DECOHERENCE, SUPERCONDUCTING QUBITS, AND THE POSSIBILITY OF QUANTUM COMPUTING - DRAFT

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Abstract

Is it possible to implement a fully controllable, unambiguously quantum computer? While most in the field believe that the answer is in the affirmative, uncertainty and skepticism still exist among academics and industry professionals. In particular, decoherence is often spoken of as an insurmountable challenge. This thesis argues that there are no fundamental mathematical or physical properties that would preclude the possibility of implementing a fully controllable quantum computer using superconducting qubits. The proof is in key results from the past 30 years in math, physics and computer science; this thesis is a sketch of these results. It begins with the well known theoretical results that have motivated the field - namely quantum algorithmic speed up and efficient error correction - and continues with an overview of the well developed theory of decoherence, arguing that decoherence has been and can still be significantly reduced. These theoretical results are related to superconducting qubits throughout. The thesis concludes with a summary of recent experimental progress with superconducting qubit circuits.

Preface

This work is a synthesis of well established material from various subfields of quantum computing. Equations, mathematical derivations, and experimental results from published papers and books are carefully referenced. This work was submitted in partial fulfillment of the requirements for the degree of Master of Arts in Philosophical Foundations of Physics at Columbia University.

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Chapter 1

Introduction

The spirit of quantum computing - the motivating questions, fundamental issues, and suggestions for future goals - is contained in Feynman's keynote speech and subsequent paper from the 1981 Conference on Physics and Computation at MIT (*Simulating Physics with computers* [19]). The following is a redaction of this speech.

1.1 Feynman's Speech

What kind of computer can be used to simulate physics? There are the approximate kinds of simulations, which use numerical algorithms based on simplifying assumptions in order to roughly compute the energy of the physical system, or characterize the system dynamics. But what about the *exact* simulation of a physical system? Is there a possibility that a computer will simulate *exactly* what nature does?

There is a worry that not all of the laws of physics can be discretized and encoded for simulation. For example, the laws of physics allow space go down to infinitesimal distances, wavelengths to increase to infinite length, sum terms in infinite order - it would be difficult, if not impossible to simulate these laws on a real, physical computer. However, it is not inconceivable that physicists could discretize space and time (although we are still ways away from this).

Another worry is that the natural laws of physics are reversible, while computer logic is not. In order to simulate a reversible system exactly, wouldn't computer logic need to be reformulated in terms of reversible logic gates? This worry is not of much concern, as it was shown by Charles Bennett, Edward Fredkin and Tommaso Toffoli that computer logic *can* be formulated in terms of reversible logic gates.¹

A more serious problem is posed by quantum mechanics. Quantum mechanics involves probability - and simulating probability is computationally problematic. If a description of a physical system in nature with N variables requires a general function of N variables, and if a computer simulates this by actually computing or storing this function, then doubling the size of nature $(N \rightarrow 2N)$ would require an exponentially explosive growth in the size of the simulating computer. It is therefore impractical (or impossible) to simulate by calculating all the probabilities exactly.

Another approach would be to simulate the probabilities of nature with a computer which is itself probabilistic. It might not give the *exact* result that nature gives - but it will give results with

¹Edward Fredkin and Tommaso Toffoli actually attended the conference; some of the work Feynman is referring to can be found in Toffoli's 1980 book *Reversible Computing* [40]. A more recent book authored by both Edward Fredkin and Toffoli is *Conservative Logic* (2002) [22].

the same probability of nature. And by repeating the probabilistic simulation many times, it will give the frequency of a given final state proportional to the number of times with approximately the same rate. Is this actually possible?

The more interesting question is: why not let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws? What kind of computation could be possible with this "quantum computer?" The implication is that a quantum computer would be able to simulate a quantum system. But the more general implication is that the capabilities of such a computer would be far *greater* than any "classical" computer.

There is a worry that a computer made of quantum components might not be able to simulate all the classes of quantum problems. However, there are many phenomena in field theory that are imitated by phenomena in solid state theory - so maybe there is a set of classes of quantum mechanical systems that are "intersimulatable." For example, maybe maybe finite and discrete quantum mechanical systems could be simulated by a Hamiltonian involving only spin-one-half lattice annihilation, creation, number and identity operators locally coupled to corresponding operators on other space-time points. And finally, maybe there is even a "universal" class that can simulate *every* possible quantum system - a sort of "universal quantum simulator?" Unsurprisingly, these questions still drive the field today.²

1.2 The Golden Age?

On September 2, 2014, Google Research Director of Engineering Hartmut Neven unceremoniously posted the following announcement on the Google Research Blog [2]:

The Quantum Artificial Intelligence team at Google is launching a hardware initiative to design and build new quantum information processors based on superconducting electronics. We are pleased to announce that John Martinis and his team at UC Santa Barbara will join Google in this initiative. John and his group have made great strides in building superconducting quantum electronic components of very high fidelity. He recently was awarded the London Prize recognizing him for his pioneering advances in quantum control and quantum information processing. With an integrated hardware group the Quantum AI team will now be able to implement and test new designs for quantum optimization and inference processors based on recent theoretical insights as well as our learnings from the D-Wave quantum annealing architecture. We will continue to collaborate with D-Wave scientists and to experiment with the Vesuvius machine at NASA Ames which will be upgraded to a 1000 qubit Washington processor.

The announcement was quickly picked up and shared within the academia and industry based quantum computing communities (see the *Tech Crunch* and *Wired* articles, [1] and [3]). There are many research groups attempting to build quantum computers using gate model architecture with qubit hardware ranging from photons to ion traps to NMR; Martinis's group (along with a smattering of other research groups at Yale and elsewhere), is well known in the field for making

²He concluded the speech: "The program that Fredkin is always pushing, about trying to find a computer simulation of physics, seems to me to be an excellent program to follow out. He and I have had wonderful, intense, and interminable arguments, and my argument is always that the real use of it would be with quantum mechanics...And I'm not happy with all the analyses that go with just the classical theory, because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy." [19]

phenomenal progress in the past fifteen years on superconducting qubit systems. And Google isn't the only computer company placing its bets on superconducting qubit hardware - the IBM quantum computing group at IBM research has also focused recent efforts on superconducting qubits as well [13].

The fact that large tech corporations are investing in quantum computing research means that the field has matured significantly. Are real, physical quantum computers possible? Martinis and others, including Google and IBM, clearly believe that the answer is *yes*. If so, how so?

1.3 The Possibility of Quantum Computing

Feynman essentially posed the following three questions (we will tackle the first two):

- 1. Is it possible to build a computer with quantum components?
- 2. Many problems in physics and computer science are computationally inefficient. Can quantum models of computing tackle these problems more efficiently?
- 3. Would such a computer be able to simulate all quantum systems?

Without getting into too much detail, some of the important (and weird) properties of quantum mechanics are "coherent superposition" and "measurement" (we'll ignore "entanglement," or quantum correlation, for now). If we let $|0\rangle$ represent one possible state of a quantum system, and $|1\rangle$ another possible state of a system, the "superposition" of these two states $|0\rangle$ and $|1\rangle$ is *also* a possible state of the quantum system:

$$\alpha \left| 0 \right\rangle + \beta \left| 1 \right\rangle \tag{1.1}$$

where α and β are real or imaginary numbers that satisfy the simple property $|\alpha|^2 + |\beta|^2 = 1$. Quantum measurement occurs when a superposition is *irreversibly* "collapsed" to a single component of superposition components:

$$\alpha |0\rangle + \beta |1\rangle \longrightarrow |0\rangle \quad \text{or} \quad |1\rangle$$

$$(1.2)$$

The probability of either outcome is given by $|\alpha|^2$ for $|0\rangle$ and $|\beta|^2$ for $|1\rangle$. Thus if $|\alpha|^2 = 1/4$ and $|\beta|^2 = 3/4$, then the probability of measuring $|1\rangle$ on the superposition state $\alpha |0\rangle + \beta |1\rangle$ is 75%. A qubit is a quantum system that can be described by the states $|0\rangle$, $|1\rangle$ or any superposition of $|0\rangle$ and $|1\rangle$ as defined by (1.1). If we treat a qubit as a single unit of information, a qubit could encode a value of $|0\rangle$, $|1\rangle$ or any superposition $\alpha |0\rangle + \beta |1\rangle$ of these. Often times, a qubit is described as a unit of information that can magically store both a "0 and 1 simultaneously." While this is one way to describe the mathematical property of "superposition," it is important to remember that measuring the qubit, however, would collapse any superposition and give a probabilistic outcome of $|0\rangle$ or $|1\rangle$.

The combination of two quantum systems, say $|1\rangle$ and $|1\rangle$, is described by the (tensor) product $|1\rangle \otimes |1\rangle$, which is often abbreviated to $|1\rangle|1\rangle$ or $|11\rangle$. If each of the two quantum systems is in superposition, say the superposition (1.1), the entire two-system ensemble can be described by:

$$(\alpha |0\rangle + \beta |1\rangle) \otimes (\alpha |0\rangle + \beta |1\rangle) \tag{1.3}$$

This could represent a two qubit ensemble. If we multiply this out, we get:

$$= \alpha |0\rangle \otimes (\alpha |0\rangle + \beta |1\rangle) + \beta |1\rangle \otimes (\alpha |0\rangle + \beta |1\rangle)$$

$$(1.4)$$

$$= \alpha^{2} |0\rangle |0\rangle + \alpha\beta |0\rangle |1\rangle + \beta\alpha |1\rangle |0\rangle + \beta^{2} |1\rangle |1\rangle$$
(1.5)

The first thing to note is that two qubits in superposition can encode four possible units of information - 00,01,10 and 11. Three qubits in superposition can encode $2^3 = 8$ possible bits of information - 000,001,010,100,011,101,110 and 111. It follows that N qubits can encode 2^N bits of information, which is a big deal. 500 qubits can encode 2^{500} bits of information (which is roughly on the order of 10^{150} bits). This is enormous compared to a Terabyte -which is a measly 8×10^{12} bits. Given this property of quantum bits, one might expect stellar computational parallelism!

Before getting too excited about this, however, it is important to remember the next rule of quantum mechanics - Born's rule of probabilistic outcomes. That is, when we measure a quantum computer, the result we get is probabilistic - and the probabilities depend on how we prepare and manipulate the qubits. In the above equation, the outcomes are: $|0\rangle |0\rangle$ with probability $|\alpha^2|^2$, $|0\rangle |1\rangle$ and $|1\rangle |0\rangle$ with probabilities $|\alpha\beta|^2$ each, and $|1\rangle |1\rangle$ with probability $|\beta^2|^2$. For $\alpha \gg \beta$, the most likely outcome of measurement is $|0\rangle |0\rangle$. If α and β are equal and normalized to $\alpha, \beta = 1/\sqrt{2}$, then each of the four outcomes have equal measurement probability of 1/4. The outcome, of course, is a 2-bit number.

The unfortunate reality is that even if we could prepare and manipulate 500 qubits (2^{500} bits) , we would only be able to read *one* of those 500-qubit vectors after measurement, in the form of a 500-bit number. If all the qubits were prepared in an equal superposition of $1/\sqrt{2}(|0\rangle + |1\rangle)$, then the probability of measuring any one of the unique 2^{500} bit combinations would be $1/2^{500}$, a miniscule number indeed. And so if we cared about the outcome of *one* of those, but not the rest, we would have to somehow skew the probabilities of the measurement outcome such that we would get the desired value with a sufficiently high probability $(1/2^{500} \text{ is not particularly good - a probability of } 1/2 \text{ would be much better})$. This was and still is one of the main challenges of quantum computing.

The early goals of quantum computing were to *map* the language of quantum mechanics to the language of computing, and then to *tease* out the special properties of this new kind of computing. This would take advantage of some of the unique properties of quantum mechanics such as quantum superposition, entanglement and coherence to perform certain algorithms more efficiently - or more "interestingly," at the least. Deutsch's various problems were stabs at this - they were a series of short "proof of principle" algorithms that inspired the field. Then came along two important algorithms in 1994 and 1996 called *Shor's algorithm* for number factorization, and *Grover's algorithm* for "unsorted database search." These two algorithms have many practical applications, and have been the main motivation for building quantum computers [39], [25].

When Shor's algorithm and Grover's algorithm were first created, they did not take into account the serious problems posed by quantum error. The worry was that the unique computational speed-up provided by these algorithms would be lost with the necessary incorporation of error correction schemes. In the years that followed, a handful of quantum error correction schemes as well as threshold theorems were proposed, and the general consensus among physicists and computer scientists alike was that *provided* the physical error rates of individual qubits and gates were *below* a certain threshold, Shor's and Grover's algorithms could be implemented with quantum error correction schemes and still maintain algorithmic speed-up.

A growing group of physicists believe that it is indeed possible to *physically build* a quantum computer using superconducting Josephson junctions, or "superconducting qubits." How would this be possible? Unlike quantum algorithms, there wasn't much progress in quantum computing experiments until the past two decades. Superconducting qubits, for example, weren't even seriously

considered viable qubit-like systems until the early 2000s. The idea of a superconducting qubit is to create a quantum system that behaved mathematically, like a 2-state quantum system. The energy ground state of the system could represent $|0\rangle$ and the excited state could represent $|1\rangle$. If it behaved quantum mechanically, it could be in a superposition as well.

In addition to having these properties, the superconducting system would have to be *addressable* - that is, we would have to be able to control it, initialize it, manipulate it with logic gates, and measure it - while it maintained its quantum properties of entanglement and superposition. This was in fact possible with superconducting qubits; at their core, they consist of a Josephson junction (a thin barrier between two superconductors) that at low temperatures allows for tunneling. Interestingly, the current (or the flux) can behave like a quantum variable and form coherent superpositions. The superconducting Josephson junctions could be cleverly arranged to become two level systems, and these two level systems could in turn be tuned and controlled simply changing the current frequency and phase.

There was a looming problem, however, and this was the issue of decoherence. In the early 2000s, these superconducting qubits had *very* fast decoherence times - that is, they did not maintain their quantum behavior for more than a few nanoseconds - not much time to perform algorithms. The real success of these qubits was the dramatic increase in coherence time during the past 15 years - the coherence times have increased by at least five orders of magnitude. This was in no small part due to a good understanding of decoherence theory as well as improvements in materials and fabrication techniques. Today, superconducting qubits are seen as similar or even better than the best qubit technologies (such as trapped ions). Superconducting qubits are also fabricated like classical computer chips - on silicon wafer - and are thus not difficult design and manufacture.

While they claim to be close as of September 2015, Martinis's group has not yet been able to implement the 2D surface code - although he has succeeded in improving coherence times past the surface code threshold [29]. Reaching these thresholds - and maintaining them as the architectures scale - requires understanding the underlying physics in order to improve qubit coherence. But he and most of the scientists in his subfield believe that there are no fundamental limits in sight - and that quantum computers built from superconducting circuits are unambiguously within reach. The skepticism surrounding quantum computing ranges from ignorant to extremely nuanced. This next section discusses some of this skepticism topically - the more rigorous discussion, of course, ensues in the subsequent chapters.

1.3.1 General Skepticism

Those with a rudimentary understanding of quantum mechanics might worry that quantum computers are not feasible simply because the quantum and classical worlds don't mix. Versions of the traditionalist Copenhagen interpretation of quantum mechanics are often taught in undergraduate physics courses; according to these accounts, the "microscopic" world obeys quantum mechanics, and the "macroscopic" world obeys classical mechanics, and never the twain shall meet (this duality is often referred to as Heisenberg's cut). In addition, any sort of human manipulation or intervention is equivalent to a measurement (in the sense described above) and hence collapse. Therefore, it is not possible to "harness" the quantum world - or so the thinking goes.

There is an easy answer to this basic skepticism - a rich, developed theory exists that does a far better job at explaining the quantum-to-classical transition than the early interpretations of quantum mechanics. This is the theory of decoherence developed by H. Dieter Zeh, Anthony Leggett, WojciechZureck and others in the 1970s and 1980s, that explains how quantum particles and systems can effectively lose their quantum coherence simply by being entangled with an "environment" with many degrees of freedom. Although they are not new fundamental axioms of quantum mechanics, the insights of decoherence have been applied to countless theoretical systems and experimental set ups with great success. In this context, measurement can be understood as a "decoherence inducing process," and manipulations can be decoherence inducing or coherence preserving, depending on how they are implemented. We can interact with and take advantage of the quantum world in novel and exciting ways.

The real proof that we can harness the quantum world, however, is with the plethora of physical prototypical systems of qubits, such as photons, ion traps, NMR, and of course superconducting qubits. These systems essentially are qubit systems that can be initialized, logically manipulated, entangled, and measured in most of the ways necessary to implement quantum circuits. Some of these technologies are further ahead than others - superconducting qubits are currently considered one of the most viable technologies, for reasons that will become clear in Chapter 5 (for a general comparison of the pros and cons of the various technologies, see the review article by Ladd et al. *Quantum Computers* (2010) [30]).

Another basic worry, which was an entirely open question at first (but has now been quite elegantly addressed although not completely resolved) has to do with the limitations of computing. As Feynman hinted at in his speech, how can we be sure that a quantum computer - assuming such a contraption could be built - wouldn't just be a souped up machine with the same fundamental limitations as a classical computer? After all, there are a myriad of ways to implement computation; most of them, however, can be fundamentally described by the classical theory of computation. Although we might have reason to believe that a quantum computer would be different, how can this be shown rigorously?

As mentioned above, a quantum computer could theoretically manipulate many more bits of information than a classical computer - that N qubits could encode 2^N bits of information, and that a single quantum timestep could operate on all superpositions/combinations simultaneously. Even today, this "quantum parallelism" is often touted in the media as the panacea to all computing and memory problems. The catch of course - and this was also recognized early on - was that measurement that did not favor any particular outcome can render quantum parallelism useless. Early skeptics did not believe that algorithms could be designed that could overcome this problem in a way that would be as efficient or more efficient as classical computers.

While it was shown in the mid-late 1980s that any classical algorithm could be mapped onto a quantum computer, it was not until the discovery of Shor's algorithm in 1994 and Grover's algorithm in 1996 that it became clear that quantum computers could actually execute particular algorithms *significantly* faster than the most powerful classical computers. While some lament that there has not been much progress in algorithms in the past decade, there is no doubt that quantum computers are in a significant category of their own.

1.3.2 Contemporary Skepticism

A more nuanced - and legitimate - worry, is that error correction is insurmountable. What does this mean exactly? It is conceivable that in order to account for quantum error, elaborate error correction schemes would have to be incorporated such that logical qubits were comprised of many individual qubits, and logical gate operations on these logical qubits were comprised of many individual operations on the individual qubits. One legitimate worry is that the increased cost in number of qubits and the timesteps of operation could be *so great* that it cancels any efficiency gained from the quantum aspect of the computation. The second, more serious worry is that necessary error correction might render quantum algorithms significantly worse than classical algorithms in terms of computation efficiency. In the mid to late 1990s, a few threshold theorems were formulated that allayed these fears, first for uncorrelated (Markovian) errors, and then for various forms of correlated errors. While there are still a few skeptics (usually mathematicians) who argue that correlated errors fundamentally preclude the possibility of efficient quantum computing with error correction, their tone has softened in recent years due to the success of recent experiments.

The final worry has to do with physics. We understand decoherence to a large extent, but how can we be sure that a particular physical implementation of a qubit - whether a trapped ion or a superconducting qubit - does not have some *fundamental physical "decoherence limit.*" Sure it might be possible to improve coherence times - but they cannot improve indefinitely. Where is the limit? And if there *is* a limit, then how do we know that is is above the error correction threshold?

The answer to this question is not so clear. On the one hand, a fully "error corrected" circuit (let alone computer) has not been successfully built yet. On the other hand, coherence times are improving at a dizzying pace, with no real end in site.

Skepticism	Response	Chapter(s)
We can't control the quantum world	Superconducting Qubits, Decoherence	2, 4, 5
Quantum computers are no more efficient than classical computers	Shor and Grover algo- rithms	2
Error correction renders quantum algorithms no bet- ter than classical algorithms	Threshold theorems	3
Coherence cannot be improved enough to make full error correction feasible	Decoherence theory	5, 6

Table 1.1: Skepticism

The foundations of quantum mechanics and quantum computing, as well as Shor's and Grover's algorithms, are covered in **Chapter 2**. **Chapter 3** covers various quantum error correction schemes and various threshold theorems, while **Chapter 4** covers the physics of Josephson junctions and superconducting qubits, including basics of qubit initialization, gate manipulation, and read out. **Chapter 5** discusses the physics models behind the general theory of decoherence, including the spin-boson model and the spin-bath model, and relates them to superconducting qubits. Recent experimental results of interest are discussed in the final chapter. All of the material in this thesis assumes familiarity with quantum mechanics at the level of the well known textbook by Griffiths [24].

