Robust Optimal Control of the Cross-Resonance Gate in Superconducting Qubits

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Abstract

Superconducting circuits are one of the leading architectures in quantum computing. To undertake quantum computing one must be able to perform quantum gates; however, two-qubit gates are still limited in fidelity and gate time. The cross-resonance gate is a two-qubit gate that uses direct microwave drives and has seen much success in its implementation; but, there are theoretical indications that it has not yet reached the coherence limited fidelity value and its gate time is still relatively long compared with other quantum gate methods. Quantum optimal control theory is a powerful tool in the design of controls for quantum operations and has shown the capability to improve gate fidelities and reduce gate times. Robust quantum optimal control methodologies have further built on this to develop high fidelity quantum gates that are robust to uncertainties and noise in the system. In this thesis we use robust quantum optimal control theory to achieve these goals for the cross-resonance gate in a variety of superconducting qubit architectures. First, we investigate two superconducting qubits embedded in a common 3D microwave cavity in which the control drive is implemented via the common cavity mode of the cavity. We determine pulse shapes that implement the cross-resonance gate that are robust to uncertainty in the qubit transition frequencies for both a strictly two-level superconducting qubit and a three-level qubit. Second, we look at the cross-resonance gate with direct drives on each qubit, finding the minimal time to perform the cross-resonance gate with pulses that are robust to uncertainty in a measured system parameter for three cases: two three-level qubits with no drive crosstalk, two three-level qubits with some drive crosstalk, and two two-level qubits. Lastly, we report on simulations undertaken towards implementing a robust, high fidelity cross-resonance gate in a novel superconducting quantum device known as the coaxmon.
Declaration

This thesis and the work to which it refers are the results of my own efforts. Any ideas, data, images or text resulting from the work of others (whether published or unpublished) are fully identified as such within the work and attributed to their originator in the text, bibliography or in footnotes. This thesis has not been submitted in whole or in part for any academic degree or professional qualification. I agree that the University has the right to submit my work to the plagiarism detection service TurnitinUK for originality checks. Whether or not drafts have been so-assessed, the University reserves the right to require an electronic version of the final document (as submitted) for assessment as above.

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Publications

The work presented in this thesis is based in part on the following articles and conference presentations. Figures which have been reproduced with permission from these publications are noted below:

Journal Articles


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Oral Presentations


**Poster Presentations**


• J. L. Allen, R. Kosut, E. Ginossar, *Robust Control of Two Qubits in 3D Circuit QED*, Microphoton, National Physics Laboratory, UK (2016)

Contents

Abstract i

Declaration ii

Acknowledgements iii

Publications v

1 Introduction 1

I Background 7

2 Superconducting Quantum Computing 8

2.1 Superconducting Qubits 9

2.1.1 LC Oscillator 9

2.1.2 Transmission Line Resonator 11

2.1.3 Nonlinearity - towards a superconducting qubit 13

2.1.4 Charge Qubit Hamiltonian 14

2.1.5 Transmon 16

2.2 Coupling Transmons 19

2.3 Quantum Information Processing with Superconducting Qubits 22

2.3.1 External Microwave Driving 22

2.3.2 Single-qubit gates 24

2.3.3 Two-qubit gates 27
CONTENTS

2.3.4 Fault-tolerant Quantum Computing ........................................... 29

3 Quantum Optimal Control ............................................................... 34

3.1 Theory ......................................................................................... 36

3.1.1 Optimal Control Problem .......................................................... 36

3.1.2 Time Evolution of Quantum Systems ........................................... 36

3.1.3 Cost Functions .......................................................................... 37

3.1.4 Quantum Control Landscape ....................................................... 40

3.1.5 Robust Control Technique .......................................................... 42

3.2 Numerical Optimisation ................................................................. 43

3.2.1 Parameterisation of the Problem .................................................. 43

3.2.2 Sequential Convex Programming ............................................... 44

3.2.3 Constraints .............................................................................. 47

3.3 Minimal Time Quantum Control ..................................................... 49

II Novel Contributions ......................................................................... 51

