings between systems. Now suppose the spins are naturally coupled yet we can still only apply external local unitary control. How much entanglement can we preserve? This question is considerably interesting, because if we could preserve entangled states in the presence of decoherence, even when the ground state was unentangled, we would be making baby steps towards persistent quantum memory.

The short approach to this question would be a detailed analysis of the Lindblad generator of the amplitude damping process. We would need to work in the coherence vector representation and invert the matrix to solve for the optimal open loop controllers. This would be exactly like the calculations in Chapter 5.

The problem with such a scheme is generating the representation of the relaxation process in the coherence vector formalism. As discussed earlier, there is no symmetry in this matrix as the process does not preserve the identity. Nonetheless, it still may be tractable, and could possibly be investigated using common numerical search methods.

If we found a plausible unitary correction procedure for preserving entanglement, testing such a scheme might even be feasible experimentally. Using a temporal labeling scheme as describe in [KCL98], we can prepare an effective pure state in liquid state NMR of the form

$$\rho = (1 - \epsilon)\mathbf{1} + \epsilon|\psi\rangle\langle\psi| \tag{9.1}$$

The perturbation to the maximally mixed state $|\psi\rangle\langle\psi|$ behaves as a pure state and its dynamics can be measured using a standard NMR apparatus. Indeed, all quantum computations to date in liquid state NMR use effective pure states, not real pure states.

Using our effective pure state, we can apply a unitary correction scheme to sustain some density matrix with a large entanglement. In doing so, we will be able to experimentally verify the preservation of quantum information.

9.2 Feedback

All of the work presented in this thesis is open loop control. We never investigate the power of feeding back our measurement processes into our next correction step. While we

have shown that open loop control is useful in its own right, we would like to discuss the potentially interesting avenues we could investigate by using closed loop control.

First consider the ability to perform weak measurements as described in Chapter 6. Lloyd and Slotine have shown that the feedback of such measurements can be used to implement an arbitrary nonlinear Shrödinger equation [LS00]

$$\frac{d\rho}{dt} = -i[H(\rho), \rho] \tag{9.2}$$

Indeed this provides ample motivation for investigating the addition of closed loop control. Perhaps more compelling, if we can perform projective measurements, then we can implement quantum error correcting codes and if our decoherence process is slow enough we can sustain an arbitrary quantum state for an arbitrarily long time.

How to proceed in this direction is unclear. Our initial work in Chapter 7 has been to investigate how to steer a one spin system to its steady state using closed loop estimation of the decoherence parameters, but the stability of such an implementation and its time optimality are far from certain. Nonetheless, applications to spectroscopy without power amplifiers and the implementation of nonlinear dynamics in quantum systems makes the study of feedback an exciting area for future work.

9.3 Final Remarks

The study of how quantum systems return to equilibrium still is an open and daunting problem in physics. Finding intuition on how to construct Kraus operators, generators for the Lindblad equation, or coherence vector differential equations would not only be of interest to the quantum information community, but to all physicists working in the quantum domain.

We have presented a new avenue of thought in the field of open quantum systems. Perhaps the most useful contribution is noting that different types of quantum noise yield to different correction schemes. We noted that dephasing operations, are not only impossible to correct with unitary operations, but are also an overly restrictive view of quantum noise processes. Relaxing processes occur throughout atomic and molecular quantum physics, and are perhaps even more realistic models of quantum noise than pure dephasing operations.

To date, most papers on quantum error correction and decoherence free subspaces focus

on dephasing operations. Decoherence free subspaces do not even exist for a relaxation process as relaxation perturbs all axes of the coherence vector. An interesting piece of future work is an analysis of the performance and behavior of error correction models on dephasing versus relaxation processes.

We have shown unitary correction to be a useful concept in quantum information processing and a useful vehicle for understanding the quantum processes of decoherence and relaxation. Its application to quantum information, nuclear magnetic resonance, and perhaps even imaging are only just emerging.

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