There is a real need for the material in this thesis. At the granular level, many fundamental quantum computing references such as the book by Nielsen and Chuang [34] hardly mention superconducting qubits or the surface code for error correction. More generally, however, very few quantum computing resources are written specifically for physicists, and topics such as quantum computing or decoherence are not usually included in undergraduate or graduate physics courses on quantum mechanics. Possibly as a result, very few physics students understand the foundations of quantum computing even though it is simply an extension of the already familiar quantum mechanics. While the narrow purpose of this thesis is to argue that quantum computing is possible, the more general goal of this thesis is to present both the foundations of quantum computing and some of the exciting recent trends in the field in a comprehensive manner.

Chapter 2

Foundations of Quantum Computing

Quantum computing is built on the hallowed principles of quantum mechanics. This chapter begins with a quick, dense review of the mathematical framework of quantum mechanics, motivated by the important question: What exactly are the non-classical features of quantum mechanics? "Superposition," "measurement" and "entanglement" are common parlance in the world of quantum computing, but how exactly are they defined? The next part of the chapter systematically explains how can we use the mathematical framework of quantum mechanics for computation: how to encode information in qubits, what logical manipulations are allowed, and how they fit together to form quantum circuits. Finally, the chapter concludes a brief overview of the great promises of quantum computing - algorithmic speed up. This includes early "proof of principle" algorithms such as the various Deutsch problems, as well as Shor's algorithm and Grover's algorithm.

2.1 Principles of Quantum Mechanics

What is it about quantum systems - and the theory of quantum mechanics - that is so unique? Let's begin with the basic mathematical postulates:

- 1. State Vector: The properties of a quantum system are completely defined by specification of its state vector $|\Psi\rangle$. The state vector is an element of a complex Hilbert space \mathcal{H} called the space of states.¹
- 2. **Observables:** With every physical property \mathcal{O} (energy, position, momentum, angular momentum, etc.) there exists an associated linear, Hermitian² operator \hat{O} (usually called an observable), which acts in the space of states. The eigenvalues of the operator are the possible values of the physical properties.
- 3. Born rule: If $|\psi\rangle$ is the vector representing the state of a system and if $|\phi\rangle$ represents another physical state, there exists a probability of finding $|\psi\rangle$ in state $|\phi\rangle$, which is given by the squared

¹Remember that the mathematical concept of a Hilbert space generalizes the notion of Euclidean space by extending the methods of vector algebra and calculus from the two-dimensional Euclidean plane and three-dimensional space to spaces with any finite or infinite number of dimensions. It is an abstract vector space with the structure of an inner product that allows length and angle to be measured

²A Hermitian matrix is a square matrix with complex entries that is equal to its own conjugate transpose. If the conjugate transpose of a matrix A is denoted by A^{\dagger} , then the Hermitian property can be expressed as $A = A^{\dagger}$.

modulus of the scalar product on \mathcal{H} : $|\langle \psi | \phi \rangle|^2$. If \hat{O} is an observable with eigenvalues λ_k and eigenvectors $|k\rangle$ such that $\hat{O} |k\rangle = \lambda_k |k\rangle$, the probability of obtaining λ_k as the outcome of the measurement \hat{O} is $|\langle k | \psi \rangle|^2$. After the measurement the state is left in the state projected on the subspace of the eigenvalue.

4. Unitary Evolution: The evolution of a closed system is unitary.³ The state vector $|\psi(t)\rangle$ at time t is derived from the state vector $|\psi(t_0)\rangle$ at time t_0 by applying unitary operator $\hat{U}(t, t_0)$ called the *evolution operator*.

How are superposition, entanglement, measurement and decoherence embedded in these postulates?

2.1.1 The Schrodinger Equation

The Schrodinger equation is a partial differential equation that describes how a quantum state of a physical system changes with time

$$\hat{H}\Psi(r,t) = i\hbar \frac{d}{dt}\Psi(r,t)$$
(2.1)

 \hat{H} is the Hamiltonian, which in most cases characterizes the total energy of the any given wavefunction. If \hat{H} is time independent, then the solution has the following form

$$\Psi(r,t) = e^{-i\hat{H}t/\hbar}\Psi(r,t), \quad \hat{U}(t) = e^{-i\hat{H}t}$$
(2.2)

where $\hat{U}(t)$ is the *evolution operator*. This simple evolution operator will come up again and again both in the context of applying gates to qubits and the various decoherence models). The familiar time independent formulation has the following structure for a single, non-relativistic particle:

$$E\Psi = \hat{H}\Psi, \text{ and } E\Psi(r) = \left[-\frac{\hbar}{2\mu}\nabla^2 + V(r)\right]\Psi(r)$$
 (2.3)

(although this will not come up much in the context of quantum computing). While the overall *form* of the Schrodinger equation was not particularly surprising when it was first formulated - as it was originally motivated by the classical wave equation - it does lead to some unusual and experimentally verified predictions such as the quantization of energy levels and the quantization of angular momentum (position, time and momentum are not quantized, however).

2.1.2 "Coherent" Superposition

Superposition lies at the heart of quantum mechanics. Superposition is the property linear combinations of quantum states, represented by vectors in Hilbert space, are also quantum states. For example, if $|\psi_1\rangle$ is a quantum state, and $|\psi_2\rangle$ is a quantum state, then

$$|\Psi\rangle = \sum_{n} c_n |\psi_n\rangle \tag{2.4}$$

is also a quantum state. Similarly, if we start off with a spin-1/2 "spin up" state $|\uparrow\rangle$ in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis, according to the superposition principle the state $|\Xi\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$ is also a quantum state.

³A matrix U is unitary if $U^{\dagger}U = UU^{\dagger} = I$. The importance of this to quantum logic is discussed in the following section.

The double slit experiment is a well known experimental verification of superposition. Electrons are directed towards two slits, and produce an interference pattern on a distant screen, which is really just a measure of spatial variation of density pattern with distribution $\rho(x)$ of particles. If each electron that passed through either one of the slits was simply either in the $|\psi_1(x)\rangle$ state or the $|\psi_2(x)\rangle$ state, then the distribution of electron buildup on the screen over time would be

$$\varrho(x) \propto |\psi_1(x)|^2 + |\psi_2(x)|^2$$
(2.5)

However, the classic result is

$$\varrho(x) = \frac{1}{2}|\psi_1(x) + \psi_2(x)|^2 = \frac{1}{2}|\psi_1(x)|^2 + \frac{1}{2}|\psi_2(x)|^2 + \operatorname{Re}\{\psi_1(x)\psi_2^*(x)\}$$
(2.6)

where the last term is responsible for the characteristic interference pattern on the screen. This shows that the particles cannot be described as one and only one of the wavefunctions $|\psi_1(x)\rangle$ or $|\psi_2(x)\rangle$, but must be described instead as a superposition of these wave functions $|\Psi(x)\rangle = (|\psi_1(x)\rangle + |\psi_2(x)\rangle)/\sqrt{2}$. The poing its that we must be careful to emphasize a state that is a superposition of other states does not simply represent a classical probabilistic ensemble of components where the system really "is" just one of the components, but we do not know which one. It is a new physical state of an individual system and not just a statistical distribution of component states.

Unitarity is an important element of quantum mechanics - as we stated above, the operator which describes the progress of a physical system in time must be a unitary operator. Why is this so? Unitarity is essentially a restriction on the allowed evolution of quantum systems that ensures that the sum of all possible outcomes is 1 (the Born rule). Unitarity is defined as

$$U^{\dagger}U = UU^{\dagger} = I \tag{2.7}$$

We can show how unitarity maintains the Born rule with the following sketch: since the probability is the square of the amplitude, it can be obtained as the inner products of vectors. The probability amplitude of $|X\rangle$, $|Y\rangle$ at initial time t, is $\langle X|Y\rangle$, and the probability amplitude of $|X'\rangle$, $|Y'\rangle$ at time time t' is $\langle X'|Y'\rangle$. In order for these probability amplitudes to remain the same (assuming measurement has not occurred), the time evolution operator must have the property that

$$\hat{U}|X\rangle = |X'\rangle, \quad \hat{U}|Y\rangle = |Y'\rangle \longrightarrow \langle X|Y\rangle = \langle X'|Y'\rangle = \langle X|\hat{U}^{\dagger}\hat{U}|Y\rangle$$
(2.8)

and hence, any evolution of a quantum system must be unitary. The importance of this for quantum computing cannot be understated: *if we wish to implement algorithms that maintain the quantum properties of qubits such as superposition, the operations we apply must be unitary.*

2.1.3 Measurement and the Quantum-to-Classical Transition

The Measurement Problem is the problem of how or whether the wavefunction collapses during an observation. The wavefunction evolves deterministically according to the Schrodinger equation as a linear superposition of orthogonal states, but actual measurements always find that the physical system is in one of the states. It is a very strange thing, really.

How does measurement occur? One early way of understanding measurement is by postulating a duality between quantum and classical worlds, famously known as **Heisenberg's cut**. Below the cut everything is governed by quantum mechanics of the wave function, and above the cut everything can be described classically. Since observation and measurement are in the classical regime (i.e. they require macroscopic observers with macroscopic forces), any interaction with the microscopic, quantum world would immediately induce collapse of the wavefunction. This is part of the Orthodox, or Copenhagen interpretation, and is problematic for multiple reasons (both physical and philosophical - see Chapter 8 of Schlosshauer [37] for a more extensive discussion).

The process of measurement is better described in terms of **von Neumann collapse** (which is the ancestor to decoherence theory). Von Neumann attempted to describe quantum measurement entirely in quantum terms as an interaction between a measured system and a measuring apparatus (which could be large or small, conscious or unconscious). The basic schematic is as follows. If the measurement apparatus starts out in the "ready" state $|a_r\rangle$ and the system to be measured is in the $|a_1\rangle$ state, after the measurement interaction the combined system is described as

$$|s_i\rangle |a_r\rangle \to |s_i\rangle |a_i\rangle \tag{2.9}$$

where the measurement has established a one-to-one correspondence between the state of the system and the state of the apparatus. In this scheme, the measurement has not altered the state of the system, and no entanglement has occurred thus far.

However, if the initial system-to-be-measured is in a superposition, then the linearity of the Schrodinger equation implies that the system apparatus combined will evolve according to:

$$|\psi\rangle |a_r\rangle = \left(\sum_i c_i |s_i\rangle\right) |a_r\rangle \to |\Psi\rangle = \sum_i c_i |s_i\rangle |a_i\rangle$$
(2.10)

This of course leaves the apparatus in an entangled, superimposed state. As Schlosshauer writes, "we can no longer attribute an individual state vector to the system or the apparatus."⁴ Entanglement has occurred, and it has occurred at the macroscopic level if the apparatus is macroscopic. This unitary evolution is referred to as premeasurement. So what happens next? According to von Neumann, there are two possibilities: (1) the system can either remain entangled, or (2) collapse of the wavefunction can occur. This second option is referred to as strong measurement.

The measurement problem still holds, however. How does "strong measurement" actually occur? In this vein, Schrodinger's cat was a thought experiment devised by Schrodinger in 1936 in order to highlight the weirdness of quantum mechanics at the macroscopic level - and the problem of how probabilities are converted to well-defined outcomes. Various interpretative frameworks were developed, such as Hugh Everett's **many-worlds interpretation**, De Broglie-Bohm theory of **Bohmian mechanics**, objective collapse models such as **GRW collapse**, and others to resolve this issue. The literature on these interpretations is vast; see David Albert's *Quantum Mechanics and Experience* [5] for a simple introduction to the measurement problem, David Wallace's book *The Emergent Multiverse* [41] for a rigorous explanation of the many-worlds interpretation, Roland Omnes's Interpretation of Quantum Mechanics [36] and Maximillian Schlosshauer's Decoherence and the Quantum-to-Classical Transition [37] for rigorous explanations of the measurement problem and how it relates to decoherence theory.

2.1.4 Decoherence

Our view of entanglement and collapse of the wave function has changed slightly since the 1930s and 1940s. Quantum effects have been observed in the lab in the mesoscopic (i.e. decidedly larger than microscopic) domain. In addition, it was realized that discussing and modeling quantum systems as *isolated* systems was not valid in many instances. The implicit assumption that we could always shield our systems from unwanted environmental disturbances was simply obscuring certain aspects of quantum theory. In the 1970s and 1980s, new research efforts began treating quantum systems as open systems - with *a lot* of success in the area of quantum optics. It was also realized that the

⁴The von Neumann scheme for ideal quantum measurement is described extensively in Schlosshauer pp. 50-53 [37].

"isolated system" assumption had in fact been a crucial obstacle to understanding the quantum-toclassical transition. Theorists such as H. Dieter Zeh and E. Joos were able to show that the openness of quantum systems could actually *explain* how quantum systems lose some of their superposition components (more on this in subsequent chapters).

It is worth mentioning in the context of decoherence and measurement that most devices capable of detecting a single particle and measuring its position strongly modify the particle's state in the measurement process (e.g. photons are destroyed when striking a screen). Less dramatically, the measurement may simply perturb the particle in an unpredictable way; a second measurement, no matter how quickly after the first, is then not guaranteed to find the particle in the same location.

However it is possible to measure a system (and collapse it if it is in a superposition) twice (or more) without changing the value of the measured system. This is a **Quantum Nondemoli**tion (QND) measurement, and it is used frequently in physical qubit systems. Note that the term "nondemolition" does not imply that the wave function fails to collapse.

2.1.5 Spin

For completeness, we state here that a "spin" S is a discrete degree of freedom that transforms like angular momentum under rotations and corresponds to an observable describing the spin of a spin 1/2 particle, in each of the three spatial directions. It is a uniquely quantum object with a finite state space. The Pauli spin matrices are set of three 2×2 complex matrices that are unitary, and they feature significantly in the quantum computing formalism.

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(2.11)

For a spin 1/2 particle, the spin operator is given by $\hat{S}_i = \frac{\hbar}{2}\hat{\sigma}_i$. A spin Hamiltonian (almost always) consists of a sum of one-spin and two-spin terms. This is very analogous to the Hamiltonian of a particle system, where one has one-body terms (an external potential) plus two-body terms (particle-particle interactions). For example, a general spin Hamiltonian can be be composed of a magnetic field coupling $\mathcal{H}_B = -\hat{H}_B \sum g_i \mu_B \hat{S}_i$ where \hat{H}_B is the magnetic field, and an exchange interaction (sometimes called Heisenberg Exchange Hamiltonian) $\mathcal{H}_{ex} = -\sum_{i,j} J_{ij} \hat{S}_i \cdot \hat{S}_j$. In a crystal, generalization of the Heisenberg Hamiltonian in which the sum is taken over the exchange Hamiltonians for all the (i, j) pairs of atoms of the many-electron system gives:

$$\mathcal{H}_{Heis} = \frac{1}{2} \left(-2J \sum_{i,j} \hat{S}_i \cdot \hat{S}_j \right) = -\sum_{i,j} J \hat{S}_i \cdot \hat{S}_j \tag{2.12}$$

We will see a similar Hamiltonian used for spin-bath coupling decoherence models in Chapters 5 and 6. Unsurprisingly, two level quantum systems can be described using the spin operator formalism. Since information is traditionally encoded in 0s and 1s, it makes sense to describe the quantum bit as a binary system as well i.e. a two dimensional complex Hilbert space with orthonormal bases $\{|0\rangle, |1\rangle\}$.

For completeness, we mention here that the Bloch sphere is a useful visualization of pure state of a two level quantum system.

$$|\Psi\rangle = e^{i\gamma} \left(\cos(\frac{\theta}{2})|0\rangle + e^{i\phi}\sin(\frac{\theta}{2})|1\rangle\right)$$
(2.13)



Figure 2.1: Bloch Sphere

where γ, θ and ϕ are real numbers. Typically $e^{i\gamma}$ is omitted, as it is not observable in most scenarios. We will reference the Bloch sphere frequently.

2.1.6 Entanglement

One of the most fascinating, disturbing and revolutionary, non-classical elements of quantum mechanics is entanglement. An entangled system is defined as a composite state of two or more systems which cannot be written as a tensor product of the original component systems. It can be understood as arising from the superposition principle combined with the linearity of the Schrodinger time evolution. For example, the Bell states are four maximally entangled states:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$
 (2.14)

$$|\Phi^{-}\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \tag{2.15}$$

$$|\Psi^{+}\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$
 (2.16)

$$|\Psi^{-}\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$
 (2.17)

It is easy to check that we cannot write these Bell states as tensor products of two individual states in the $\{|0\rangle, |1\rangle\}$ basis (e.g. $|\Phi^+\rangle \neq |\psi_1\rangle \otimes |\psi_2\rangle$ where $|\psi_i\rangle = \alpha|0\rangle + \beta|1\rangle$). But what does entanglement mean, and how are quantum correlations different from classical correlations? We say that there is a measurement correlation between quantum systems. However in classical systems, we often come across correlations due to conservation laws. If an object at rest splits into two equal fragments, and we measure the momentum of one of the fragments we can infer (immediately) the momentum of the other fragment due to conservation of momentum. In the case of an entangled system, when we measure one of the particles/subsystems, the quantum correlations are "transformed" into classical (purely statistical) correlations. However, the outcome of the first measurement is random - we have no way of predicting with 100% accuracy which particular outcome will be obtained. It would appear...that after the first measurement, the outcome is "instantaneously" transmitted to the other particle, which may be separated by an arbitrary distance. While this was originally considered a troubling aspect of the theory of quantum mechanics (see the famous 1935 "EPR" paper *Can quantum mechanical description of physical reality be considered complete?* by Einstein, Podolsky and Rosen [18]), entanglement is now considered an indisputable part of quantum mechanics. John Bell's book *Speakable and Unspeakable in Quantum Mechanics* [9] contains a more extensive discussion on entanglement and the role it plays in our current understanding of quantum mechanics.

The maximally entangled Greenberger-Horne-Zeilinger (GHZ) state is simply an extension of the Bell $|\Psi^+\rangle$ state for N > 2 qubits:

$$|GHZ\rangle = \frac{|0\rangle^{\otimes N} + |1\rangle^{\otimes N}}{\sqrt{2}}$$
(2.18)

where $|0\rangle^{\otimes N}$ is the N-tensor product. For example, the simplest entangled state N = 3 is:

$$|GHZ\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}}$$

As we shall see later, many experiments (e.g. [8] and [29]) create and maintain GHZ states as a measure of how well their hardwares can entangle their qubits. This is particularly important because by various measures of entanglement (there is no standard measure), the GHZ is considered maximally entangled.⁵ If one of the qubits is measured (as either 0 or 1), however, the states are no longer entangled. In contrast, the W state is defined as:

$$|W\rangle = \frac{1}{\sqrt{N}} (|100..0\rangle + |010...0\rangle + ... + |00...01\rangle)$$
(2.19)

and has multiparticle entanglement such that when one qubit is measured, the remaining qubits are still entangled.

2.2 Quantum Computing Basics: The Quantum Circuit Model

It was once thought that logic gates were fundamentally irreversible. Theoretical research in the area of reversible computing established that the irreversible logic of classical computers could be reformulated in terms of reversible gates (one-to-one maps of input and output). Since quantum evolutions are unitary, reversible logic is the paradigm of choice for quantum computing. Standard quantum computing theory begins with the definition of the primary units of information - qubits - orthogonal states in a two level quantum system. We define these two component vectors in the $\{|0\rangle, |1\rangle\}$ basis as

$$|0\rangle = \begin{bmatrix} 1\\0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0\\1 \end{bmatrix}$$
(2.20)

It is also common to use the $\{|+\rangle, |-\rangle\}$ basis

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\1 \end{bmatrix}$$
(2.21)

⁵Interestingly, it wasn't explicitly studied until 1989 by Daniel Greenberg, Michael Horne and Aaron Zeilinger in *Going Beyond Bell's Theorem* [23].



Figure 2.2: Classical Computing Logic Gates (Irreversible)

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\ -1 \end{bmatrix}$$
(2.22)

We define the tensor product of two qubits as:

$$|0\rangle \otimes |0\rangle = |00\rangle = \begin{bmatrix} 1\\0 \end{bmatrix} \otimes \begin{bmatrix} 1\\0 \end{bmatrix} = \begin{bmatrix} 1 \times \begin{bmatrix} 1\\0\\0\\1\\0 \end{bmatrix} = \begin{bmatrix} 1\\0\\0\\0 \end{bmatrix}$$
$$|01\rangle = \begin{bmatrix} 0\\1\\0\\0 \end{bmatrix}, \quad |10\rangle = \begin{bmatrix} 0\\0\\1\\0 \end{bmatrix}, \quad |11\rangle = \begin{bmatrix} 0\\0\\0\\1 \end{bmatrix}$$

The tensor product of 3 qubits gives vectors of length $2^3 = 8$, and so on (we can see that the Dirac bra-ket notation makes dealing with the tensor product of many qubits less cumbersome than vector notation).