4 Optimal Control of Two Qubits via a Single Cavity Drive in Circuit Quantum Electrodynamics ................................. 52

4.1 "Cross-Resonance" with global cavity driving ................................. 53

4.2 Relevant experimental constraints .................................................. 57

4.3 Two-level Optimal Control ............................................................. 59

4.4 Multilevel transmon model ............................................................. 65

4.5 Discussion ..................................................................................... 69

4.6 Conclusion .................................................................................... 70

5 Time Optimal Robust Cross-Resonance Gate ..................................... 72

5.1 Coupled Multi-Level Systems with Direct Drives .............................. 73

5.2 Cross-resonance Simulation and Optimal Control ............................ 75

5.2.1 Desired Operation .................................................................... 75

5.2.2 Dressed Frame for Hamiltonian .................................................. 77
List of Figures

2.1 A simple LC circuit diagram. .............................................................. 10
2.2 A transmission line resonator can be modelled as a chain of $N$ LC oscillators in the limit $N \to \infty$. .............................................................. 11

4.1 Examples of piece-wise constant pulses before and after the Gaussian filter is applied. (a) Piece-wise constant pulse when the control dimension is set as $N = 25$ constant amplitudes. (b) Pulse shape produced when applying the Gaussian filter to the pulse in Figure 4.1a. (c) Piece-wise constant pulse when the control dimension is set as $N = 50$ constant amplitudes. (d) Pulse shape produced when applying the Gaussian filter to the pulse in Figure 4.1c. .......................... 59
4.2 Flat-top Gaussian with 16 piecewise constant amplitude .............................. 60
4.3 Optimized two-level pulse with no robustness .............................................. 61
4.4 Entanglement $E$ versus pulse number ................................................... 62
4.5 Optimal pulses without filter and with filter .............................................. 63
4.6 Fidelity after optimizing for robustness in two-level approximation .................. 64
4.7 Fidelity after optimizing for robustness in two-level approximation with a filter transfer function ................................................... 64
4.8 Fidelity after optimizing for robustness in both qubit parameters for the two-level approximation with a filter transfer function .................................. 65
4.9 Fidelity of optimized pulses using a multilevel system Hamiltonian comprised of two Duffing oscillators each coupled to a common cavity mode with a single cavity drive. ................................................... 67
LIST OF FIGURES

4.10 Variation in the fidelity $F$ with changing $\omega_a^{(2)}$ for a pulse given without taking into account an error in this parameters during optimisation. ........................................ 68

4.11 Fidelity versus sampled parameter range for multilevel systems ........................................ 68

5.1 Minimum and average infidelity versus time for two coupled three-level qubits with no classical crosstalk and no uncertainty. ....................................................... 79

5.2 Average infidelity versus time for two coupled three-level qubits with no classical crosstalk for uncertainties ranging from 1% to 10%. ....................................................... 80

5.3 Average infidelity versus time for two coupled three-level with some classical crosstalk and no uncertainty compared with the no crosstalk average infidelity results. ....................................................... 82

5.4 Average infidelity versus time for two coupled three-level qubits with some classical crosstalk for uncertainties ranging from 1% to 10%. ....................................................... 82

5.5 Average infidelity versus time for two coupled two-level with no classical crosstalk and no uncertainty. This is compared with the two coupled three-level qubit infidelity results for no crosstalk and some crosstalk. ....................................................... 84

5.6 Representation of leakage for 10 ns, 20 ns, 40 ns, and 80 ns pulses from the results of the three-level simulations with no crosstalk and no uncertainty. ....................................................... 85

5.7 Average infidelity versus time for two coupled two-level qubits with some classical crosstalk for uncertainties ranging from 1% to 10%. ....................................................... 85

6.1 Initial pulse shape for the single-qubit gate optimization ....................................................... 98