2.2.1 Qubit Manipulations and Gates

The natural choice of unitary transformations to use for two level quantum systems are:

$$\mathbf{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{Y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \mathbf{Z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
(2.23)

which are the same matrices as the Pauli σ matrices mentioned above. Interpreted in the context of logic operations, the Pauli-X is simply a NOT gate

$$\mathbf{X} |0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle, \quad \mathbf{X} |1\rangle \rightarrow |0\rangle$$

as it flips the state $|0\rangle$ to $|1\rangle$ and the state $|1\rangle$ to $|0\rangle$. The Z-gate has no classical analogy, as it rotates $|1\rangle$ to $-|1\rangle$ but does nothing to $|0\rangle$:

$$\mathbf{Z} |1\rangle = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \rightarrow -\begin{bmatrix} 0 \\ 1 \end{bmatrix} = -|1\rangle$$

Gates can also be applied one after another.⁶

While the above gates are the most obvious operators to introduce into the quantum circuit model, there are three more important single qubit gates that play a role in the quantum algorithms to come. These gates are the Hadamard gate H, the phase gate S, and the shift gate T (also called the $\pi/8$ -gate).

$$\mathbf{H} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1\\ 1 & -1 \end{bmatrix}$$
(2.24)

$$\mathbf{S} = \begin{bmatrix} 1 & 0\\ 0 & i \end{bmatrix} \tag{2.25}$$

$$\mathbf{T} = e^{i\pi/8} \begin{bmatrix} e^{-i\pi/8} & 0\\ 0 & e^{i\pi/8} \end{bmatrix} = \begin{bmatrix} 1 & 0\\ 0 & e^{i\pi/4} \end{bmatrix}$$
(2.26)

The Hadamard gate has the important property of putting the $|0\rangle$ and $|1\rangle$ states in superpositions. This is equivalent to switching from the $\{|0\rangle, |1\rangle\}$ basis to the $\{|+\rangle, |-\rangle\}$ basis:

$$\mathbf{H} | 0 \rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) = |+\rangle, \quad \mathbf{H} |1\rangle = |-\rangle$$
$$\mathbf{H} |-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 \\ 2 \end{bmatrix} = |1\rangle, \quad \mathbf{H} |+\rangle = |0\rangle$$

Pauli spin matrices exponentiated⁷ give rise to three useful classes of unitary matrices called *rotation*

$$\begin{aligned} \mathbf{X}\mathbf{Z} \left| 0 \right\rangle &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \left| 1 \right\rangle \\ \mathbf{Z}\mathbf{X} \left| 0 \right\rangle &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = -\left| 1 \right\rangle \end{aligned}$$

Both of these are distinct from $\mathbf{X} \otimes \mathbf{Z} |0\rangle \otimes |1\rangle = \mathbf{X} |0\rangle \mathbf{Z} |1\rangle$, where $\mathbf{X} \otimes \mathbf{Z}$ is a 2-qubit operator, or a 4×4 matrix. ⁷Note that the function of an operator can be expressed as $f(\hat{A}) = \sum_i f(\lambda_i) |a_i\rangle \langle a_i|$, where λ_i is an eigenvalue and $|a_i\rangle$ is an eigenvector. Since the eigenvectors of \mathbf{Z} are $|0\rangle$ and $|1\rangle$ with eigenvalues 1 and -1, we can write $e^{-i\theta \mathbf{Z}/2} = e^{-i\theta(1)/2} |0\rangle \langle 0| + e^{-i\theta(-1)/2} |1\rangle \langle 1| = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}$

 $^{^{6}\}mathrm{These}$ matrices are operators, and order matters. Conventionally, the rightmost operator is applied first, such that:

Gate	Notation	Matrix				
NOT (Pauli-X)	- <u>X</u> -	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$				
Pauli-Z	- <u>Z</u> -	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$				
Hadamard	-H	$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1\\ 1 & -1 \end{bmatrix}$				
CNOT (Controlled NOT)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$				

Figure 2.3: Quantum Gates

operators:⁸

$$R_x(\theta) \equiv e^{-i\theta \mathbf{X}/2} = \cos(\frac{\theta}{2}\mathbf{I} - i\sin\frac{\theta}{2}\mathbf{X}) = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$
(2.27)

$$R_y(\theta) \equiv e^{-i\theta \mathbf{Y}/2} = \cos(\frac{\theta}{2}\mathbf{I} - i\sin\frac{\theta}{2}\mathbf{Y}) = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$
(2.28)

$$R_z(\theta) \equiv e^{-i\theta \mathbf{Z}/2} = \cos(\frac{\theta}{2}\mathbf{I} - i\sin\frac{\theta}{2}\mathbf{Z}) = \begin{bmatrix} e^{-i\theta/2} & 0\\ 0 & e^{i\theta/2} \end{bmatrix}$$
(2.29)

For any unitary operation U on a qubit, there exist real numbers α , β , γ , δ such that $U = e^{i\alpha}R_x(\beta)R_z(\gamma)R_x(\delta)$. This generalizes for all non-parallel vectors \hat{m} , \hat{n} such that $U = e^{i\alpha}R_{\hat{n}}(\beta)R_{\hat{m}}(\gamma)R_{\hat{n}}(\delta)$. This is an important result, as it states that any single qubit operation can be decomposed into this form.⁹ This is called the X-Z decomposition for a single qubit.

There are a few notable two-qubit gates, including the Control NOT (CNOT) and SWAP gates:

$$\mathbf{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad \mathbf{SWAP} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

These gates have the following transformations:

$$\begin{array}{ll} \mathbf{CNOT} \left| 00 \right\rangle \rightarrow \left| 00 \right\rangle, \quad \mathbf{CNOT} \left| 01 \right\rangle \rightarrow \left| 01 \right\rangle, \quad \mathbf{CNOT} \left| 10 \right\rangle \rightarrow \left| 11 \right\rangle, \quad \mathbf{CNOT} \left| 11 \right\rangle \rightarrow \left| 10 \right\rangle \\ \mathbf{SWAP} \left| 00 \right\rangle \rightarrow \left| 00 \right\rangle, \quad \mathbf{SWAP} \left| 01 \right\rangle \rightarrow \left| 10 \right\rangle, \quad \mathbf{SWAP} \left| 10 \right\rangle \rightarrow \left| 01 \right\rangle, \quad \mathbf{SWAP} \left| 11 \right\rangle \rightarrow \left| 11 \right\rangle \\ \end{array}$$

 CNOT is particularly important, as any unitary transformation on n qubits can be decomposed into

⁸Nielsen and Chuang, pp. 174-175 [34]

⁹The following corollary can be used to build multi-qubit unitary operations. For a single qubit unitary gate, there exist single qubit operators A,B,C such that ABC = I and $U = e^{i\alpha}AXBXC$ where α is an overall phase factor.

a sequence of CNOT and single qubit gates.

The Toffoli gate, also known as CCNOT, is a 3-qubit gate that flips the third qubit if the first two qubits are $|1\rangle$:

$$CCNOT = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Since the state space of a 3-qubit vector has length 2^3 , 3-qubit gates are 8×8 matrices.

The Fredkin gate (also known as CSWAP, or controlled SWAP) is a reversible three-qubit gate that swaps the last two qubits if the first qubit is $|1\rangle$:

	[1	0	0	0	0	0	0	0
	0	1	0	0	0	0	0	0
	0	0	1	0	0	0	0	0
CCWAD	0	0	0	1	0	0	0	0
CSWAP =	0	0	0	0	1	0	0	0
	0	0	0	0	0	0	1	0
	0	0	0	0	0	1	0	0
	0	0	0	0	0	0	0	1

Note that the majority of these gates (e.g. Fredkin and Toffoli gates) were formulated in the context of reversible computing, which preceded the quantum circuit model formalism. The notation for quantum gates was developed by Adriano Barenco, Charles Bennett, Richard Cleve, David DiVincenzo, Peter Shor and others. See *Elementary Gates for Quantum Computation* by Barenco et al. [6] for a more extensive discussion on one and two-qubit gates.

A universal set of gates is a finite set of gates which, when combined, can model any arbitrary operation. In classical computing, the set of AND and NOT gates is universal. In reversible (classical) computing, the 3-qubit Toffoli gate is a universal reversible logic gate, as any reversible circuit can be constructed from it. In quantum computing, the set of Toffoli/CCNOT (3 qubit) is universal, as various combinations of CCNOT can model all of the aforementioned one, two and three-qubit gates. The set of CNOT (two-qubit), H (one-qubit) and T (one-qubit) is also universal for the same reason.

2.2.2 No Cloning Theorem

There is an interesting and important result, called the "no cloning theorem," which states that it is impossible to create an identical copy of an *arbitrary* unknown quantum state.¹⁰ We can easily show this mathematically. Let's assume that there exists a unitary "copier" operator \hat{C} that somehow copies the state $|\phi\rangle$ onto the state $|e\rangle$ in the following way:

$$\hat{C}|\phi\rangle_A|e\rangle_B = |\phi\rangle_A|\phi\rangle_B \tag{2.30}$$

 $^{^{10}}$ William Wootters and Wojciech Zurek were the first to point this out explicitly in their 1982 paper A single quantum cannot be cloned [42].

for all possible states $|\phi\rangle$ in the state space. It must be unitary if it is a non-measurement, time evolution on the state. This seems fine; however, if we select an arbitrary pair of states $|\phi\rangle_A$ and $|\psi\rangle_A$ and try to copy them we run into trouble. Because \hat{C} is unitary, it preserves the inner product, so the inner product after the copier is applied must remain the same:

$$\langle e|_B \langle \phi|_A |\psi\rangle_A |e\rangle_B = \langle e|_B \langle \phi|_A \hat{C}^{\dagger} \hat{C} |\psi\rangle_A |e\rangle_B = \langle \phi|_B \langle \phi|_A |\psi\rangle_A |\psi\rangle_B, \qquad (2.31)$$

Equating the left hand side and right hand sides

$$\langle \phi | \psi \rangle_A \langle e | e \rangle_B = \langle \phi | \psi \rangle_A = \langle \phi | \psi \rangle_{AB}^2$$

This implies that either $\langle \phi | \psi \rangle = 1$ or $\langle \phi | \psi \rangle = 0$, so we obtain either $\phi = \psi$ or ϕ and ψ are orthogonal. However, this cannot be the case for two arbitrary states (e.g. $\phi = \frac{1}{2} |0\rangle + \frac{\sqrt{3}}{2} |1\rangle$ and $\phi = \frac{1}{\sqrt{2}} |0\rangle + \frac{1}{\sqrt{2}} |1\rangle$ whose inner product is equal to $\frac{1+\sqrt{3}}{2\sqrt{2}}$). Therefore a single universal gate \hat{C} cannot clone a *general* quantum state. However, a copier could clone equal or orthogonal states.

The implications of the no cloning theorem for quantum algorithms and quantum error correction are important. Let's say we manipulate some qubits as part of a routine (i.e. as part of a general quantum algorithm or as part of a an error correction protocol), and want to duplicate the results of this routine without measurement in order to proceed to the next part of the algorithm. The no cloning theorem states that this is simply not possible.

2.3 Early Quantum Algorithms

Thus far we have not discussed any algorithms that take advantage of the unique properties of quantum systems described at the beginning of the chapter. The grand vision of quantum computing is for there to be a class of algorithms comprising of many unitary operations run repeatedly with correct (or desired) answers represented by the distribution of probabilistic outcomes. The theory of reversible computation had already established that *classical* computation could be achieved with reversible gates, albeit without speed up. The algorithms described below are simple "proof of principle" algorithms designed to highlight the *possible speed up* due to the properties of quantum mechanics. The following sections roughly follow the format of David Deutsch's seminal 1985 paper *Quantum theory, the Church-Turing principle and the universal quantum computer* [15].

Quantum Parallelism: We are interested in constructing a circuit whose input is x and whose output is f(x) with probability 1, while also computing f(x) more efficiently than a classical circuit. A single qubit $|x\rangle$ has two possible values, $|0\rangle$ and $|1\rangle$. The possible values of the function are $|f(x)\rangle = |0\rangle$ or $|f(x)\rangle = |1\rangle$. The Fredkin gate transforms two qubits in the following way:

$$|x\rangle|y\rangle \rightarrow |x\rangle|y \oplus f(x)\rangle$$

Where $|x\rangle|y\rangle$ is a suitable input observable, \oplus is addition modulo 2, and $|x\rangle|y\oplus f(x)\rangle$ is a suitable output observable. Note that the third input f(x) is hardwired into the circuit (this is one of the properties of Fredkin gates). If the second qubit is set to $|y\rangle = |0\rangle$, then the transformation carried out by the Fredkin gate is:

$$|x\rangle|0\rangle \to |x\rangle|0 \oplus f(x)\rangle = |x\rangle|f(x)\rangle \tag{2.32}$$

where we obtain $|f(x)\rangle$ from $|x\rangle$. Note that nothing particularly exciting has happened yet - (2.32) simply takes x and spits out f(x), just like any classical circuit might. However, things change when $|x\rangle$ is in a superposition of two output qubits:

$$|x\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \longrightarrow f\left(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right) = \frac{1}{\sqrt{2}}(|f(0)\rangle + |f(1)\rangle)$$

Already we can see that the Fredkin gate will process information about both $|f(0)\rangle$ and $|f(1)\rangle$. Mathematically this turns into:

$$|x\rangle|0\rangle \to |x\rangle|f(x)\rangle$$
 (2.33)

$$\frac{1}{\sqrt{2}} \Big(|0\rangle + |1\rangle \Big) |0\rangle \to \frac{1}{2} \Big(|0\rangle + |1\rangle \Big) \Big(|f(0)\rangle + |f(1)\rangle \Big)$$
(2.34)

$$= \frac{1}{2} \Big(|0\rangle |f(0)\rangle + |1\rangle |f(0)\rangle + |0\rangle |f(1)\rangle + |1\rangle |f(1)\rangle \Big)$$
(2.35)

The output therefore contains information both about $|f(0)\rangle$ and $|f(1)\rangle$. This is quantum parallelism, and it can mathematically be extended to *n* qubits.¹¹ Thus quantum parallelism allows us to construct the entire truth table of a quantum gate array with 2^n entries in a single time step.

The trouble, of course, is that when we measure the output, we can only observe one value of (2.33) i.e. one value of the truth table, with probability 1/4. If we repeat the measurement, we are equally as likely to get any of the four table entries. Obtaining all four entries would require at least 4 measurements. This of course would have no advantage over a classical algorithm whatsoever, as a classical algorithm would simply calculate one entry in a single iteration, and all four entries in 4 iterations (maximum). So in order to actually exploit quantum parallelism, clever algorithms need to manipulate the probabilities associated with each value. "Deutsch's Problem" is one such algorithm.

"Deutsch's Problem" (1985): Lets say that a programmer is interested in calculating $f(0) \oplus f(1)$ instead of just f(x). By modular arithmetic:

$$0 \oplus 0 = 0, \quad 0 \oplus 1 = 1, \quad 1 \oplus 0 = 1, \quad 1 \oplus 1 = 0$$

So if f(0) = f(1), then $f(0) \oplus f(1) = 0$, and if $f(0) \neq f(1)$, then $f(0) \oplus f(1) = 1$. Classically, calculating $f(0) \oplus f(1)$ requires calculating both f(0) and f(1) with a total time of 2T. A quantum algorithm can reduce that time to T. All we need to do is create the state:

$$\frac{1}{\sqrt{2}} \Big(|0\rangle |f(0)\rangle + |1\rangle |f(1)\rangle \Big)$$
(2.36)

And find the inner product with a new output observable in the following non-degenerate basis:

$$|zero\rangle = |0\rangle|0\rangle - |0\rangle|1\rangle + |1\rangle|0\rangle - |1\rangle|1\rangle$$
(2.37)

$$|one\rangle = |0\rangle|0\rangle - |0\rangle|1\rangle - |1\rangle|0\rangle + |1\rangle|1\rangle$$
(2.38)

$$|fail\rangle = |0\rangle|0\rangle + |0\rangle|1\rangle + |1\rangle|0\rangle + |1\rangle|1\rangle$$
(2.39)

$$|error\rangle = |0\rangle|0\rangle + |0\rangle|1\rangle - |1\rangle|0\rangle - |1\rangle|1\rangle$$
(2.40)

(each pair on the RHS has a normalization coefficient of 1/2). The surprising result is that if the observed value is $|zero\rangle$, then it must be the case that f(0) = f(1), and if the observed value is $|one\rangle$, then it must be the case that $f(0) \neq f(1)$. The probability of measuring a value for $f(0) \oplus f(1)$ (either $|zero\rangle$ or $|one\rangle$) is 1/2, and the probability of not measuring a value (i.e. $|fail\rangle$) is also 1/2.

¹¹See Marinescu pp.205-206 [31] for a simple proof.

Thus the quantum algorithm computes $f(0) \oplus f(1)$ in a single step with a probabilistic success rate of 1/2.

In 1992, David Deutsch and Richard Jozsa improved this idea with a *deterministic* algorithm (generalized to a function which takes n bits input). Unlike Deutsch's Problem, this algorithm required two function evaluations instead of only one. Further improvements to the Deutsch-Jozsa algorithm were made by Richard Cleve and others in *Quantum algorithms revisited* [12] resulting in the *Deutsch-Jozsa Algorithm* that is both deterministic and requires only a single query of f(x). The Deutsch-Jozsa algorithm provided inspiration for Shor's algorithm and Grover's algorithm, which we shall cover later in this chapter. The next algorithm below is a special case of the general Deutsch-Jozsa algorithm.

"Deutsch's Algorithm" (1998): Similar to above, we want to check whether a function is either balanced or constant; i.e. if f(0) = f(1) or $f(0) \neq f(1)$. If $f(0) \oplus f(1) = 0$, then functions are balanced, and if $f(0) \oplus f(1) = 1$, then the functions are constant. We are given a quantum implementation of the function f(x) that maps $|x\rangle |y\rangle$ to $|x\rangle |f(x) \oplus y\rangle$. First apply the Hadamard gate to each qubit

$$\mathbf{H}\mathbf{H}|0\rangle|1\rangle = \mathbf{H}|0\rangle\mathbf{H}|1\rangle \longrightarrow \frac{1}{2}(|0\rangle + |1\rangle)(|0\rangle - |1\rangle)$$
(2.41)

$$= \frac{1}{2} |0\rangle (|0\rangle - |1\rangle) + \frac{1}{2} |1\rangle (|0\rangle - |1\rangle)$$
(2.42)

apply function f(x) via the unitary gate $U_{f(x)}$

$$= \frac{1}{2} |0\rangle (|f(0) \oplus 0\rangle - |f(0) \oplus 1\rangle) + \frac{1}{2} |1\rangle (|f(1) \oplus 0\rangle - |f(1) \oplus 1\rangle)$$
(2.43)

$$= \frac{1}{2} (-1)^{f(0)} |0\rangle (|0\rangle - |1\rangle) + \frac{1}{2} (-1)^{f(1)} |1\rangle (|0\rangle - |1\rangle)$$
(2.44)

$$= (-1)^{f(0)} \frac{1}{2} \left(|0\rangle + (-1)^{f(0) \oplus f(1)} |1\rangle \right) \left(|0\rangle - |1\rangle \right)$$
(2.45)

(this requires some algebra). We ignore the global phase, and apply the Hadamard gate to each qubit:

$$= (-1)^{f(0)} \mathbf{H} \frac{1}{\sqrt{2}} \Big(|0\rangle + (-1)^{f(0) \oplus f(1)} |1\rangle \Big) \mathbf{H} \frac{1}{\sqrt{2}} \Big(|0\rangle - |1\rangle \Big)$$
(2.46)

$$= \frac{1}{2} \Big(|0\rangle + (-1)^{f(0) \oplus f(1)} |0\rangle \Big) |1\rangle + \frac{1}{2} \Big(|1\rangle - (-1)^{f(0) \oplus f(1)} |1\rangle \Big) |1\rangle$$
(2.47)

$$= \frac{1}{2} \left(1 + (-1)^{f(0) \oplus f(1)} \right) |0\rangle |1\rangle + \frac{1}{2} \left(1 - (-1)^{f(0) \oplus f(1)} \right) |1\rangle |1\rangle$$
(2.48)

When the first qubit is measured, if the function is *balanced* the outcome will be $|0\rangle$ with probability 1, and if the function is *constant* the outcome will be $|1\rangle$ with probability 1. This deterministically returns an answer in a single algorithmic iteration. While this algorithm doesn't have many practical purposes, it undoubtedly proves the *possibility* of algorithmic speedup with quantum computers.

2.4 The Quantum Fourier Transform (QFT)

The Quantum Fourier Transform (QFT) is the quantum analogue of the discrete fourier transform, and is an important part of many quantum algorithms including Shor's algorithm. The QFT gate



Figure 2.4: The general Deutsch-Josza algorithm begins with the n + 1 bit state $|0\rangle^{\otimes n}|1\rangle$ and examines the probability of measuring $|0\rangle^{\otimes n}$, $|\frac{1}{2^n}\sum_{x=0}^{2^n-1}(-1)^{f(x)}|^2$ which evaluates to 1 if f(x) is constant and 0 if f(x) is balanced.

acts on quantum state $\sum_{i=0}^{N-1} x_i |i\rangle$ and maps it to a quantum state $\sum_{i=0}^{N-1} y_i |i\rangle$ according to the formula

$$y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j e^{2\pi i j k/N}$$
(2.49)

where ω is often substituted for $e^{2\pi i/N}$. This is possible because the fourier transform is unitary and can be expressed as a unitary matrix F_N

$$F_N = \begin{bmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \dots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \dots & \omega^{2(N-1)} \\ 1 & \omega^3 & \omega^6 & \omega^9 & \dots & \omega^{3(N-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \omega^{3(N-1)} & \dots & \omega^{(N-1)(N-1)} \end{bmatrix}$$

For example, for N = 4, w = i and

$$F_4 = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{bmatrix}$$

The QFT can be implemented simply by a series of Hadamard and rotation gates. See Nielsen and Chuang pp. 216-221 [34] and Marinescu pp. 210-224 [31] for extensive discussions and examples of the Quantum Fourier Transform.



Figure 2.5: Quantum Fourier Transform Circuit for N = 3

2.5 Quantum Phase Estimation

The quantum phase estimation algorithm is a quantum algorithm that finds many applications as a subroutine in other algorithms. The algorithm allows us to estimate the eigenphase θ of an eigenvector $|\psi\rangle$ of a unitary gate U (where $U |\psi\rangle = e^{i\theta} |\psi\rangle$), given access to a quantum state proportional to the eigenvector and a procedure to implement the unitary gate conditionally. Note that the Quantum Fourier Transform is part of the phase estimation algorithm. See Nielsen and Chuang pp. 221-247 [34] for a rigorous treatment of quantum phase estimation and its role in Shor's algorithm.

2.6 Shor's Algorithm

Shor's algorithm is quantum algorithm for integer factorization, formulated in 1994 by Peter Shor [39]. The problem posed is: given a composite integer N, find a factor (any nontrivial factor will do). It is substantially faster than the fastest known classical number factorization algorithm, called the general number field sieve (although it is possible that an unknown faster classical algorithm might exist).¹² Much of the excitement surrounding Shor's algorithm has to do with the possibility that it could be used to break public-key encryption schemes such as RSA, which is based on the assumption that factoring large numbers is computationally intractable.

Shor's algorithm consists of two parts: (1) reducing the factoring problem to the problem of *order-finding* (2) solving the order finding problem with a quantum algorithm, which can be thought of as the quantum phase estimation algorithm in disguise. Scott Aaronson explains the algorithm well without much mathematical formalism; the following sketch is based off his explanation [4]. A more rigorous explanation of Shor's algorithm and the derivation of its computational complexity can be found in Nielsen and Chuang pp. 226-247 [34] and Marinescu pp. 224-247 [31].

As we hinted at previously, an efficient quantum algorithm needs to exploit some structure of the problem in order to "skew" the measurement outcome such that the outcome is probabilistically correct. The integer factorization problem does have some structure - *in fact, it can be reduced to period finding.* What exactly is period finding, then?

We start off by noticing that we can express the powers of 2 as powers of 2 mod 15:

 $2, 4, 8, 16, 32, 64, 128, 256, 512, 1024, \ldots \rightarrow 2, 4, 8, 1, 2, 4, 8, 1, 2, 4, \ldots$

It is clear from this that the powers of 2 mod 15 are periodic. The powers of 2 mod 21 are also periodic: 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024, $\dots \rightarrow 2, 4, 8, 16, 11, 1, 2, 4, 8, 16$, etc. The generalization of this by Euler states that if N is product of two prime number p and q, then the sequence:

$$x \mod N, \quad x^2 \mod N, \quad x^3 \mod N, \quad x^4 \mod N, \quad \dots$$
 (2.50)

will repeat with some period that evenly divides (p-1)(q-1), provided x is not divisible by p or q. It follows that if N = 15, then the prime factors of N are p = 3 and q = 5, so (p-1)(q-1) = 8. And the period of 2 mod 15 is 4, which evenly divides 8. Similarly, for N = 21, then p = 3 and q = 7, so (p-1)(q-1) = 12. And the period of 2 mod 21 is 6, which evenly divides 12. This means that, if we can find the period of a sequence that van be expressed in the form of (2.50), then we can uncover a "hidden" structure of the prime factors of N (namely, a divisor of (p-1)(q-1)). And in order to find the period, we simply need to apply the (quantum) Fourier transform over the superposition of

¹²Specifically, the cost of Shor's algorithm is $O((\log N)^3)$ using fast multiplication, which is polynomial in the number of bits needed to represent N, or "polylog N." It is substantially faster than the general number field sieve, which works in "sub-exponential time" about $O(e^{1.9(\log N)^{1/3}(\log \log N)^{2/3}})$ [39]

xmod N, $x^2 \mod N$, $x^3 \mod N$ etc. (luckily it is possible to generate this superposition). The reason this is not efficient on a *classical* computer is that the period of the sequence might be extremely large, i.e. it could have N might have hundreds or thousands of digits, and it is therefore impractical to store or manipulate on a classical computer. This of course is not an issue for a quantum computer with an N-qubit register that encodes 2^N bits of information. So if we apply the Quantum Fourier Transform to this particular superposition of states, the outcome will be a new superposition of states which is probabilistically weighted towards the vector/state representing the period. This is repeated, and the outcomes are used to reconstruct the original prime factors.

Until now the Quantum Fourier Transform was simply a unitary operation - a tool and not an algorithm. When included in Shor's algorithm, however, it is the *key* to quantum algorithmic efficiency. This is because the outcome of the QFT depends on the input i.e. the superposition of states. So when a problem can be reduced to a question of finding the period, the Quantum Fourier Transform can be used to skew the measurement statistics.

2.7 Grover's Algorithm

Grover's algorithm finds unique input to a black box function that produces a particular output value using just $O(N^{1/2})$ evaluations of the function, where N is the size of the function's domain. This only produces *quadratic* speed up as opposed to the *exponential* speed up of Shor's algorithm. While it was originally described as a database search algorithm, it is better described as an inverting function, i.e. for a function $y = f(\omega)$, calculate ω given y.

f is the function which maps database entries to 0 or 1 where $f(\omega) = 1$ if and only if ω satisfies the search criterion. The algorithm relies on the existence of "quantum black box" access to a subroutine U_{ω} which is a unitary operator with the following properties:

$$U_{\omega} |\omega\rangle = - |\omega\rangle$$

$$U_{\omega} |x\rangle = |x\rangle \quad \text{for all } x \neq \omega$$

Assuming such a subroutine exists and is efficient, the goal is to identify index $|\omega\rangle$. The algorithm is simply:

1. Initialize the system to a superposition over all states

$$|s\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle$$

- 2. Perform the Grover iteration r(N) times: this is defined as applying operator U_{ω} , then applying the Grover diffusion operator $U_s = 2 |s\rangle \langle s| I$.
- 3. Measure: the result will be eigenvalue λ_{ω} with probability approaching 1 for $N \gg 1$. From λ_{ω}, ω may be obtained

Note that if we are dealing with a database, it is not represented explicitly but rather by index -reading a full database item by item could take a much longer time than Grover's search algorithm. Nielsen and Chuang pp. 248 - 261 [34] and Marinescu pp. 246-261 [31] discuss Grover's algorithm in more detail.

Chapter 3

Quantum Error

"The marvel of the present result [re the threshold theorem] is that it proves that, to the best of our current knowledge, no principle in physics will limit quantum computers from being realized someday" Nielsen and Chuang, p.494

It was understood early on that quantum systems are inherently noisy. How difficult it would be to manage this quantum noise was studied in the mid-90s by Landauer, Unruh, and others. The worry, of course, was that implementing error correction on quantum circuits would render any "quantum algorithmic efficiency" (such as that achieved by Shor's algorithm) useless. It would be even worse if quantum error correction required such an overhead of resources that it made quantum computers significantly *worse* than classical computers.

Luckily, these fears never materialized, and in the ensuing years various efficient error correction schemes were designed (such as Shor's code, CSS, the surface code and others) that cleverly tackled the issue of error correction. Of particular importance were the various threshold theorems, which showed that a quantum computer could simulate an ideal quantum computer, provided the level of noise is below a certain threshold. These threshold theorems imply that the error in quantum computers can be controlled as the number of qubits scales up. They also imply that algorithms like Shor's algorithm and Grover's algorithm would *still* be more efficient than classical algorithms even with error correction. Of all the error correction schemes, the surface code takes advantage of particular properties of qubits such as parity to reduce the threshold necessary to implement efficient computation (this is why it is favored among supperconducting qubit research groups). The stabilizer code, for example, has a threshold around $p_{th} \approx 10^{-4}$ while the surface code has a threshold around $p_{th} \approx 10^{-2}$. Depending how much better coherence is than the minimum threshold for a particular implementation, it is estimated that error correction will account for the majority of quantum information processing (which is not the most exciting prospect).

The main sources for this section are Nielson and Chuang [34], Schlosshauer [37] and Martinis's extensive surface code paper [21]. Unfortunately this chapter is somewhat topical and covers just enough material to understand error correction in the context of quantum computing. Where the noise comes from, and how exactly it affects these systems, is discussed in subsequent chapters.

3.1 Quantum Error Formalism

3.1.1 A Simple Understanding

How do we model noise in a classical system? Let's start with a simple example of bit 0 that has probability p of flipping to 1 through some noisy process, and similarly for bit $1 \rightarrow 0$. If X is initial state of the bit, and Y is the final state of the bit, probability dictates:

$$p(Y = y) = \sum_{x} p(Y = y | X = x) p(X = x)$$

where conditional probabilities p(Y = y | X = x) are called transition probabilities. Rewriting in matrix form with p_0, p_1 as initial probabilities that the bits are in the states 0 and 1, and q_0, q_1 as corresponding probabilities after noise has occurred

$$\left[\begin{array}{c} q_0 \\ q_1 \end{array}\right] = \left[\begin{array}{cc} 1-p & p \\ p & 1-p \end{array}\right] \left[\begin{array}{c} p_0 \\ p_1 \end{array}\right]$$

where the center matrix is evolution matrix E. This assumes that consecutive noise processes are independent, is physically reasonable in many situations. More generally, it treats results as stochastic Markov processes. Although quantum errors are quite different from classical errors, we can generalize this probabilistic paradigm to the class of quantum errors by simply assuming that at every time step of a quantum manipulation, there is an associated probability of error p.

There are five general kinds of quantum errors:

amplitude damping - If a qubit is in excited state $|1\rangle$, amplitude damping causes qubit to "relax" to the ground state $|0\rangle$ by losing energy to the environment (for example, in the form of a photon when a single atom coupled to a single mode of electromagnetic radiation undergoes spontaneous emission). However, if a qubit is in the ground state, no change occurs.

phase damping - Phase damping (also called the **phase flip**) is a noise process that describes a change in phase of the quantum state. For example, a $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ state might transform to a $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ state. Phase damping is uniquely quantum mechanical, and can even describe loss of quantum information without loss of energy. As Nielsen and Chuang write that "phase damping is one of the most subtle and important processes in the study of quantum computation and quantum information."¹ As an aside, T_2 is often referred to as the "Transverse coherence time" or "phase damping time" and it essentially describes how long the phase term of the qubit can be controlled. This will be discussed further in the discussion of decoherence.

bit flip - This noise simply flips the qubit from $|0\rangle$ to $|1\rangle$ (and vice versa).

bit-phase flip - The bit-phase flip is a combination of the bit flip and the phase flip (noting that $\mathbf{Y} = i\mathbf{X}\mathbf{Z}$). Thus, $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \longrightarrow -\frac{1}{\sqrt{2}}(|1\rangle + |1\rangle)$ is an example of a bit-phase flip.

depolarizing channel - This is a channel where the amplitude of the state uniformly contracts, regardless of value or phase.

¹Nielsen and Chuang, p. 385 [34]

3.2 Quantum Error Correction (QEC)

3.2.1 Simple Error Correction: the Shor Code

In order to protect against the effects of these possible errors, we can *encode* information by including redundant information. One simple example is to replace a single qubit with three qubits $|0\rangle \rightarrow |000\rangle = |0_L\rangle$, $|1\rangle \rightarrow |111\rangle = |1_L\rangle$ which we call a logical qubit. Suppose initial state $a |0\rangle + b |1\rangle$ was logically encoded such that $|0_L\rangle + b |1_L\rangle = a |000\rangle + b |111\rangle$, and that a *bit flip* occurred on one of the qubits. A simple error correction procedure to recover the original state would be:

1. Error Detection (syndrome diagnosis): perform an operation that indicates which qubit flipped, if any. There are four projection operators:

$$\begin{array}{ll} P_0 \equiv |000\rangle \left\langle 000| + |111\rangle \left\langle 111\right| & \text{no error} \\ P_1 \equiv |100\rangle \left\langle 100| + |011\rangle \left\langle 011\right| & \text{bit flip qubit 1} \\ P_2 \equiv |010\rangle \left\langle 010| + |101\rangle \left\langle 101\right| & \text{bit flip qubit 2} \\ P_3 \equiv |001\rangle \left\langle 001| + |110\rangle \left\langle 110\right| & \text{bit flip qubit 3} \end{array} \right.$$

Note that the syndrome only contains information about which error has occured, but no information about the value of a or b (i.e. no information about the state being protected).

2. **Recovery** Use value of error syndrome to decide which procedure to use to recover initial state. If P_0 do nothing, if P_1 then flip first qubit, etc.

This correction scheme works well provided bit flips occur on no more than one of the three qubits. This occurs with probability $(1-p)^3 + 3(1-p)^2 = 1 - 3p^2 + 2p^3$ and the probability of the error *not* being corrected is therefore $3p^2 - 2p^3$. If p < 1/2, then the probability of the error being corrected is > 1/2. However, if the probability of error is > 1/2, then the probability of the error being corrected is < 1/2.

This only applies to bit flip errors - however as we saw above, there are other kinds of errors. Interestingly, there is a simple way to convert the phase flip channel into a bit flip channel. The phase flip operator \mathbf{Z} is applied to state $a |0\rangle + b |1\rangle$ such that it becomes $a |0\rangle - b |1\rangle$. In $\{|+\rangle, |-\rangle\}$ basis the \mathbf{Z} operator acts as a bit flip: $\mathbf{Z} |+\rangle = |-\rangle$. Hence for phase-flip correction, we can simply encode logical qubits as $|0_L\rangle = |+++\rangle$, $|1_L\rangle = |---\rangle$. All operations needed for error correction are performed in a similar manner to the bit flip channel but in the $\{|+\rangle, |1\rangle\}$ by including the Hadamard transform \mathbf{H} where necessary. The Shor code is a simple quantum code which can protect against the effects of arbitrary error on single qubit. It takes advantage of the three qubit bit flip and phase flip codes. First encode using the phase flip code $|0\rangle \rightarrow |+++\rangle, |1\rangle \rightarrow |---\rangle$ and then encode each of the three qubits using the bit flip code, such that each $|+\rangle \rightarrow \frac{1}{2\sqrt{2}}(|000\rangle + |111\rangle)$ and $|-\rangle \rightarrow \frac{1}{2\sqrt{2}}(|000\rangle - |111\rangle)$. The result is a **nine qubit code**:

$$|0\rangle \rightarrow |0_L\rangle \equiv \frac{1}{2\sqrt{2}} (|000\rangle + |111\rangle) (|000\rangle + |111\rangle) (|000\rangle + |111\rangle)$$
$$|1\rangle \rightarrow |1_L\rangle \equiv \frac{1}{2\sqrt{2}} (|000\rangle - |111\rangle) (|000\rangle - |111\rangle) (|000\rangle - |111\rangle)$$

The Shor code was one of the first error correction schemes.

3.2.2 Stabilizer Codes

Stabilizer codes (or additive quantum codes) are an important class - many states can be more easily described by working with the operators that stabilize them than by working explicitly with the state itself. And many error correction schemes (including Shor's code and CSS) can be more compactly described using stabilizer formalism than state vector formalism. Stabilizer formalism also allows for systematic construction procedures for encoding, decoding and error-correction.

3.2.3 Fault Tolerance

The basic idea of fault-tolerance is to compute directly on encoded states without decoding them. If we assume noise can affect every element of computation (state preparation, quantum gates, measurement procedure, transmission of quantum information along wires, etc.), we must replace each qubit in the original circuit with an encoded block of qubits and replace each gate with a *procedure* for performing *encoded gate* acting on the encoded state. Applying error correction periodically is not sufficient to prevent the build up of errors

- 1. Encoded gates can cause errors to propagate. Therefore encoded gates must be designed carefully such that failure during procedure can only propagate to a small number of qubits in each block (called *fault tolerant* procedures).
- 2. Error correction itself can introduce errors on encoded qubits, so this must be accounted for as well

The fault tolerance of a procedure is defined as the property that if only one component o the procedure fails, then the failure causes at most one error in each encoded block of qubits output from the procedure.²

3.2.4 Threshold Theorems

There is a remarkable result - the threshold theorem - that arbitrarily good quantum computation can be achieved even with faulty logic gates provided only that error probability per gate is below a constant threshold. The result is based on concatenated codes which can be used to reduce the effective error rate achieved by computation even further. We can recursively apply a particular scheme for simulating a circuit using an encoded circuit by constructing a hierarchy of circuits. If failure of physical qubit is p, then failure at one level of encoding is cp^2 , at two levels of encoding is $c(cp^2)^2$. Concatenating k times, probability of failure at highest level is $(cp)^{2^k}/c$, while the size of the simulating circuit goes as d^k times the size of the original circuit (d is a constant representing maximum number of operations used in fault tolerant procedure to do encoded gate and errorcorrection).

One of the earlier threshold theorems stated the following:

Threshold Theorem A quantum circuit containing p(n) gates may be simulated with probability of error at most ϵ using

 $O(poly(\log p(n)/\epsilon)p(n))$

gates on hardware whose components fail with probability at most p provided p is below some constant threshold $p < p_{th}$ and given reasonable assumptions about the noise in the underlying hardware.

 $^{^2\}mathrm{Nielsen}$ Chuang p. 476 [34]

For the Steane code, $p_{th} \approx 10^{-4}$. The most important result of error correction codes is the result that provided noise in individual quantum gates is below a certain constant threshold, it is possible to efficiently perform an arbitrarily large quantum computation. The conclusion, then, is that quantum error does not pose an existential threat for quantum computation.

It is important to note the assumptions made for the early threshold theorems. It is certainly reasonable that physical implementations of qubits might experience more varied forms of noise that don't fit into the above formulation, such as

- 1. Correlated error in time (i.e. the noise is non-Markovian)
- 2. Correlated error due to spatial considerations

Finally, it is important to realize that threshold result requires parallelism, and doesn't take into account classical communication elements, inclusion of ancilla qubit generation etc. However, many more sophisticated models have been developed since the first threshold theorems, and the general idea of a threshold still holds for these as well.

3.2.5 Surface Codes

Surface codes are a particular class of code that take advantage of symmetrical properties of groups of qubits (such as parity) to correct quantum errors. They were somewhat obscure until recently, and are not mentioned in Nielsen and Chuang. Some consider it an even more robust type of error correction that only needs nearest neighbor correlation and has lower threshold values than the traditional codes mentioned above. Surface codes: Towards practical large-scale quantum computation by Fowler, Mariantoni, Martinis and Cleland 2012 [21] is a fantastic resource with a wealth of information about surface codes. Below is one figure from this paper.


Figure 3.1: Surface Code (a) A two-dimensional array implementation of the surface code. Data qubits are open circles, measurement qubits are solid circles, with measure-Z qubits colored green (dark) and measure-X qubits colored orange (light). Away from the boundaries, each data qubit contacts four measure qubits, and each measure qubit contacts four data qubits; the measure qubits perform four-terminal measurements. On the boundaries, the measure qubits contact only three data qubits and perform three-terminal measurements, and the data qubits contact either two or three measure qubits. The solid line surrounding the array indicates the array boundary. (b) Geometric sequence of operations (left), and quantum circuit (right) for one surface code cycle for a measure-Z qubit, which stabilizes $\hat{Z}_a \hat{Z}_b \hat{Z}_c \hat{Z}_d$. (c) Geometry and quantum circuit for a measure-X qubit, which stabilizes $\hat{X}_a \hat{X}_b \hat{X}_c \hat{X}_d$. The two identity \hat{I} operators for the measure-Z process, which are performed by simply waiting, ensure that the timing on the measure-X qubit matches that of the measure-Z qubit, the former undergoing two Hadamard \hat{H} operations. The identity operators come at the beginning and end of the sequence, reducing the impact of any errors during these steps [21].