6.2 Pulse shapes for the four different constraint cases for the $X_{\pi/2}$ gate. The blue line gives the pulse shape for $c_{1, X}(t)$, the orange line is $c_{1, Y}(t)$, the yellow line is $c_{2, X}(t)$, and the purple line is $c_{2, Y}(t)$. (a) Pulse shape for no frequency constraint or Gaussian filter. (b) Pulse shape with only Gaussian filter during search. (c) Pulse shape with frequency constraint only. (d) Pulse shape with both frequency constraint and Gaussian filter ....................................................... 100

6.3 Pulse shapes after Gaussian filter is applied ....................................................... 101
6.4 Frequency components of the pulse shapes for the four different constraint cases for the $X_{\pi/2} I$ gate. Here, $c_1'(f)$ is the Fourier transform of $c_{1,X}(t)$, $c_2'(f)$ is for $c_{1,Y}(t)$, $c_3'(f)$ is for $c_{2,X}(t)$, and $c_4'(f)$ is for $c_{2,Y}(t)$. (a) Frequency components for no bandwidth constraint or Gaussian filter. (b) Frequency components for only Gaussian filter during search. (c) Frequency components for bandwidth constraint only. (d) Frequency components for both bandwidth constraint and Gaussian filter. 

6.5 Logarithmic plot of pulse infidelity against time in the cases where there is no uncertainty in the system. 

6.6 Logarithmic plot of pulse minimum infidelity against time in the cases where there is uncertainty in the system.
Chapter 1

Introduction

In this modern age of information science, there is a constant need and desire to design better and faster computers to process data and find solutions to more complex problems. As computers became more advanced, more complex problems were discovered and developed; there has been much investment in supercomputers to solve such complex problems. Nonetheless, there are still many problems that are too complex for modern computers to solve. Moore’s Law, in which it is stated that the number of transistors in a circuit doubles approximately every two years, has held true since it was first stated in 1965 [1, 2]. However, it is beginning to reach a saturation point as the transistors become so small that quantum effects begin to become important. Even at this saturation point, there are still complex problems outside of the grasp of modern computers.

In 1959, Richard Feynman suggested the possibility of using quantum effects for computation and further went on to propose using quantum systems to simulate other more complex quantum systems in 1982 [3, 4]. Simulating complex quantum systems is one such example of a problem that is too difficult for modern computers to handle due to the complexity of quantum systems. This suggestion would revolutionise the field of information science by making seemingly impossible to solve problems possible. However, at first the quantum information science field was slow to find interest as it was seen to be an extremely difficult problem; there had been no major examples of the power of quantum systems for information processing. In 1984, the world’s first quantum cryptography protocol was developed in which quantum
effects were used to encode a private key for use in a one-time pad encryption scheme [5]. The nature of quantum mechanics means that it is impossible for an eavesdropper to hack the key undetected and therefore any hacked private key can be discarded to ensure privacy. Using something as fundamental as quantum mechanics for encryption is inherently more secure than the current methods for encryption as the laws of quantum mechanics cannot be broken. Nonetheless, even with the development of this algorithm, interest in the field was still initially fairly minimal.

In 1994, Peter Shor developed a quantum algorithm which would allow a quantum computer to find the prime factors of large integers in a time exponentially faster than the best known classical computers [6]. This breakthrough garnered serious interest in the field as the widely used RSA encryption scheme is based on the assumption that finding the prime factors of very large integers is computationally extremely difficult [7, 8]. Shor’s algorithm demonstrated that with a quantum computer most of the world’s encryption schemes could be hacked. From this demonstration, the quantum information science field grew more rapidly, with more algorithms developed such as the Grover search algorithm in 1996, among many others still being developed [9–13]. From these initial beginnings of quantum computing demonstrations, the quantum information science field grew to encompass many aspects such as quantum metrology [14], quantum cryptography [15], quantum simulation [4], quantum teleportation [16], and of course quantum computing [17].