Chapter 4

Superconducting Qubits

While we have reviewed much of the theoretical foundation of quantum computing, from the circuit model to quantum error correction, the question still remains: how is it possible to physically implement a qubit -and for that matter, a quantum computer? While there are many possible physical implementations of qubits, including photons, ion traps and NMR, superconducting qubits are currently considered one of the most successful and feasible technologies. This has to due with the fact that, over the past decade, the quantum coherence of superconducting qubits has increased more than five orders of magnitude (more on this in subsequent chapters).

Superconducting qubits are essentially variations of Josephson junction circuits with inductors, capacitors and resonators in addition to Josephson junctions. The circuits are very similar to dissipationless LC circuits (i.e. simple harmonic oscillators) at extremely low temperatures, except that the Josephson junctions behave like nonlinear inductive elements and affect the oscillator potential such that it becomes *anharmonic*. The anharmonicity, of course, is key as it means that the different energy levels may be addressed at different frequencies. When tuned appropriately, higher energy levels can be ignored and the circuit becomes a two level system (with a ground state and an excited state) which is a robust representation of a qubit.

The qubit can be controlled by applying a sinusoidal driving force (similar to a classical circuit). The frequency of the driving wave causes rotations about the z-axis, and the *phase* of the driving voltage causes rotations about the x and y axis. This allows for complete control of the state of the qubit. Finally, measurement can be done by reading the signal from a resonator coupled to the qubit.

In this way, with superconducting qubits we have:

- 1. Representation of quantum information
- 2. Application of unitary transforms
- 3. Preparation of a fiducial input state
- 4. Measurement of output

The majority of the material in this chapter was referenced from Superconducting Quantum Bits (2008) by Clarke and Wilhelm [11], Steven Girvin's chapter on circuit QED from Quantum Machines: Measurement and Control of Engineered Quantum Systems: Lecture Notes of Les Houches Summer School (chapter 3) [16], Superconducting Qubits: A Short Review by Devoret, Wallraff and Martinis [17], as well as great course notes by Andreas Wallraff, and Theo Walter from the ETH

Zurich QSIT 2015 course.¹ All of these resources discuss the physics of superconducting circuits extensively. Unfortunately the standard reference for quantum computing, Nielson and Chuang [34], only mentions superconducting qubits in a single paragraph.

4.1 Macroscopic Quantum Behavior and Josephson Junctions

There are two important definitions related to Josephson junctions:

1. flux quantization, whereby magnetic flux in superconducting ring is quantized

$$\Phi_0 = h/2e \approx 2.07 \times 10^{-15} \text{Tm}$$
(4.1)

2. Josephson Tunneling, where cooper pairs can tunnel through energy barrier coherently. Supercurrent I through the barrier is related to the gauge invariant phase difference $\delta(t)$ between the phases of the two superconductors:

$$I = I_0 \sin(\delta(t)) \tag{4.2}$$

where I_0 is the critical current, a phenomenological property of the junction. The phase difference changes in time as $\hbar \frac{d\delta(t)}{dt} = \hbar \omega = 2eV$, where ω is the angular frequency at which the supercurrent oscillates.

We introduce the operators $\hat{\delta}$ and \hat{N} associated with the **Josephson coupling energy** $E_j = I_0 \Phi_0/2\pi$ and the **charging energy** $E_c = (2e)^2/2C$.

When Josephson junctions were fist investigated in the 1960s, it was found that macroscopic quantum tunneling occured and that energy levels were quantized [28]. Cooper pairs tunnel from $|0\rangle$ state through barrier when $I < I_0$ and then run freely down the washboard potential, generating a voltage of $2\Delta_s/e$, which can be detected easily. Energy quantization was found by irradiating junction with microwaves, since each energy level has a unique frequency due to the anharmonic nature of the potential.

In the 1980s, Anthony Leggett predicted that it would be possible to demonstrate a superposition of macroscopic flux states in Josephson junction devices. This was not achieved experimentally until 1997 and 2000 by Nakamura with a charge qubit and Friedman and Caspar Van der Waal with flux qubits.

The next step is to show that the nonlinear inductance alters the Hamiltonian of the LC circuit in order to solve for the new energy levels of the system. There are many different ways of doing this - either with a coax line, capacitor or inductor coupled with voltage. The so called "phase qubit" is with coax line and forms a natural phase basis, the "charge qubit" is with a capacitor and forms a charge basis, and the "flux qubit" is with an inductor and forms a flux basis. The Cooper pair box, or charge qubit is currently the most used configuration, and is the basis of the quantronium, transmon and then xmon qubits. We will therefore focus on the charge qubit.

 $^{^{1}} These notes can be accessed at qudev.ethz.ch/node/114091 and qudev.ethz.ch/content/QSIT15/QSIT15_Super_L02_slides.pdf$

Circuit Equations 4.2

The following is a rough and simple derivation of the quantum analogue to the LC Circuit. The classical circuit equations are:

$$\Phi = LI \quad V_L = -L\frac{dI}{dt} \quad Q = CV_C \tag{4.3}$$

$$E_{mag} = \frac{1}{2}LI^2 \quad E_{elec}\frac{1}{2}CV^2 \tag{4.4}$$

where Φ magnetic flux of the inductor, L is inductance, I is the current, Q is the total charge on capacitor C is the capacitance, V_L is the voltage across inductor, V_C is the voltage across the capacitor, and E is the energy stored in inductor capacitor respectively. Ignoring resistance, the basic circuit Hamiltonian is:

$$H_{LC} = \frac{1}{2}CV^2 + \frac{1}{2}LI^2 = \frac{1}{2}\frac{Q^2}{C} + \frac{1}{2}\frac{\Phi^2}{L}$$
(4.5)

If we treat Q as p and Φ as x, recalling that:

$$\frac{\delta H}{\delta p} = \dot{x} \quad \frac{\delta H}{\delta x} = -\dot{p}, \quad \frac{\delta H}{\delta \Phi} = \frac{\Phi}{L} = I = \dot{Q} \quad \frac{\delta H}{\delta Q} = \frac{Q}{C} = V = -L\dot{I} = -\dot{\Phi} \tag{4.6}$$

Making the jump from classical to quantum by treating x and p as operators \hat{x} and \hat{p} , we have the quantum Hamiltonian:

$$\hat{H}_{q} = \frac{1}{2}\frac{\hat{Q}^{2}}{C} + \frac{1}{2}\frac{\hat{\Phi}^{2}}{L} = \frac{1}{2}\frac{\hbar}{C}\frac{\delta^{2}}{\delta\Phi^{2}} + \frac{1}{2}\frac{1}{L}\hat{\Phi}^{2}$$
(4.7)

Which has all the expected properties of a quantum harmonic oscillator such as energy E_n = $\hbar\omega\left(n+\frac{1}{2}\right)$. This can be expressed in second quantization form:

$$\hat{H} = \hbar\omega(\hat{a}_{LC}^{\dagger}\hat{a}_{LC} + \frac{1}{2}) \tag{4.8}$$

$$\hat{a}_{LC} = \frac{1}{\sqrt{2\hbar Z_C}} \left(Z_C \hat{Q} + i\hat{\Phi} \right) \quad \hat{a}_{LC}^{\dagger} = \frac{1}{\sqrt{2\hbar Z_C}} \left(Z_C \hat{Q} - i\hat{\Phi} \right) \tag{4.9}$$

$$\hat{a}_{\dagger} = \sqrt{n+1} |n+1\rangle \quad \hat{a} |n\rangle = \sqrt{n} |n-1\rangle \quad \hat{a}^{\dagger} \hat{a} |n\rangle = n |n\rangle \quad [\hat{a}^{\dagger}, \hat{a}] = 1$$
(4.10)

where $Z_C = \sqrt{L/C}$ is the characteristic impedance, with no dissipation.² We now move on to the **RLC Circuit**. If we include resistance in parallel with the inductor and

²The same would hold with the following substitutions: $\hat{V} = \frac{\hat{Q}}{C}$ $\hat{I} = \frac{\hat{\Phi}}{L}$

capacitor, the dynamic equation for current through the inductor is

$$\frac{d^2}{dt}I_L + \frac{R}{L}\frac{d}{dt}I_L + \frac{1}{LC}I_L = 0$$
(4.11)

$$\frac{d^2}{dt}I_L + 2\alpha \frac{d}{dt}I_L + \omega_0^2 I_L = 0$$
(4.12)

 α , and ω_0 , are both in units of angular frequency. α , is called the neper frequency, or attenuation, and is a measure of how fast the transient response of the circuit will die away after the stimulus has been removed, and ω_0 is the angular resonance frequency. For the case of the series RLC circuit these two parameters are given by: $\alpha = R/2L$ and $\omega_0 = 1/\sqrt{LC}$. The damping factor is $\zeta = \frac{\alpha}{\omega_0} = \frac{R}{2}\sqrt{\frac{C}{L}}$, which has the general solution

$$I_L(t) = A_1 e^{t(-\alpha + \sqrt{\alpha^2 - \omega_0^2})} + A_2 e^{t(-\alpha - \sqrt{\alpha^2 - \omega_0^2})}$$
(4.13)

For an underdamped response $\zeta < 1$

$$I_L = A e^{-\alpha t} \sin(\omega_0 \sqrt{1 - \zeta^2} t + \phi) \tag{4.14}$$

The equation implies that the lower the resistance, the less the decay - as would be expected from our understanding of the LC circuit. The general solution is sinusoidal with an amplitude that decays with characteristic time, corresponding to energy dissipation.

The Q factor is a widespread measure used to characterize resonators. It is defined as the peak energy stored in the circuit divided by the average energy dissipated in it per radian at resonance. Low Q circuits are therefore damped and lossy and high Q circuits are underdamped. Q is related to bandwidth; low Q circuits are wide band and high Q circuits are narrow band (Q is the inverse of fractional bandwidth). For a resistor in series

$$Q = \frac{1}{\omega_0 RC} = \frac{\omega_0 L}{R} = \frac{1}{R} \sqrt{\frac{L}{C}}$$
(4.15)

In order to control the circuit, we need to make energy gap between ground state and first excited state much larger than thermal energy of the system. Luckily, the energy spectrum of superconductors is ideal for this. While the energy spectrum of valence electrons is a continuum above superconducting temperatures, at critical temperature, electrons bind into cooper pairs and form bosonic states. At sufficiently low temperatures, all the cooper pairs reach ground state (since they are bosonic). And thus we get split energy levels!

This leads us to superconductors. At typical temperatures of 10^{-2} K, superconductors have with quality factors Q on the order of 10^4 (due to limitation of size of inductors and capacitors which are roughly 1 nH and 1 pF, leading to typical resonant frequency on order of 5 Hz).

The fundamental challenge of *building* a quantum computer lies in the tension between decoupling and coupling; in order for a qubit to have quantum properties, it must be isolated/decoupled from other sources (e.g. noise from other qubits or noise from external controls). However, some level of coupling is necessary in order to initialize, control, and read out the qubit. Many qubit implementations based on microscopic degrees of freedom, such as electron spins and atomic dipoles have difficulty creating inter-qubit coupling without introducing unwanted decoherence. However, as we shall see, superconducting qubits can be manipulated and measured quit elegantly.

4.3 The Charge Qubit (Cooper pair Box)



Figure 4.1: Cooper pair Box (a) schematic (b) energy levels and (c) $\langle n \rangle$

The charge qubit is an island of charge, sandwiched between an external capacitor and Josephson junction. Initially, the island is charge neutral. When the gate voltage is turned on, charges build up at the capacitor and charges begin to polarize both in the circuit and on the "island" without any net charge being added to the system. As polarization increases, charges begin to tunnel onto the island through the Josephson junction. As the voltage continues to increase, there is an *increase* in the number of Cooper pairs that tunnel to the island. When the voltage is removed, these Cooper pairs tunnel back. The charge qubit therefore treats the presence or absence of Cooper pairs on island as the two states of a qubit (e.g. ground state is represented by no extra pairs on the island, while the excited state is represented by one extra Cooper pair on island).

The Hamiltonian can be simply expressed as the sum of total energy stored in the electric and magnetic fields $H = H_E + H_B$. The energy stored in the electric field is related to the capacitor, and there are two capacitors and extra Cooper pair charges. Since we are concerned with the *difference* in the number of Cooper pairs, we want to keep track of charge $Q_{\Sigma} = Q_{cooper} - Q_G$. If we call C_{Σ} the net capacitance of island, we get this from the sum of the gate capacitor and junction capacitor which are in parallel (i.e. they can be added) $C_{\Sigma} = C_G + C_J$. We also want to represent the charge of Cooper pairs in terms of number of Cooper pairs, so $\hat{Q}_{cooper} = 2e\hat{N}_{cooper}$ (since each pair has net charge of 2e). It follows that the gate capacitor has $Q_G = 2eN_G = C_GV_G$. Therefore

$$H_E = \frac{1}{2} \frac{Q_{\Sigma}^2}{C_{\Sigma}} = \frac{4e^2}{2C_{\Sigma}} \left(\hat{N}_{cooper} - N_G \right)^2 \tag{4.16}$$

where charging energy is $E_C = 4e^2/2C_{\Sigma}$. (Beware - this is still somewhat classical, haven't fully derived results). The Hamiltonian is parabolic in nature, and is centered at every discrete value of N_{cooper} . Note that we are not considering any sort of dissipation or interaction.

On he other hand, the energy stored in the magnetic field (stored by Josephson junction due to

its inductor-like properties) is $H_B = -E_{J_0} \cos \hat{\delta}$

$$H = E_C \left(\hat{N}_{cooper} - N_G \right)^2 - E_{J_0} \cos \hat{\delta} = E_C \left(-i\frac{d}{d\delta} - N_G \right)^2 - E_{J_0} \cos \hat{\delta}$$
(4.17)

Rewritten in the charge number basis as

$$\hat{H} = \sum_{N} \left[E_C (\hat{N}_{cooper} - N_G)^2 |N\rangle \langle N| - \frac{1}{2} E_{J_0} (|N\rangle \langle N+1| + |N+1\rangle \langle N|) \right]$$
(4.18)

(4.19)

If we make the two level approximation (i.e. assume that we only care about the lowest two) such that $N = \{0, 1\}$, we can rewrite the Hamiltonian in terms of the familiar Pauli spin matrices,

$$\hat{H} = -\frac{1}{2}E_C(1 - 2N_G)\hat{\sigma}_z - \frac{1}{2}E_{J_0}\hat{\sigma}_x$$
(4.20)

and solve for energy eigenvalues³

$$E_{\pm} = \pm \frac{1}{2} \sqrt{E_C^2 + E_{J_0}^2 + 4N_G E_C^2 (N_G - 1)}$$
(4.21)

What we see is that the magnetic component of Hamiltonian proportional to E_J creates energy gaps at degeneracy points! Gap size between ground and first excited state is E_J , and this energy decreases with each level. This, of course, is anharmonic and allows for precise control of transitions! More importantly, E_C is a function of the voltage, while E_j is a function of the flux. These correspond to effective magnetic fields in the z-direction and x-direction respectively. Therefore, we have effectively created a tunable atom!

4.3.1 Tuning Junction

The relevant tuning parameters in the Hamiltonian are the charging energy E_C , the number of gate charges N_G and the Josephson energy E_J . E_C is inversely proportional to net capacitance on island, so we could add more capacitors to change capacitance. Since N_G is proportional to the externally applied voltage, tuning the voltage changes N_G . While the Josephson energy E_J can be manufactured to specification (e.g. surface area and thickness of Josephson substrate). Finally, the phase difference depends on magnetic flux through junction; two junctions in parallel change dependence of cosine term in E_J according to magnetic flux through loop of junctions.

4.3.2 Manipulation

The next question is, how driving force will affect qubit? If we tune the frequency of the driving oscillator near the transition frequency of system, we would expect system to transition from ground state to first excited state (corresponding to an X-gate)

Using the rotating wave approximation (see Appendix), we can derive the following Hamiltonian that relates the driving frequency and the driving phase to the Pauli spin matrices

$$\hat{H}_{rot} = \frac{1}{2} (\omega_q - \omega_d) \hat{\sigma}_z + \frac{1}{2} \bar{A} (\cos \phi \hat{\sigma}_x + \sin \phi \hat{\sigma}_y)$$
(4.22)

³Note that the above Hamiltonian differs slightly depending on particular circuit

The long and short of it is that the frequency of the driving voltage controls z-axis rotations, and the phase of the driving voltage controls x and y-axis rotations!

4.3.3 Qubit-Qubit Coupling and Quantum Non-Demolition (QND) Readout

The final piece to the superconducting qubit schematic is qubit measurement. This is done by coupling the qubit to a resonator and measuring the effective resonant frequency. The mathematics is somewhat involved and draws from the well researched field of cavity quantum electrodynamics (cavity QED). The goal is to convert the Hamiltonian of the resonator qubit system into the form of the Jaynes-Cummings Hamiltonian, which is a template Hamiltonian used in qavity QED. The Jaynes-Cummings Hamiltonian looks like

$$\hat{H}_{Jaynes-Cummings} = \hbar\omega \left(\hat{a}^{\dagger} \hat{a} + \frac{1}{2} \right) + \frac{1}{2} \hbar\omega \hat{\sigma}_z + \frac{1}{2} \hbar g \left(\hat{a} \hat{\sigma}^+ + \hat{a}^{\dagger} \hat{\sigma}^- \right)$$
(4.23)

where ω_c is the frequency of the mode of oscillation of the radiation in the cavity, ω_a is the transition frequency of the atom trapped in the cavity, g is the coupling factor, and $\hat{\sigma}^{\pm}$ are the raising and lowering operators of the atom. If we ignore the high frequencies (since contributions to evolution of the system are too fast for consideration), we can rewrite original Hamiltonian into Jaynes-Cummings form

$$\hat{H} = \hbar\omega_r \left(\hat{a}^{\dagger} \hat{a} + \frac{1}{2} \right) + \frac{1}{2} E_J \hat{\sigma}_z + \frac{1}{2} \hbar g \left(\hat{a} \hat{\sigma}^+ + \hat{a}^{\dagger} \hat{\sigma}^- \right)$$
(4.24)

with

$$g = E_C \frac{C_G}{2e} \sqrt{\frac{\hbar\omega_r}{2C}} \tag{4.25}$$

where C_G is the capacitance of the capacitor in the qubit, and C is the capacitance of the capacitor in the LC resonator circuit. Coupling between resonator and qubit take energy from resonator and give to qubit ($\alpha\sigma^+$) or vice versa.

In order to actually measure the qubit, we detune the resonant frequency of the resonator and the qubit so that when a signal is sent to qubit through the resonator, the resonator is hardly perturbed. We simplify the Hamiltonian further (since it is weakly coupled) and fin that the effective frequency of the resonator ω_r when coupled to the qubit, is dependent on the state of the qubit. Once the resonator and qubit are detuned (dispersive regime), we can measure ω_r to determine state of qubit without disturbing qubit (i.e. Quantum Non Demolition). It is then possible to perform basic spectroscopy on resonator, and hence measure the system. We mention here that qubit-qubit coupling differs between various physical implementations, but are usually similar to the methods described above. See the Girvin chapter [16] or the review article by Devoret et al. [17] for more details.

Chapter 5

The Physics of Decoherence

Decoherence is the loss of coherence or ordering of the phase angles between the components of a system in a quantum superposition due to energy dissipation and/or pure dephasing. This represents one of the most difficult and unique challenges to quantum computing, as the entire theory requires that coherence times are better than particular fault tolerant thresholds. Fortunately, decoherence theory allows us to understand which parameters are important for *improving* coherence times, and it does not seem like there are any theoretical principles that limit coherence times below the fault tolerant thresholds.

In this chapter, the theory is developed carefully, first with toy models and then with the canonical spin-boson model and spin bath model. We also emphasize how coherence times might be improved from a mathematical perspective.

Density matrices and reduced density matrices play an important role in decoherence theory. This is because, when entanglement occurs (say, between the system of interest and the environment), we cannot describe the entangled system in terms of a single quantum state vector (see section 2.1.6). However, the measurement statistics of such entangled systems can be elegantly described with reduced density matrices. The following exposition on density matrices and decoherence models roughly follows Schlosshauer, Chapters 2-5 [37]. Maximilian Schlosshauer's Decoherence and the Quantum to Classical Transition is an extremely well written book that covers the above topics in much more depth. Roland Omnes' well known book The Interpretation of Quantum Mechanics [36] is also a good introduction to the general subject of decoherence and the role it plays in the interpretation of quantum mechanics. Finally, Joos Zeh and others wrote a well regarded (and more advanced) volume on the subject called Decoherence and the Appearance of a Classical World in Quantum Theory [27].