Since these initial developments, the quantum computing field has grown exponentially and there is currently extensive active research being undertaken by many different research groups. The field has already demonstrated some of the quantum computing algorithms such as Shor’s algorithm, first demonstrated in 2001 on a small scale quantum computer and further demonstrated on another device in 2009 [18, 19]. The field has now developed commercial interest as large companies have begun to invest in the technologies to develop their own quantum computers. IBM, Google, Intel are among some of the global companies that are directly contributing to the development of quantum computers. Additionally, there are many start-up companies beginning to be formed to develop their own quantum computers such as Rigetti Computing in California and Quantum Circuits Inc in Connecticut. Europe and the
UK are also investing in quantum technologies. In 2014 the UK started a network of four research hubs in different areas of quantum information science, with collaborations initially beginning between 17 universities and 132 companies. Further investments in new hubs are now being made. In 2018 Europe also launched its quantum flagship programme to develop quantum technologies.

To develop a quantum computer, one must be able to create and control a coherent quantum state. The key component of a quantum computer is a quantum bit, or qubit, which is a two-level system \[17\]. These qubits can exist in a state of either 0 or 1, much like their counterpart the classical bit. However, due to being quantum states they can also exist in superpositions of the two different states. This leads to a more powerful computer due to the amount of information accessible during the computation before measurement. Additionally, the qubits have the ability to be entangled. This is a purely quantum phenomenon in which qubits that are entangled can no longer be described separately, they are now one quantum state. This additional feature is what truly gives quantum computers an advantage over classical computers.

There are many different candidates for realising these two-level systems including (but not limited to) NMR states \[20, 21\], trapped ions \[22\], quantum dots \[23\], and nitrogen vacancies in diamond \[24\]. Another promising candidate is the superconducting circuit \[25, 26\]. These devices are created using a circuit that is constructed to act as an effective one-dimensional resonator and a superconducting element known as a Josephson junction \[27\]. This element creates the anharmonicity necessary to isolate two levels in the otherwise harmonic state of the one-dimensional resonator\[28\]. Superconducting elements have zero electrical resistance and, as such, exhibit and maintain quantum coherence. Due to the system being macroscopic in size, and operating in the microwave frequency regime, these systems have the advantage of benefiting from the wide range of pre-existing fabrication techniques developed for the electronics and telecommunications industry. As opposed to other systems that are microscopic objects with parameters determined by nature, these systems can be designed to have specific parameters that may be required for certain experiments. Superconducting circuits have been designed to replicate many effects that are seen in cavity
quantum electrodynamics (CQED), which studies lights interaction with matter[29]. However, superconducting systems can be designed in a way to reach regimes previously unreachable in CQED such as the strong-coupling regime [30]. This has led to the development of the field of circuit quantum electrodynamics (cQED).

Quantum information processing requires the ability to precisely manipulate the quantum system in order to perform a desired function. Just as classical computers have logic gates to be performed in order to carry out information processing, quantum computers have quantum gates that are used to perform quantum information processing. To keep the quantum nature of the system it must be sufficiently isolated so that there is no noise, which will then protect the qubits coherence. However, to perform quantum operations on the qubits and measure the outcomes, the system must be exposed to some external interaction. This immediately opens up avenues of environmental noise which then causes decoherence and limits the ability to perform quantum information processing [31]. There are several methods for controlling the qubits in a superconducting device and there has been much progress in engineering these controls to minimise decoherence, however there is still scope for improving the controls. Given that it is now possible to shape control pulses to achieve a desired operation, optimal control theory applied to quantum systems has been shown to be a powerful for designing pulses toward driving quantum gates with high precision [32, 33].

This thesis investigates the use of optimal control techniques to design pulse shapes to achieve a particular quantum operation in various superconducting quantum devices. The aim was to achieve this operation with high fidelity while ensuring robustness to uncertainty in the device. Additionally, it was sought to ensure that the results produced from the optimal control simulations that were directly applicable to experiments and the operation times were shorter than the state-of-the-art implementations. The rest of this introduction outlines the contents of the remaining chapters of the thesis.

Chapter 2 provides the framework for the process of quantum computing with superconducting quantum devices. It introduces superconducting circuits by deriving the Hamiltonian for a one-dimensional resonator and then applies the Josephson junction to the circuit to determine the level structure of the superconducting qubit of choice and show how this is
used to define a qubit. The chapter further discusses ways to couple multiple qubits and how to control them. In particular, the two-qubit entangling gate of interest to this thesis, the cross-resonance gate, is defined. This gate is widely used in superconducting circuits due to its success and relative simplicity of operation.

Chapter 3 lays out quantum optimal control theory and defines the problem to be solved. It discusses the application of optimal control theory to quantum systems by casting the evolution of such systems in a way that is applicable to optimal control theory. Cost functions are defined which define how well the control is performing compared with the solution being sought; these cost functions lead to an area known as quantum control landscapes which are used to search for the optimal control and define the controls optimality. The chapter then goes on to discuss the methods used for designing controls that are robust to uncertainty. There are various ways of searching the control landscape for the optimal solution; this chapter presents one such method that is used in this work. Additionally, experimentally relevant considerations are discussed and methods for including them in the search are defined.

Chapter 4 investigates the implementation of the cross-resonance gate in a 3D superconducting cavity device where the drive is applied via the cavity. This work uses optimal control to design pulses to perform the cross-resonance gate with a global drive on both qubits via the cavity and to ensure this is robust against the uncertainty in measuring the qubit parameters. This work is of great interest as it would reduce the control channels of the system to ensure the decoherence channels are minimised, leading to favourable conditions for scaling up the device to large scale quantum computing. In particular, this work was driven by a collaboration with LeekLab in Oxford university where they were designing 3D cavities for use in superconducting experiments.

Chapter 5 looks at the more traditional implementation for the cross-resonance gate in which the control drives are applied directly to the qubits. Using this system, the minimal time of operation of the cross-resonance gate is sought while still achieving high fidelity robust pulses for some uncertainty in the system. The aim is also to achieve a pulse that is experimentally viable. The simulations are run for three different circumstances: three-level qubits with no classical control crosstalk, three-level qubits with some classical control
crosstalk, and two-level qubits.

Finally, Chapter 6 reviews simulations undertaken toward the implementation of the cross-
resonance gate in a novel superconducting quantum device from LeekLab in Oxford University: the coaxmon device. The simulations undertaken built on the work of the previous chapters to find robust, fast, high fidelity control sequences that were experimentally feasible.
Part I

Background
Chapter 2

Superconducting Quantum Computing

Among the many architectures for building a quantum computer, superconducting circuits are currently one of the most promising [26]. This is due, in part, to the advantage offered by the man-made, macroscopic nature of the system. The devices can be engineered to exhibit ideal parameter regimes for particular experiments using the wide range of pre-existing lithographic fabrication techniques that ensure the parameters are accurately met [34]. The benefit of the use of pre-existing fabrication techniques is further promising as it means the systems could be mass produced once the regime of large scale quantum computation is reached.

Superconducting qubits are created by using a superconducting element, the Josephson junction, in conjunction with standard circuit elements [25]. A general circuit will not exhibit quantum coherence due to resistance which will cause dissipation, meaning any coherence is rapidly lost. Superconducting elements have no resistance due to the electrons forming Cooper pairs and Bose-Einstein condensing once the element reaches its critical temperature [35, 36], with the condensate containing a gap in its energy spectrum. If the gap is larger than the thermal energy of the ionic lattice in the superconductor then the Cooper pairs will not be scattered by the lattice, therefore experiencing no resistance [37]. In these systems, therefore, coherence can be preserved. When combined in the correct orientation with the correct components the circuit can form effective two-level systems which can be used as qubits. These qubits can be coupled to cavities to form superconducting qubit-cavity systems which can reproduce many results from cavity quantum electrodynamics (CQED) and even
reach regimes not previously achievable in CQED. This has produced a rich field of research called circuit quantum electrodynamics (cQED). Circuit quantum electrodynamics systems can be used to investigate fundamental physics, but can also be used as the building blocks of quantum computers [26].