5.1 Density Matrices

We begin with a density matrix of a **pure state** (i.e. unentangled). We can define the density operator $\hat{\rho}$ corresponding to a pure state $|\psi\rangle$ as $\hat{\rho} \equiv |\psi\rangle \langle \psi|$, which is the projection operator onto the state $|\psi\rangle$. If we reexpress $|\psi\rangle$ as a superposition of basis states $|\phi_i\rangle$ such that $|\psi\rangle = \sum_i c_i |\phi_i\rangle$ with a corresponding *density operator*

$$\hat{\rho} = |\psi\rangle \langle \psi| = \sum_{ij} c_i c_j^* |\phi_i\rangle \langle \phi_j|$$
(5.1)

This can be written in matrix form, and is called the *density matrix*

$$\rho_{ij} = c_i c_j^* \langle \phi_i | \psi \rangle \langle \psi | \phi_j \rangle = c_i c_j^* \langle \phi_i | \hat{\rho} | \phi_j \rangle$$

$$\begin{bmatrix} c_1 c_1^* \langle \phi_1 | \hat{\rho} | \phi_1 \rangle & c_1 c_2^* \langle \phi_1 | \hat{\rho} | \phi_2 \rangle & \dots \end{bmatrix}$$
(5.2)

$$\rho = \begin{vmatrix} c_2 c_1^* \langle \phi_2 | \hat{\rho} | \phi_1 \rangle & c_2 c_2^* \langle \phi_2 | \hat{\rho} | \phi_2 \rangle \\ \vdots & \ddots \end{vmatrix}$$
(5.3)

While the i = j terms are called the diagonal terms, the $i \neq j$ terms are called the off-diagonal terms, or *interference terms*. These interference terms are the embodiment of coherent superposition discussed in section 2.1.2. It is important to keep in mind, however, that these interference terms should always be understood in terms of a particular basis (in this case $\{|\phi_i\rangle\}$. A basis in which the density matrix becomes diagonal always exists, and there will be no interference in this basis. As Schlosshauer emphasizes, we should not assume that a diagonal density matrix implies a system that "does not have quantum properties" or "behaves classically."¹ Note that the two ways of describing the system (either as a pure state $|\psi\rangle$ or as a pure state density operator $\hat{\rho} = |\psi\rangle \langle \psi|$) are entirely equivalent formally and physically.

The density matrix formalism turns out to be much more useful when dealing with **mixed states**, or statistical ensembles of several pure states. In such scenarios, insufficient information is known about the system - it is in a pure state, but the observer does not know which pure state. We can therefore ascribe probabilities p_i to each of the pure states $|\psi_i\rangle$. The density matrix is the quantum-mechanical analogue to a phase-space probability measure (probability distribution of position and momentum) in classical statistical mechanics. The mixed state itself represents a classical ensemble, where the origin of the probabilities is purely classical. Supposing that a quantum system may be found in state $|\psi_1\rangle$ with probability p_1 , or in state $|\psi_2\rangle$ with probability p_2 , and so on, the density operator for this system is

$$\hat{\rho} = \sum_{i} p_i |\psi_i\rangle \langle \psi_i| \tag{5.4}$$

where $\{|\psi_i\rangle\}$ need not be orthogonal and $\sum_i p_i = 1$. By choosing an orthonormal basis $\{|u_m\rangle\}$, one may resolve the density operator into a density matrix or density operator:

$$\rho_{mn} = \sum_{i} p_i \langle u_m | \psi_i \rangle \langle \psi_i | u_n \rangle = \langle u_m | \hat{\rho} | u_n \rangle, \quad \hat{\rho} = \sum_{mn} | u_m \rangle \rho_{mn} \langle u_n |$$
(5.5)

For an operator \hat{O} , which describes an observable O of the system, the expectation value $\langle \hat{O} \rangle$ is given by

$$\langle \hat{O} \rangle = \sum_{i} p_{i} \langle \psi_{i} | \hat{O} | \psi_{i} \rangle = \sum_{i} p_{i} \langle \psi_{i} | u_{n} \rangle \langle u_{n} | \hat{O} | u_{m} \rangle \langle u_{m} | \psi_{i} \rangle$$
(5.6)

$$=\sum_{mn} \langle u_m | \hat{\rho} | u_n \rangle \langle u_n | \hat{O} | u_m \rangle = \sum_{mn} \rho_{mn} O_{nm} = \operatorname{Tr}(\hat{\rho} \hat{O})$$
(5.7)

where the trace operation Tr acting on an operator \hat{O} in the basis $\{|\psi_i\rangle\}$ is defined as $Tr(\hat{O}) \equiv \sum_i \langle \psi_i | \hat{O} | \psi_i \rangle$ (i.e. the sum of the diagonal elements). In other words, the expectation value of \hat{O} for the mixed state is the sum of the expectation values of \hat{O} for each of the pure states $|\psi_i\rangle$ weighted by the probabilities p_i and can be computed as the trace of the product of the density matrix with

¹Schlosshauer, p. 35 [37].

the matrix representation of \hat{O} in the same basis. We also note here that for an entangled system, the density operator $\hat{\rho}$ of the composite system cannot be written as the tensor product of the two subsystems $\hat{\rho_1} \otimes \hat{\rho_2}$.

Now the real motivation to introduce this formalism is to use **reduced density matrices** to describe the dynamics of an open quantum system - a system where the environment is significantly influencing the quantum system of interest. If a quantum system has two or more subsystems that are entangled, then each subsystem must be treated as a mixed state even if the complete system is in a pure state. The basic example is for a quantum system \mathcal{A} entangled with a quantum system \mathcal{B} . The combined quantum system \mathcal{AB} may be pure, but we can only access (i.e. perform measurements on) one of the systems, \mathcal{A} . The most appropriate way to express all the information available to the observer of system \mathcal{A} is with the reduced density matrix

$$\hat{\rho}_{\mathcal{A}} \equiv \mathrm{Tr}_{\mathcal{B}}\hat{\rho} \tag{5.8}$$

where $\operatorname{Tr}_{\mathcal{B}}$ is the trace performed using the orthonormal basis of the Hilbert space $\mathcal{H}_{\mathcal{B}}$ of system \mathcal{B} , or the partial trace. We can interpret this as averaging over the observed degrees of freedom of the unobservable system \mathcal{B} . Importantly, this definition seems to hint that the system \mathcal{B} plays some role in the dynamics of \mathcal{AB} , and that this is part of the outcome of \mathcal{A} when system \mathcal{A} is observed.

In order to derive this reduced density matrix, consider an entangled state of systems \mathcal{A} and \mathcal{B}

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|a_1\rangle |b_1\rangle + |a_2\rangle |b_2\rangle) \tag{5.9}$$

where $|a_i\rangle$, $|b_i\rangle$ are arbitrary normalized but not necessarily orthogonal states of \mathcal{A} and \mathcal{B} . The pure state density matrix (i.e. of the total system \mathcal{AB} , which is pure) is:

$$\hat{\rho} = |\Psi\rangle \langle \Psi| = \frac{1}{2} \sum_{ij=1}^{2} |a_i\rangle \langle a_j| \otimes |b_i\rangle \langle b_j|$$
(5.10)

This bipartite density matrix isn't particularly insightful.² We want to calculate expectation values for \mathcal{A} -observables, which we call $\hat{O} = \hat{O}_{\mathcal{A}} \otimes \hat{I}_{\mathcal{B}}$ with $\{|\psi_k\rangle\}$ and $\{|\phi_l\rangle\}$ as orthonormal bases of the Hilbert spaces $\mathcal{H}_{\mathcal{A}}$ and $\mathcal{H}_{\mathcal{B}}$ of \mathcal{A} and \mathcal{B} . Since the expectation value $\langle \hat{O} \rangle$ of any observable can be computed using the trace rule (5.6), we can write

$$\langle \hat{O} \rangle = \operatorname{Tr}(\hat{\rho}\hat{O}) = \sum_{kl} \langle \phi_l | \langle \psi_k | \hat{\rho} \left(\hat{O}_{\mathcal{A}} \otimes \hat{I}_{\mathcal{B}} \right) | \psi_k \rangle | \phi_k \rangle$$
(5.11)

$$=\sum_{k} \langle \psi_{k} | \left(\sum_{l=1} \langle \phi_{l} | \hat{\rho} | \phi_{l} \rangle \right) \hat{O}_{\mathcal{A}} | \psi_{k} \rangle$$
(5.12)

$$=\sum_{k} \langle \psi_{k} | (\operatorname{Tr}_{\mathcal{B}} \hat{\rho}) \hat{O}_{\mathcal{A}} | \psi_{k} \rangle$$
(5.13)

$$= \operatorname{Tr}_{\mathcal{A}}\left((\operatorname{Tr}_{\mathcal{B}}\hat{\rho})\hat{O}_{\mathcal{A}}\right) = \operatorname{Tr}_{\mathcal{A}}\left(\hat{\rho}_{\mathcal{A}}\hat{O}_{\mathcal{A}}\right)$$
(5.14)

²This can be expressed as $\frac{1}{2} \Big(|a_1\rangle \langle a_1| \otimes |b_1\rangle \langle b_1| + |a_2\rangle \langle a_1| \otimes |b_2\rangle \langle b_1| + |a_1\rangle \langle a_2| \otimes |b_1\rangle \langle b_2| + |a_2\rangle \langle a_2| \otimes |b_2\rangle \langle b_2| \Big)$ or alternatively as $\frac{1}{2} \Big(|a_1b_1\rangle \langle a_1b_1| + |a_2b_2\rangle \langle a_1b_1| + |a_1b_1\rangle \langle a_2b_2| + |a_2b_2\rangle \langle b_2b_2| \Big)$

For the bipartite state, the reduced density operator is

$$\hat{\rho}_{\mathcal{A}} = \frac{1}{2} \sum_{ij=1}^{2} |a_i\rangle \langle a_j| \langle b_j|b_i\rangle$$
(5.15)

$$=\frac{1}{2}\left|a_{1}\right\rangle\left\langle a_{1}\right|+\frac{1}{2}\left|a_{2}\right\rangle\left\langle a_{2}\right|+\frac{1}{2}\left(\left|a_{1}\right\rangle\left\langle a_{2}\right|\left\langle b_{2}\right|b_{1}\right\rangle+\left|a_{2}\right\rangle\left\langle a_{1}\right|\left\langle b_{1}\right|b_{2}\right\rangle\right)$$
(5.16)

Where the two terms in the brackets are the off diagonal interference terms. It is clear that the influence of system \mathcal{B} is interconnected with with off diagonal \mathcal{A} terms. And here is the key - if the states $|b_1\rangle$ and $|b_2\rangle$ are orthogonal, then the off diagonal terms - and hence any indication of interference - vanish. This will become more evident in the next example.

Also note that this result can be generalized for entanglement between N subsystems:

$$\hat{\rho}_i = \operatorname{Tr}_{1,\dots,i-1,i+1,\dots,N}(\hat{\rho}), \quad \text{and} \quad \langle \hat{O} \rangle = \operatorname{Tr}(\hat{\rho}\hat{O}) = \operatorname{Tr}_i(\hat{\rho}_i\hat{O}_i)$$
(5.17)

The insight here is that by tracing over all or a fraction of the degrees of freedom of the environment, we can obtain a complete and exhaustive description of the measurement statistics for the system of interest.

5.2 Simple Model for Decoherence

As an instructive example to build on the above result, let us consider a two-qubit system where the second qubit is "environmental noise" \mathcal{B} . The interaction Hamiltonian between two, two-level systems is described by the Heisenberg Hamiltonian equation 2.12 (with $\hbar = 1$)

$$\hat{H} = \frac{J}{4} \hat{\sigma}_z^{(\mathcal{A})} \otimes \hat{\sigma}_z^{(\mathcal{B})}$$
(5.18)

where J is simply a coupling constant. Starting with the product state $|\Psi(t_0)\rangle = |+\rangle_{\mathcal{A}} \otimes |+\rangle_{\mathcal{B}} = |++\rangle$, we let the system unitarily evolve with operator $\hat{U}(t) = e^{-i\hat{H}t}$ (equation 2.2) and then perform the trace operation on the \mathcal{B} -qubit to understand how the \mathcal{A} -qubit evolved (and how it was influenced by the \mathcal{B} -qubit). We can write the density operator $\hat{\rho}_{\mathcal{A}}$

$$\hat{\rho}_{\mathcal{A}} = |+\rangle_{\mathcal{A}} \langle +|_{\mathcal{A}} = \frac{1}{2} (|0\rangle \langle 0| + |1\rangle \langle 1| + |0\rangle \langle 1| + |1\rangle \langle 0|)$$
(5.19)

and the density matrix as

$$\rho_{\mathcal{A}} = \frac{1}{2} \begin{pmatrix} 1 & 1\\ 1 & 1 \end{pmatrix} \tag{5.20}$$

at time t we have

$$|\Psi(t)\rangle = U(t) |+\rangle_{\mathcal{A}} |+\rangle_{\mathcal{B}} = e^{-iJt\hat{\sigma}_{\mathcal{A}}\hat{\sigma_{\mathcal{B}}}/2} |+\rangle |+\rangle$$
(5.21)

(5.22)

The state of the \mathcal{A} -qubit at time t is given by

$$\rho_1(t) = \operatorname{Tr}(|\Psi(t)\rangle \langle \Psi(t)|) = \frac{1}{2} \begin{pmatrix} 1 & \cos(Jt/2) \\ \cos(Jt/2) & 1 \end{pmatrix}$$
(5.23)

The algebra for equation 5.23 is a bit cumbersome³. It is evident that while the diagonal elements are constant, the off-diagonal elements change with time. This means that the coherence is periodically completely lost and then completely regained (albeit with sign changes) at intervals of π/J . The coherence is regained when The real consequences of this changing coherence are highlighted in the next example.

In 1982, Wojciech Zurek created one of the first basic models to illustrate basic features of environment induced decoherence [43]. The model consists of a two level quantum system \mathcal{S} linearly coupled to an environment \mathcal{E} that is comprised of N other quantum two level systems (this is a generalization of the above toy model). Although it is overly simplified for most purposes, it can be applied to certain real, physical systems.⁴ Two basis states of \mathcal{S} are $|0\rangle$ and $|1\rangle$ while the basis states of the N two level systems of environment \mathcal{E} are $|\uparrow\rangle_i, |\downarrow\rangle_i$ where i = 1, 2, ...N. The total systemenvironment combination is a 2^{N+1} dimensional tensor product Hilbert space $\mathcal{H} = \mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{E}_{1...N}}$. Assuming that the interaction Hamiltonian \hat{H}_{int} dominates the evolution (i.e. ignoring intrinsic dynamics of each system), we have

$$\hat{H} = \frac{1}{2}\hat{\sigma}_z \otimes \left(g_1\hat{\sigma}_z^{(1)} \otimes \hat{I}_{2,3,\dots N} + g_2\hat{\sigma}_z^{(2)} \otimes \hat{I}_{1,3,\dots N} + \dots\right)$$
(5.24)

$$=\frac{1}{2}\hat{\sigma}_z \otimes \left(\sum_{i=1}^N g_i \hat{\sigma}_z^{(i)} \bigotimes_{i' \neq i} \hat{I}_{i'}\right)$$
(5.25)

$$=\frac{1}{2}\hat{\sigma}_z\otimes\hat{E}\tag{5.26}$$

Each element in the environment couples to the central system \mathcal{S} , but they do not couple with each other (the identity is only necessary when $i' \neq i$, and is implicit in E). The qubit couples linearly through z-spin component to each of the environmental spins, where q_i for i = 1, 2, ... N is the coupling strength, while the Hamiltonian is in diagonal form. Since the Hamiltonian commutes, it is a conserved quantity and no energy is exchanged and therefore no dissipation needs to occur. We can describe the energy eigenstates of the environment part \hat{E} of the Hamiltonian as $|n\rangle =$ $|\uparrow\rangle_1 |\downarrow\rangle_2 \dots |\uparrow\rangle_N$, and associate energy ϵ_n with each eigenstate $|n\rangle$

$$\epsilon_n = \sum_{i=1}^N (-1)^{n_i} g_i \tag{5.27}$$

where we define $n_i = 1$ if ith environmental spin is in the down state $|\downarrow\rangle$ and $n_i = 0$ if ith environmental spin is in the up state $|\uparrow\rangle$ any arbitrary pure state of \mathcal{SE} can be represented as:

$$|\Psi\rangle = \sum_{n=0}^{2^{N}-1} (c_n |0\rangle |n\rangle + d_n |1\rangle |n\rangle)$$
(5.28)

³We can notice that the eigenvectors of the 4×4 matrix $\hat{\sigma}_z \otimes \hat{\sigma}_z$ are $|00\rangle$, $|11\rangle$, $|01\rangle$, $|10\rangle$ with eigenvalues 1, 1, -1, -1 respectively. Remembering that the function of an operator can be expressed as $f(\hat{A}) = \sum_i f(\lambda_i) |a_i\rangle \langle a_i|$, where λ_i is an eigenvalue and $|a_i\rangle$ is an eigenvector, we can write $e^{-iJt\hat{\sigma}_z\hat{\sigma}_z/2}|+\rangle|+\rangle = \left[e^{-iJt/2}(|00\rangle\langle 00|+|11\rangle\langle 11|)+e^{iJt/2}(|01\rangle\langle 10|+|10\rangle\langle 01|)\right]|++\rangle$ etc.

⁴Schlosshauer p. 90 [37]

Assuming that S and \mathcal{E} are uncorrelated at t = 0,

$$|\Psi\rangle = (a|0\rangle + b|1\rangle) \sum_{n=0}^{2^{N}-1} c_{n}|n\rangle$$
(5.29)

As above, the time evolution of the total system \mathcal{SE} can be expressed as

$$|\Psi(t)\rangle = e^{-i\tilde{H}t} |\Psi(0)\rangle = a |0\rangle |\mathcal{E}_0(t)\rangle + b |1\rangle |\mathcal{E}_1(t)\rangle$$
(5.30)

$$|\mathcal{E}_0(t)\rangle = \sum_{n=0}^{2^{n-1}} c_n e^{-i\epsilon_n t/2} |n\rangle$$
(5.31)

Already we can see that the basis states $|0\rangle$, $|1\rangle$ of S are correlated with the relative states $|\mathcal{E}_0(t)\rangle$, $|\mathcal{E}_1(t)\rangle$ of the environment \mathcal{E} . The smaller the overlap between $\langle \mathcal{E}_1(t)|\mathcal{E}_0(t)\rangle$, the more information is encoded in the environment that distinguishes between states $|0\rangle$ and $|1\rangle$. $\langle \mathcal{E}_1(t)|\mathcal{E}_0(t)\rangle$ is interpreted as the *decoherence factor* r(t), given by

$$r(t) \equiv \langle \mathcal{E}_1(t) | \mathcal{E}_0(t) \rangle \equiv \sum_{n=0}^{2^N - 1} |c_n|^2 e^{-i\epsilon_n t}$$
(5.32)

Taking the trace in the $\{|0\rangle, |1\rangle\}$ basis

$$\hat{\rho}_{\mathcal{S}}(t) = \operatorname{Tr}_{\mathcal{E}}\hat{\rho}(t) \equiv \operatorname{Tr}_{\mathcal{E}}|\Psi(t)\rangle \langle \Psi(t)|$$
(5.33)

$$= |a|^{2} |0\rangle \langle 0| + |b|^{2} |1\rangle \langle 1| + ab^{*}r(t) |0\rangle \langle 1| + a^{*}br^{*}(t) |1\rangle \langle 0|$$
(5.34)

Finally, we see that if $r(t) \rightarrow 0$, the interference terms disappear. Hence r(t) describes local damping of interferences between $|0\rangle$ and $|1\rangle$.

But how does r(t) change overtime, and how is it affected by the number of spins N in the environment? Cucchietti, Paz and Zurek [14] were able to show that:

- 1. The degree of suppression of coherence scales exponentially with size N of the environment
- 2. For sufficiently large N, r(t) follows an approximately Gaussian decay with time $r(t) \approx e^{-\Gamma^2 t^2}$, where Γ^2 is a decay constant determined by the initial state of the environment and the distribution of couplings g_i
- 3. As long as the number of degrees of freedom of the environment \mathcal{E} is finite, there exists a characteristic recurrence time for which the decoherence factor will return to it's initial value of one (this is because equation 5.32 is a sum of periodic functions, which is in turn periodic). In physically relevant situations, the characteristic recurrence time is extremely long (and can even exceed the lifetime of the universe). Thus even with this simple model, loss of coherence is for all practical purposes irreversible.
- 4. There are a few unique states/boundary conditions: for example, if the each element in the environment system was initially in the $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$, then r(t) would be $\cos^{N}(gt)$, which is periodic with frequency $g/2\pi$. However these do not usually apply in physical situations.

This particular model highlights a few important points. Most importantly, we see that including "the environment" in a model can essentially explain the quantum to classical transition. Why

don't we see coherence at the macroscopic level? Because coherence is suppressed by environmental interactions. In addition, the interactions in this particular model were energy conserving - so despite the fact that there was no energy exchanged/dissipated, decoherence did occur. The fact that decoherence can occur without energy dissipation makes it very clear that decoherence is a uniquely quantum phenomenon. In the more "realistic" models we will see soon, of course, decoherence usually does include dissipation.

5.3 Scattering Models

The next well known type of models are the scattering induced decoherence models. Although the derivations are too lengthy for this context, a few comments are in order. Many of the ideas of open quantum systems and environmentally induced decoherence were developed in the 1970s and 1980s. It is now understood that any interaction between a massive object and a particle may lead to entanglement and hence decoherence. The larger the object, the larger the scattering cross section, the faster the decoherence. Interestingly, scattering induced decoherence resolves Schrodinger's historical problem of describing particles as spatially extended waves. It is generally taught in introductory physics courses that a free particle described by a locally spatialized wave packet spreads out on very short timescales. For example, if we describe a free particle with the mass of an electron ($m \approx 10^{-30}$ kg) as a gaussian wave packet with an initial width of 1 angstrom, unitary time evolution spreads the wave packet to a width on the order of 1,000 km!⁵ The seminal paper by E. Joos and H.D. Zeh in 1985 [26] showed for the first time that ubiquitous scattering of photons, air molecules and other environmental particles effectively suppresses the coherent spreading of free particles on extremely short timescales. For more detail, see Omnes Chapter 7 [36] and Schlosshauer Chapter 3.1 [37]. Ample references to original papers can be found there as well.

5.4 Canonical Decoherence Models

The beauty of decoherence theory is that it allows us to map complex systems onto canonical models. There are four main canonical models for open quantum systems, which are made up of two kinds of central systems and two kinds of environment systems:

- Central system S: The central system of interest is either modeled as (1) particles with continuous coordinates \hat{x} and \hat{p} (e.g. photons) or (2) as discrete, two level systems (TLS) (e.g. spin-1/2 particles)
- Environment \mathcal{E} : The interacting environment can either be modeled as (1) a collection of continuous harmonic oscillators, or as (2) a collection of discrete two level systems

The **spin-boson model** is a canonical model of a two level system coupled to an environment of harmonic oscillators. Generally, the model is solved with an arbitrary choice of parameters, and then "fit" to physically relevant situations by filling in parameters. Often times the same canonical model will be unique in different regimes. The purpose of these next two sections is to provide an overview of the two canonical decoherence models used for superconducting qubit theory and experiment.

Often times the two level central system is can be modeled as a particle confined to a double well potential - two energy minimums (excited and ground states) separated by a barrier. Hence the Hamiltonian can consist of a simple excitation/relaxation term, as well as a tunneling term.⁶ It

⁵A free particle $\psi(x, t = 0) = (\sqrt{\pi}\sigma)^{-1/2}e^{-x^2/2\sigma^2}$ has probability density $|\psi(x, t)|^2 = (1/\sqrt{\pi}\sigma(t))e^{-x^2/\sigma^2(t)}$. The width of the wavepacket grows as $\sigma(t) = \sigma[1 + \hbar^2 t^2/(m^2\sigma^4)]^{1/2}$ See Schlosshauer, p.119[37]

⁶The Hamiltonian of a tunneling term is $\hat{H} = -1/2\Delta_0\sigma_x$, which is simple a flip operator $|e\rangle \rightarrow |g\rangle$ or $|g\rangle \rightarrow |e\rangle$

is clear that qubits can be modeled as two level systems (TLS), and this is the most appropriate central system S. We've thus narrowed down the canonical models to the spin-boson model (with oscillator environments) and the spin-bath model (with spin environments). When do each of these models apply?

Oscillator environments are essentially a quasicontinuum of delocalized bosonic field modes. When decoherence occurs due to oscillator environments, energy and coherence are effectively irreversibly lost into the extended bosonic environment.⁷ Spin environments, on the other hand, are particularly useful for modeling low temperature, superconducting experiments. This regime is dominated by *local modes*, such as paramagnetic spins, electronic impurities, tunneling charges, defects, nuclear spins, etc. Decoherence caused by these modes are confined to small regions in space. As we shall see with superconducting qubits, even small improvements in the number of material defects can greatly improve coherence times.

The subfields of decoherence and open quantum systems have an extensive toolbox of rigorous mathematical objects (e.g. Schmidt decomposition, Wigner representation, Operator-Sum formalism, Master equations, Born Markov approximations, Lindbald form, Langevin equations). However, simple versions of the spin-boson model and the spin-bath model can be analyzed without this mathematical heavylifting.⁸

5.5 Spin-Boson Model

For the purposes of this discussion, we will consider a simplified version of the model in which the Hamiltonian of the spin system does not contain a tunneling term. Despite the fact that it is a simplified version, it still displays many of the characteristic features of decoherence.⁹

5.5.1 Set up

We begin with a Hamiltonian of the form

$$\hat{H} = \hat{H}_{\mathcal{S}} + \hat{H}_{\mathcal{E}} + \hat{H}_{int} \tag{5.35}$$

The first term is the Hamiltonian of the central system S, defined as $\hat{H}_S = \frac{1}{2}\omega_0\hat{\sigma}_z$. ω_0 is the difference in energy between the basis states $|0\rangle$ and $|1\rangle$. Note that in the more extensive model, the tunneling term would be included in \hat{H}_S as well.

- 1. Unruh, William G. "Maintaining coherence in quantum computers." Physical Review A 51.2 (1995): 992.
- Palma, G. Massimo, Kalle-Antti Suominen, and Artur K. Ekert. "Quantum computers and dissipation." Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences. Vol. 452. No. 1946. The Royal Society, 1996.
- 3. Duan, Lu-Ming, and Guang-Can Guo. "Reducing decoherence in quantum-computer memory with all quantum bits coupling to the same environment." Physical Review A 57.2 (1998): 737.
- Reina, John H., Luis Quiroga, and Neil F. Johnson. "Decoherence of quantum registers." Physical Review A 65.3 (2002): 032326.

⁷Feynman and Vernon actually showed that the interaction with any environment can be linearly mapped onto a system coupled to a an oscillator environment assuming that the interaction is weak and second-order perturbation theory can be applied [20].

⁸Schlosshauer, again, does a fantastic job motivating and explaining much of this mathematical framework in [37] ⁹Some interesting examples of physical models that make this simplifying assumption:

The second term is the Hamiltonian of the environment of harmonic oscillators, with the familiar

$$\hat{H}_{\mathcal{E}} = \sum_{i} \left(\frac{1}{2m_i} \hat{p}_i^2 + \frac{1}{2} m_i \omega_i^2 \hat{q}_i^2 \right)$$
(5.36)

where the bosonic mode *i* of the *i*th oscillator is defined by its natural frequency ω_i , mass m_i , position operator \hat{q}_i and momentum operator \hat{p}_i .

Finally, the third term describes the linear coupling between the two level system S and the environment \mathcal{E} .

$$\hat{H}_{int} = \hat{\sigma}_z \otimes \sum_i c_i \hat{q}_i \tag{5.37}$$

where the $\hat{\sigma}_z$ coordinate is coupled to the position coordinates \hat{q}_i of each harmonic oscillator with coupling strengths c_i . It is convenient to write the Hamiltonians in terms of the bosonic annihilatian and creation operators for each mode.

$$\hat{q}_i = \sqrt{\frac{1}{2m_i\omega_i}} \left(\hat{a}_i + \hat{a}_i^{\dagger} \right) \tag{5.38}$$

$$\hat{p}_i = -i\sqrt{\frac{m_i\omega_i}{2}} \left(\hat{a}_i - \hat{a}_i^{\dagger}\right) \tag{5.39}$$

and dropping the vacuum-energy term $\sum_i \omega_i/2$, we can rewrite the full Hamiltonian as

$$\hat{H} = \frac{1}{2}\omega_0\hat{\sigma}_z + \sum_i \omega_i\hat{a}_i^{\dagger}\hat{a}_i + \hat{\sigma}_z \otimes \sum_i \left(g_i\hat{a}_i^{\dagger} + g_i^*\hat{a}_i\right)$$
(5.40)

As in the in simple spin model above (equation 5.24), the property $\left[\hat{H}, \hat{\sigma}_z\right] = 0$ indicates that there is a conserved quantity. In this case, there is no induced transition between the ground and excited state of the two level system \mathcal{S} (which would involve a $\hat{\sigma}_x$ operator), and hence no energy dissipation ($|e\rangle \rightarrow |g\rangle$) or absorption (in the form of excitation $|g\rangle \rightarrow |e\rangle$). In addition, the *populations* of the two energy levels are conserved quantities. This is therefore a model of decoherence without dissipation. In circumstances where the timescale for decoherence without dissipation is much shorter than the timescale for energy relaxation, the above model suffices. Clearly the more complete model with the tunneling term allows for energy dissipation as well.

5.5.2 Solution

The strategy is to obtain a relatively workable expression for the time evolution operator. Unfortunately this involves more math than can appropriately fit here (the basic approach is to switch to the interaction picture, write the time evolution operator $\hat{U}(t)$ as a time ordered product of operators, expand in terms of a Dyson series and then express $\hat{U}(t)$ in terms of a *non* time ordered evolution operator $\hat{V}(t)$).

Making the usual assumption that S and \mathcal{E} are uncorrelated at time t = 0, we obtain the time evolution:

$$|\Psi(t)\rangle = \hat{V}(t) |\Psi(0)\rangle = \hat{V}(t)(a |0\rangle + b |1\rangle) |\Phi_{\mathcal{E}}\rangle$$
(5.41)

$$= a \left| 0 \right\rangle \prod_{i} \hat{D}(\lambda_{i}(t)/2) \left| \Phi_{\mathcal{E}} \right\rangle + b \left| 1 \right\rangle \prod_{i} \hat{D}(-\lambda_{i}(t)/2) \left| \Phi_{\mathcal{E}} \right\rangle$$
(5.42)

$$\equiv a \left| 0 \right\rangle \left| \mathcal{E}_{+}(t) \right\rangle + b \left| 1 \right\rangle \left| \mathcal{E}_{-}(t) \right\rangle \tag{5.43}$$

where $\hat{D}(\lambda_i(t))$ is an operator that generates the evolution of the i-th environmental oscillator. Unsurprisingly, the form of the $|\Psi(t)\rangle$ is similar to that obtained in the simple spin-spin model in section 5.2, equation 5.30. In both cases, the states $|0\rangle$, $|1\rangle$ of the central system \mathcal{S} and the states $|\mathcal{E}_+(t)\rangle$, $|\mathcal{E}_-(t)\rangle$ environment \mathcal{E} are clearly and elegantly correlated. The specific forms of the states $|\mathcal{E}_+(t)\rangle$, $|\mathcal{E}_-(t)\rangle$ of course depend on the initial state of the environment.

Environment in ground state: The first scenario to look at is the initial state of \mathcal{E} in the energy ground state $|\Phi_{\mathcal{E}}\rangle = \prod_i |E_0\rangle_i$ where *i* runs over all the environmental oscillators. This can be likened to a measurement like process - the state of the environment $|\Phi_{\mathcal{E}}\rangle$ gets *shifted* into the states $|\mathcal{E}_+(t)\rangle$, $|\mathcal{E}_-(t)\rangle$. And if the environment is sufficiently macroscopic, they are capable of discriminating between the states $|0\rangle$ and $|1\rangle$. The coherence will be lost from the system, and the off-diagonal elements in the reduced density matrix of the system (expressed in the basis $\{|0\rangle, |1\rangle\}$) will disappear.

It can be shown that the decoherence factor is given by

$$r(t) = \langle \mathcal{E}_{-}(t) | \mathcal{E}_{+}(t) \rangle = \exp\left(-\sum_{i} 4 \frac{|g_i|^2}{\omega_i^2} (1 - \cos \omega_i t)\right) \approx \exp\left(-\sum_{i} 2|g_i|^2 t^2\right)$$
(5.44)

where the final approximation is for t much smaller than dynamical timescales ω_i^{-1} of the modes (i.e. $\omega_i t \ll 1$, so the cosine can be approximated to $\cos(\omega_i t) \approx 1 - \frac{1}{2}\omega_i^2 t^2$). This final approximation gives a gaussian decay of coherence between the states $|0\rangle$ and $|1\rangle$.

Environment in thermal equilibrium: This is the more general case, where the environmental oscillator is in a thermal state.

If the environment is sufficiently large, we can assume a continuous density of environmental modes.

We can then analyze the decoherence factor in terms of a sum over the discrete couplings g_i to a continuous description by means of the spectral density $J(\omega)$.¹⁰ The typical approach is to consider spectral density that is ohmic for sufficiently small frequencies $J(\omega) \propto \omega$ that has a smooth high-frequency cutoff quantified by Λ . Integrating over ω , we get a result that can be separated into temperature dependent and temperature independent terms

$$\Gamma(t) = \Gamma_{fluc}(t) + \Gamma_{therm}(t) \tag{5.45}$$

where $\Gamma_{fluc}(t) = -\frac{1}{2}\ln(1+\Lambda^2 t^2)$ and $\Gamma_{therm}(t) \approx -\ln(\sinh(\pi k_B T t)/\pi k_B T t)$. Note that Γ_{fluc} is independent of the temperature, but sensitive to the cutoff frequency, while Γ_{therm} is dependent on

¹⁰This replaces the discrete sum in the modes for $J(\omega)$ with an (often phenomenologically motivated) continuous function of the environmental frequencies ω . Usually, the frequency dependence of $J(\omega)$ is taken to follow a powerlaw dependence of the form $J(\omega) \propto \omega^{\alpha}$. The most common choice for the exponent α is $\alpha = 1$, such that $J(\omega)$ increases linearly with ω . This type of spectral density is called ohmic (the nomenclature has its origin in an analysis of dissipative effects in the spin boson model). Other, less important examples include subohmic spectral densities characterized by $\alpha < 1$ and supraohmic spectral densities for which $\alpha > 1$. Schlosshauer p. 188 [37]

the temperature, and independent of Λ . It can be shown that at short and extremely short time regimes, decoherence is entirely due to quantum vacuum fluctuations. It can also be shown that for long-time regimes (much larger than the typical thermal fluctuation time), the decoherence factor r(t) decays exponentially on a timescale set by the thermal correlation time $(k_BT)^1$. It is clear from this very general model that coherence times can be improved by decreasing temperature, an obvious but important result. Schlosshauer has an extensive derivation of the above results in Chapter 5 of [37].

5.5.3 Full Spin-Boson Model

Shnirman, Makhlin and Schon review the full spin boson model and apply it to superconducting charge qubits in their 2002 paper Noise and Decoherence in Quantum Two-Level Systems [38], and also summarize what is known about relaxation and dephasing processes for spin-boson models with linear coupling. The key difference from the previous model is the addition of the tunneling term $\propto \hat{\sigma}_x$ that makes the dynamics much more rich. Again, the motivating question is: how do we get from a model to an estimation of decoherence time?

With this model, there is a dephasing timescale τ_{ϕ} as well as a relaxation timescale τ_{relax} that characterizes how the diagonal entries tend to their thermal equilibrium. The decoherence rates using the Bloch-Redfield approximation are

$$\Gamma_{\rm relax} \equiv \tau_{\rm relax}^{-1} = \frac{1}{\hbar^2} \sin^2 \theta S_X(\omega = \Delta E/\hbar)$$
(5.46)

$$\Gamma_{\phi} \equiv \tau_{\phi}^{-1} = \frac{1}{2}\Gamma_{\text{relax}} + \frac{1}{\hbar^2}\cos^2\theta S_X(\omega=0)$$
(5.47)

The "pure" dephasing rate Γ_{ϕ}^* is defined as being $\propto \cos^2 \theta$ and is entirely non-dissipative and has no classical analogue. This leads to the often quoted relation

$$\Gamma_{\phi} = \frac{1}{2}\Gamma_{\text{relax}} + \Gamma_{\phi}^{*} \tag{5.48}$$

which is sometimes also stated as

$$\boxed{\frac{1}{T_2} = \frac{1}{2T_1} - \frac{1}{T_{\phi}}}$$
(5.49)

In environment dominated regime, $\Delta E \ll \alpha k_B T$, the coupling to the bath is dominant part of Hamiltonian, and dephasing Γ_{ϕ} is much faster than relaxation Γ_{relax} .

5.6 Spin-Bath Model

The spin-bath model, or spin-spin model, is extremely useful for describing defects in superconducting states. This is the regime where decoherence correlated with temperature is weak and decoherence correlated to two-level state *local defects* are significant. Without going into much detail, the model is similar to the simple spin-bath model we encountered at the beginning of this chapter except for the inclusion of a tunneling term. Unsurprisingly, this leads to significantly different dynamics compared to the earlier static model. Schlosshauer Section 5.4.1 [37] discusses this model in detail, and McDermott [33] applies this to superconducting qubits.



Figure 5.1: "Moore's Law" for Qubits (T_2) , [35]

5.7 Decoherence in Superconducting Qubits

Coherence times for superconducting qubits have dramatically improved since the early 2000s by 5 orders of magnitude! This was due to a combination of theoretical insights and methodical experimentation. The nanosecond scale coherence in a Cooper pair by Nakamura in 1999. In 2002 Vion developed the quantronium qubit, a modified charge qubit, with a T₂ coherence time of hundreds of nanoseconds. Schoelkopf and his group at Yale developed the transmon qubit, which significantly reduced the charge sensitivity of the cooper pair box by adding a shunt interdigitated capacitor, microsecond range, and the 3D cavity transmon approach developed by Yale has increased coherence to around $100\mu s$ Logic gate fidelity has significantly improved as well [35].

Many of the theoretical insights came from complex applications of the canonical models mentioned above of various qubit systems; the experimental insights however came from various fields such as materials science and electrical engineering. There is also a lot of confusion and disagreement among the leading research groups regarding many of the underlying decoherence mechanisms. Below we will touch on some examples of theoretical insights.

Megrant and Martinis outline some of the main sources of decoherence in UCSB final report for the CSQ program: Review of decoherence and materials physics for superconducting qubits [32]. The sources are threefold: Capacitor loss, inductor loss, and radiation loss (gate fidelity is a source of error but not necessarily decoherence). Dielectric loss in the capacitor can have many possible sources; for example, charge fluctuations, quasiparticle tunneling, or phonon radiation. These in turn are often related to defects introduced in the fabrication materials and processes. Inductor loss can come from trapped vortices, critical current fluctuations, and flux noise. Qubit decoherence may also come from dissipation and noise from leads connected to the device. As per the discussion throughout this chapter, most of these sources can be modeled either as oscillator environments or as two level system environments.

In the context of superconducting qubits, a two level system (TLS) is a localized low-energy

excitation predominantly found in noncrystalline dielectric materials. A TLS can be an ion or electron that can tunnel between two spatial quantum states. It can arise due to defects in the crystal structure or the presence of polar impurites. TLS have significant impact at low temperatures, particularly when there are many TLS that form a "decoherence inducing" environment [35].

Unsurprisingly, there is some disagreement about this. Martinis and Megrant claim, for example, that "The simple TLS model is consistent with all data we have seen in the past 5 years" but note that "other groups doing transmon research have not reported significant effects from TLS." [32]



Figure 5.2: Possible Sources of Decoherence in Supercondcuting Qubits

In the 2002 paper Noise and Decoherence in Quantum Two-Level Systems by Alexander Shnirman, Yuriy Makhlin and Gerard Schon [38] we see a discussion of noise in charge qubits due to voltage fluctuations. As we saw earlier in the control Hamiltonian of the charge qubit, $\delta V(t)$ couples to σ_z and $\delta \Phi(t)$ couples to σ_x . Because these noises are derived from linear circuits, they are Gaussian and can be modeled by a bath of harmonic oscillators. They are entirely characterized by their power spectra which in turn depend on impedance $Z(\omega)$ and temperature T.

The power spectra for the gate voltage fluctuations in the control circuit would be something like

$$S_V(\omega) = 2\text{Re}\{Z_t(\omega)\}\hbar\omega \coth\left(\frac{\hbar\omega}{2k_BT}\right)$$
(5.50)

At low frequencies the circuit will behave like a resistor $Z(\omega) = R_V$ and the results for ohmic dissipation apply. The dissipation would be characterized by dimensionless parameter

$$\alpha_V = \frac{4R_V}{R_K} \left(\frac{C_g}{C_{qb}}\right)^2 \tag{5.51}$$

which depends linearly on strength of voltage fluctuations in environment and coupling to the qubit ($\propto C_g/C_{qb}$). For a typical value of voltage circuit $R_V \approx 5\Omega$ and for small effect of fluctuations $C_g \ll C_J$ can reach very weak dissipation, which theoretically allows for $\approx 10^6$ coherent single bit manipulations.

In the same paper, they begin to discuss stronger sources of noise: background charge fluctuations. They claim that they can be either modeled as two-state quantum system bath, or as approximate oscillator bath with the appropriate spectrum, but do not discuss much further.

In the 2008 paper Materials Origins of Decoherence in Superconducting Qubits by Robert Mc-Dermott [33], he states that for defect energies larger than k_BT , TLS defects behave like a "spin bath" in the quantum regime, and that the spin physics gives rise to unusual properties such as enhanced dielectric loss at low temperature and low microwave drive power. On the other hand, defects with energies less than k_BT produce low-frequency charge and dielectric noise. Hence the quantum TLS contribute to qubit energy relaxation, while the thermal TLS contribute to dephasing.

Just as resonant a magnetic field can induce transitions in a system of spins immersed in a strong static magnetic field, resonant electric fields can couple to TLS with an electric dipole moment, including transitions and dissipation. The loss tangent tan δ of the amorphous dielectric decreases due to population of the TLS excited state. However, as thermal or external microwave transitions saturate the TLS, the dielectric becomes transparent to resonant irradiation and the loss decreases

The dielectric loss of TLS can influence the qubit T_1 time in two ways: (1) lossy dielectrics incorporated in the wiring external to the qubit junction contribute a fraction α to the qubit capacitance, and (2) in the case of a large qubit junction with area $100\mu m^2$ the tunnel barrier itself contains a quasicontinuum of resonant TLS and dissipation from these states can induce qubit relaxation. Interestingly, at millikelvin temperatures and at low microwave drive powers, the integral quality factor of the tank is the inverse of the intrinsic loss tangent of the capacitor dielectric $Q_i = 1/\tan \delta_i$. It is clear that the capacitance shunting the qubit junction should be entirely free of low energy defect states. While a continuum of TLS in bulk dielectrics can lead to energy relaxation, coupling of the qubit to discrete TLS in the Josephson barrier can itself lead to the quantum coherent transfer of energy between the qubit and the TLS, and result in fidelity loss.

McDermott concludes that in order to minimize fidelity loss due to TLS in the qubit tunnel barrier, it is necessary to reduce the density of resonant TLS. This can done straightforwardly either by reducing the area of the Josephson junction or by improving the quality of barrier.



Figure 6.1: (a) Optical micrograph of the planar Xmon qubit, formed by the Al superconducting film (light) and the exposed sapphire substrate (dark). The qubit is capacitively coupled to a quarter wave readout resonator (top), a quantum bus resonator (right), and an XY control line (left), and inductively coupled to a Z control line (bottom). The Xmon arm length is L. (b) The inset shows the shadow evaporated Al junction layer in false color (blue regions). The junction size is $0.300.20 \mu m2$. The capacitor central linewidth is S, and the gap width is W. (c) The electrical circuit of the qubit. Barends et. al. 2013 [7]

Chapter 6 Recent Progress

Everything until now has been somewhat theoretical. And what a shame it would be if there was nothing more to state than a slew of theoretical results! Luckily there has been *an incredible amount of progress* in the subfield of superconducting qubits. Before concluding, it is worthwhile to review some of the most exciting experimental developments. After all, the ultimate proof is in the experiments themselves.

6.1 The Xmon Qubit (UCSB 2013)

In August 2013, Barends, Martinis and others at UCSB published *Coherent Josephson Qubit Suitable* for Scalable Quantum Integrated Circuits [7]. In this paper, they built a planar, tunable superconducting qubit which they dubbed the "xmon." One of the most impressive results was that they were able to achieve xmon T_1 energy relaxation time of up to 44 μs .

While many groups at the time were embedding "transmon" qubits into 3D superconducting cavities to minimize defects, with T_1 energy relaxation times between 30 and 140 μs , the xmon

was essentially a planar transmon that was much more versatile. Martinis saw it as a balance of coherence, connectivity and relatively easy manufacturing. What was unique about this qubit was that it was *frequency tunable*, meant that they could implement fast two-qubit gates (because there was not a concern of perturbing nieghboring qubits). They were also able to achieve the important benchmark of Control-Z in 25 ns. According to the paper, the xmon qubit "provides key ingredient for implementing a surface code quantum computer." They also found that energy relaxation depends on qubit frequency.

In this paper they also investigated dependence of qubit coherence time on capacitor geometry using six different designs - varying width of central line, gap width, and arm length. They found that overall energy relaxation time increases with width; the belief is that widening the capacitor reduced the surface participation of dipole moments residing on surface oxides ad interfaces. They also noted that lower and upper bounds of T_1 increasing with capacitor dimension seem to indicate that defects reside within the capacitor. Also in the paper, they modeled decoherence mechanism arising from a sparse bath of weakly coupled (two level) defects.

How does the modular design work? Each arm has different function - a coplanar waveguide resonator for read out, a quantum bus resonator for coupling/entanglement, XY control for frequency control and Z control for phase control. Three of the connections are made with coupling capacitor, and each coupling can be individually tuned and optimized. XY control can excite qubit in 10 ns, while T_1 of XY control is 0.3 ms. Z-control - can rapidly detune on order of 1 ns, while T_1 for z-control is ≈ 30 ms. More arms can be added for connectivity. They also noted that the limit $T_2 = 2T_1$ was not reached, indicating additional dephasing. Also note that in the paper *Qubit Architecture* with High Coherence and Fast Tunable Coupling [10] Chen, Cleland, Martinis and others were able to demonstrate that the cross coupling effects between two xmon qubits could be made small for planar integrated circuits while still allowing for multiqubit operations.

6.2 5-qubit Linear Array (UCSB 2014)

The next truly exciting experiment came in 2014. In the paper Superconducting Quantum Circuits at the Surface Code Threshold for Fault Tolerance [8] Barends, Korotkov, Cleland, Martinis and others announced that they had built a 5-qubit linear array using xmon qubits.

In this particular experiment, the UCSB group was able to demonstrate universal set of logic gates in a multi-qubit processor with single-qubit gate fidelity of 99.92% and two-qubit gate fidelity of up to 99.4%. This is very good, as it places superconducting qubits at the fault tolerance threshold for surface code error correction. They were also able to construct a 5-qubit GHZ state. As they write in the paper: "The results demonstrate that Josephson quantum computing is a high fidelity technology with a clear path to scaling up to large-scale, fault tolerant quantum circuit."

Among other technical achievements, the they were able to maintain controlled phase gate nearly 40*ns* when two qubits were brought near resonance. This was with a dispersive measurement method; where each qubit is coupled to a readout resonator with a distinct resonance frequency, enabling simultaneous readout using frequency domain multiplexing through a single coplanar waveguide. They also measured performance when simultaneously operating nearest-neighbor qubits, and fidelities were essentially unchanged (remember qubits are at different idle frequencies to minimize coupling).

They were also able to implement a two-qubit controlled phase gate by tuning one qubit in frequency along a fast adiabatic trajectory that takes two qubit state $|11\rangle$ close to the avoided level crossing with the state $|02\rangle$. This two qubit gate fidelity is comparable to highest rates reported in other qubit implementations, including NMR (99.5 %) and ion traps (99.3 %). But most importantly, they verified by simulation that gate fidelities are at the threshold for surface



Figure 6.2: a, Optical image of the integrated Josephson quantum processor, consisting of aluminium (dark) on sapphire (light). The five cross-shaped devices (Q0Q4) are the Xmon variant of the transmon qubits30, placed in a linear array. To the left of the qubits are five meandering coplanar waveguide resonators used for individual state readout. Control wiring is brought in from the contact pads at the edge of the chip, ending at the right of the qubits. b, Circuit diagram. Our architecture uses direct, nearest-neighbour coupling of the qubits (red/orange), made possible by the nodal connectivity of the Xmon qubit. Using a single readout line, each qubit can be measured using frequency-domain multiplexing (blue). Individual qubits are driven through capacitively coupled microwave control lines (XY), and frequency control is achieved through inductively coupled d.c. lines (Z) (violet). c, Schematic representation of an entangling operation using a controlledphase gate with unitary representation UCZ; (I) qubits at rest, at distinct frequencies with minimal interaction; (II) when brought near resonance, the state-dependent frequency shift brings about a rotation conditional on the qubit states; (III) qubits are returned to their rest frequency [8]

code quantum error correction. They estimated that decoherence accounts for 55 % of control phase gate error, control error accounts for 24 % error, and state leakage accounts for 21 % error.

The 5-qubit GHZ state was largest tomographic measurement of multi-qubit entanglement demonstrated in solid state, and it too had fidelity similar to ion traps. They conclude by claiming that a linear extension of the array to larger number of qubits is straightforward, and that implementing a 2D array will be somewhat more challenging (due to a more complicated wiring and readout design) but also straightforward. Within a year, they delivered on their promise.

6.3 9-qubit Linear Array (UCSB 2015)

The most recent and important experiment by far was reported in March 2015. In the paper *State* preservation by repetitive error detection in a superconducting quantum circuit [29] Kelly, Barends, Cleland, Martinis and others reported that they were able to protect classical states as well as non-classical GHZ states from environmental bit-flip errors (although not phase flip errors...yet) and demonstrate the suppression of those errors with increasing system size. They were able to track errors as they occurred by repeatedly performing projective QND parity measurements. Simplest

system demonstrating basic elements of surface code is a one-dimensional chain of qubits (a "primitive" of the surface code) which corrects **bit flip errors** (note - not phase flip errors) on both data and measurement qubits. They were also able to test first and second order fault tolerance by concatenation. Note however, that they did not implement the full surface code, and were not able to correct for phase errors.



Figure 6.3: Repetition code: device and algorithm. a, The repetition code is a one-dimensional (1D) variant of the surface code, and is able to protect against \mathbf{X} (bit-flip) errors. The code is implemented using an alternating pattern of data and measurement qubits. b, Optical micrograph of the superconducting quantum device, consisting of nine Xmon transmon qubits with individual control and measurement, with a nearest-neighbour coupling scheme. c, The repetition code algorithm uses repeated entangling and measurement operations which detect bit-flips, using the parity scheme on the right. Using the output from the measurement qubits during the repetition code for error detection, the initial state can be recovered by removing physical errors in software. Measurement qubits are initialized into the $|0\rangle$ state and need no reinitialization as measurement is QND.

6.4 4-qubit 2D Array (IBM 2015)

IBM has also been doing research in superconducting qubits, and in their most recent experiment they implemented a 4-qubit array of transmons. The paper was *Demonstration of a quantum error* detection code using a square lattice of four superconducting qubits (April 2015, Nature Communications) Corcoles, Gambetta, Chow [13].

While classical bit flip error can be corrected with a linear array, phase flip error requires a 2D lattice (for the surface code). This protocol detected an arbitrary quantum error on an encoded twoqubit entangled state via QND parity measurements via error syndrome qubits. IBM stated that this experiment "Represents building block towards larger lattices amenable to fault-tolerant quantum error correction architectures such as the surface code," which is a vision that both Martinis/Google



Figure 6.4: The optical image shows all components of the device, including the four qubits, Q1Q4, the four readout resonators R1R4 and the four coupling buses B12, B23, B34 and B41. The readout resonators also serve as qubit control lines, with single- and two-qubit gates applied at frequencies ω_i with $i\{1, 2, 3, 4\}$. Readout is performed at the resonator frequency ω_{MI} . A blowup of one of the qubits is also shown, depicting the capacitor geometry as well as the coupling lines to the readout resonator (green coupler) and to the buses (red couplers). The black scale bar represents a length of $100\mu m$ [13].

and IBM seem to share.

The chip was a 2x2 lattice of superconducting transmons, each coupled with nearest neighbors via two independent superconducting coplanar waveguide resonators serving as quantum buses. While this is an important step, they acknowledged that their system has not yet reached the fault tolerance threshold yet.

6.5 Conclusion

We carefully developed of the quantum circuit formalism of quantum computing, starting with two level quantum systems and the Pauli spin matrices and building up to the celebrated algorithms of Shor and Grover. The limitations of these algorithms were also discussed. These theoretical developments addressed some of the original questions posed by Feynman - among other things, they established that a computer built from quantum components is, indeed, fundamentally different from a classical computer.

We then developed the problem of quantum error correction, which stems from the fundamental physics of quantum systems but can be abstracted to a set of five possible transformations. The two most important of these are energy relaxation, where the qubit loses energy to the environment and relaxes from the $|1\rangle$ state to the $|0\rangle$ state, and dephasing, which changes the relative phase of a qubit in a superposition. Novel error correction schemes had to be formulated in order to correct for these possible errors, as classical error correction schemes cannot be implemented on qubits due to the no cloning theorem. We also briefly touched on the threshold theorems, and the possibility of efficient quantum computing given a probability of error below a threshold for a particular error correction scheme. The surface code has the highest (and therefore most approachable) threshold of the error correction codes, which is why it is considered an important benchmark. Although this benchmark has not been fully reached, the necessary coherence time for a single qubit in the surface code has been reached.

Next we explained the framework surrounding the physical implementation of superconducting qubits, highlighting the unique properties of the Josephson junction and the similarity of Josephson circuits with classical LC/RLC circuits. In particular, we show that the frequency and phase of the driving voltage allow for elegant manipulation of the Pauli spin matrices.

Finally, we investigated the phenomenon of decoherence more closely to understand how interaction with the environment influences a particular quantum system. We introduced the canonical spin-boson and spin-spin models, and discussed them in the context of superconducting qubits. In this discussion we explained how coherence could be improved both by clever circuit design and by better fabrication techniques. This also explains the five-fold increase in coherence times since 2000. We finished off the subject with some recent examples of superconducting qubit research.

Martinis and his group at UCSB built qubits above the surface code threshold but have not yet built a 2D array in order to correct both bit and phase flip errors. IBM *has* build a 2D array, but its qubits are below surface code threshold. It seems that:

- 1. Coherence times are improving and don't seem to have reached a ceiling
- 2. Arrays of qubits are extremely well controlled, and do not seem to change behavior when scaled up
- 3. Large scale industrial manufacturing of superconducting qubits will not be difficult given current fabrication techniques

In the face of all the theoretical results and experimental progress, it is not so hard to believe that coherence in superconducting qubits might improve *just a bit more* - at least just enough to make fault tolerant circuits and fault tolerant computing a reality.

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Appendix A

Recent UCSB Publications

Just to get a sense of the fast pace research coming out of the UCSB (now Google) group, here is a list of their most recent publications and submitted papers from the group website web.physics.ucsb.edu/martinisgroup/pu [accessed October 7, 2015]. The following are **from 2015 alone**:

- Qubit metrology for building a fault-tolerant quantum computer John M. Martinis Accepted for publication in NPJ Quantum Information (2015).
- Measuring and Suppressing Quantum State Leakage in a Superconducting Qubit Zijun Chen, Julian Kelly, Chris Quintana, R. Barends, B. Campbell, Yu Chen, B. Chiaro, A. Dunsworth, A. G. Fowler, E. Lucero, E. Jeffrey, A. Megrant, J. Mutus, M. Neeley, C. Neill, P. J. J. O'Malley, P. Roushan, D. Sank, A. Vainsencher, J. Wenner, T. C. White, A. N. Korotkov, John M. Martinis Submitted (2015). arXiv:1509.05470
- Violating the Bell-Leggett-Garg inequality with weak measurement of an entangled state T.C. White, J.Y. Mutus, J. Dressel, J. Kelly, R. Barends, E. Jeffrey, D. Sank, A. Megrant, B. Campbell, Yu Chen, Z. Chen, B. Chiaro, A. Dunsworth, I.-C. Hoi, C. Neill, P.J.J. O'Malley, P. Roushan, A. Vainsencher, J. Wenner, A. N. Korotkov, John M. Martinis Submitted (2015). arXiv:1504.02707
- Scalable extraction of error models from the output of error detection circuits Austin G. Fowler, D. Sank, J. Kelly, R. Barends, John M. Martinis Submitted (2014). arXiv:1405.1454
- Quantum theory of a bandpass Purcell filter for qubit readout Eyob A. Sete, John M. Martinis, Alexander N. Korotkov PRA 92, 012325 (2015). arXiv:1504.06030
- Tunable coupler for superconducting Xmon qubits: Perturbative nonlinear model Michael R. Geller, Emmanuel Donate, Yu Chen, Michael T. Fang, Nelson Leung, Charles Neill, Pedram Roushan, John M. Martinis PRA 92, 012320 (2015). arXiv:1405.1915
- Digital quantum simulation of fermionic models with a superconducting circuit R. Barends, L. Lamata, J. Kelly, L. Garca-Ivarez, A. G. Fowler, A. Megrant, E. Jeffrey, T. C. White, D. Sank, J. Y. Mutus, B. Campbell, Yu Chen, Z. Chen, B. Chiaro, A. Dunsworth, I.-C. Hoi, C. Neill, P. J. J. O'Malley, C. Quintana, P. Roushan, A. Vainsencher, J. Wenner, E. Solano, John M. Martinis Nature Communications 6, 7654 (2015). arXiv:1501.07703
- Traveling wave parametric amplifier with Josephson junctions using minimal resonator phase matching T.C. White, J.Y. Mutus, I.-C. Hoi, R. Barends, B. Campbell, Yu

Chen, Z. Chen, B. Chiaro, A. Dunsworth, E. Jeffrey, J. Kelly, A. Megrant, C. Neill, P.J.J. O'Malley, P. Roushan, D. Sank, A. Vainsencher, J. Wenner, S. Chaudhuri, J. Gao, John M. Martinis APL 106, 242601 (2015). arXiv:1503.04364

- Universal quantum simulation with prethreshold superconducting qubits: Singleexcitation subspace method Michael R. Geller, John M. Martinis, Andrew T. Sornborger, Phillip C. Stancil, Emily J. Pritchett, Hao You, Andrei Galiautdinov PRA 91, 062309 (2015). arXiv:1505.04990
- Qubit metrology of ultralow phase noise using randomized benchmarking P. J. J. O'Malley, J. Kelly, R. Barends, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, A. G. Fowler, I.-C. Hoi, E. Jeffrey, A. Megrant, J. Mutus, C. Neill, C. Quintana, P. Roushan, D. Sank, A. Vainsencher, J. Wenner, T. C. White, A. N. Korotkov, A. N. Cleland, John M. Martinis Phys. Rev. Applied 3, 044009 (2015). arXiv:1411.2613

Appendix B

Recent Yale Publications

The following is a list of the Devoret group's most recent publications and submitted papers from the group website qulab.eng.yale.edu/publications_page.html [accessed November 4, 2015]. The following are **from 2015**:

- Remote Entanglement by Coherent Multiplication of Concurrent Quantum Signals A. Roy, L. Jiang, A. D. Stone, M. H. Devoret Phys. Rev. Lett. 115, 150503 (2015)
- 2.5D circuit quantum electrodynamics Z. K. Minev, K. Serniak, I.M. Pop, Z. Leghtas, K. Sliwa, M. Hatridge, L. Frunzio, R. J. Schoelkopf, M. H. Devoret arXiv:1509.01619v1
- Surface Participation and Dielectric Loss in Superconducting Qubits C. Wang, C. Axline, Y. Gao, T. Brecht, L. Frunzio, M. H. Devoret, R. J. Schoelkopf arXiv:1509.01854v1
- Multilayer Microwave Integrated Quantum Circuits for Scalable Quantum Computing T. Brecht, W. Pfaff, C. Wang, Y. Chu, L. Frunzio, M. H. Devoret, R. J. Schoelkopf arXiv:1509.01127v1
- Demonstration of Micromachined Superconducting Cavities T. Brecht, M. Reagor, Y. Chu, W. Pfaff, C. Wang, L. Frunzio, M. H. Devoret, R. J. Schoelkopf arXiv:1509.01119v1
- Comparing and combining measurement-based and driven-dissipative entanglement stabilization Y. Liu, S. Shankar, N. Ofek, M. Hatridge, A. Narla, K. M. Sliwa, L. Frunzio, R. J. Schoelkopf, M. H. Devoret arXiv:1509.00860v1
- A Quantum Memory with Near-millisecond Coherence in Circuit QED M. Reagor, W. Pfaff, C. Axline, R. W. Heeres, N. Ofek, K. Sliwa, E. Holland, C. Wang, J. Blumoff, K. Chou, M. Hatridge, L. Frunzio, M. H. Devoret, L. Jiang, R. J. Schoelkopf arXiv:1508.05882v2
- Characterizing Entanglement of An Artificial Atom and a Cavity Cat State with Bell's Inequality B. Vlastakis, A. Petrenko, N. Ofek, L. Sun, Z. Leghtas, K. Sliwa, M. Hatridge, J. Blumoff, L. Frunzio, M. Mirrahimi, L. Jiang, M. H. Devoret, and R. J. Schoelkopf arXiv:1504.02512v1
- Single-Photon Resolved Cross-Kerr Interaction for Autonomous Stabilization of Photon-number States E. T. Holland, B. Vlastakis, R. W. Heeres, M. J. Reagor, U. Vool, Z. Leghtas, L. Frunzio, G. Kirchmair, M. H. Devoret, M. Mirrahimi, R. J. Schoelkopf arXiv:1504.03382v1

• Cavity State Manipulation Using Photon-Number Selective Phase Gates R. W. Heeres, B. Vlastakis, E. Holland, S. Krastanov, V. Albert, L. Frunzio, L. Jiang, R. J. Schoelkopf arXiv:1503.01496v1



Figure B.1: Thesis on a napkin