This chapter will describe the physical construction of the cQED systems and will also construct the Hamiltonians for the relevant systems. These will then be put in the context of quantum computing and will show a variety of ways that superconducting systems can be used to perform quantum operations.

2.1 Superconducting Qubits

It is well known that one can construct a quantum harmonic oscillator using circuit components; for example, the combination of an inductor and a capacitor will be shown in this section. However, in this case the level differences will not be well separated and two levels of the oscillator could not be isolated to be used as the basis for qubits. To achieve isolation of two levels from the other level structures a non-linear element can be used, but one that must be dissipationless in order to keep the coherence at a useful level; the Josephson junction is a superconducting element that meets this requirement.

This section will give an overview of the construction of a superconducting qubit Hamiltonian, starting with a quantum harmonic oscillator and show how the superconducting element adds the anharmonic term to make these systems effective two level systems.

2.1.1 LC Oscillator

There is a standard methodology for constructing a circuit Hamiltonian using the circuit diagram [38–40]. A trivial example is using the LC oscillator, as shown in Figure 2.1. Using the standard method the Lagrangian can be found for this circuit

\[
L(\phi, \dot{\phi}) = \frac{C\dot{\phi}^2}{2} - \frac{\phi^2}{2L}.
\]  

(2.1)
2.1. SUPERCONDUCTING QUBITS

Figure 2.1: A simple LC circuit diagram. This behaves as a simple harmonic oscillator when there is no dissipation.

where $C$ is the capacitance, $L$ is the inductance and $\phi$ is the magnetic flux of the inductor. This Lagrangian is constructed of a 'kinetic' term, given by the energy stored in the capacitor as a function of the voltage across it, and a 'potential' term, given by the energy stored in the inductor. From this the Hamiltonian can be found by defining $q = \partial / \partial \dot{\phi}$ and is given by

$$H = \frac{q^2}{2C} + \frac{\phi^2}{2L}.$$  \hspace{1cm} (2.2)

This can be quantised by introducing creation and annihilation operators that obey

$$[a, a^\dagger] = 1,$$ \hspace{1cm} (2.3)

$$\phi = \sqrt{\frac{\hbar Z}{2}} (a + a^\dagger),$$ \hspace{1cm} (2.4)

$$q = -i \sqrt{\frac{\hbar}{2Z}} (a - a^\dagger),$$ \hspace{1cm} (2.5)

with $Z = \sqrt{L/C}$. This then produces the standard quantum harmonic oscillator Hamiltonian

$$H = \hbar \omega \left( a^\dagger a + \frac{1}{2} \right) ,$$ \hspace{1cm} (2.6)
with $\omega = 1/\sqrt{LC}$.

### 2.1.2 Transmission Line Resonator

![Transmission Line Resonator Diagram](image)

Figure 2.2: A transmission line resonator can be modelled as a chain of $N$ LC oscillators in the limit $N \to \infty$. It can be shown that this behaves as a one-dimensional harmonic oscillator in the limit $N \to \infty$.

Another example of a commonly used device is a transmission line resonator. A transmission line resonator of length $d$, with capacitance per unit length $c$ and inductance per unit length $l$ can be treated as a chain of $N$ LC oscillators in the limit $N \to \infty$, shown in Figure 2.2. The Lagrangian for this system is given by

$$
L(\phi_1, \dot{\phi}_1, \ldots, \phi_N, \dot{\phi}_N) = N \sum_{i=1}^{N} \frac{\Delta C \phi_i^2}{2} - \sum_{i=1}^{N-1} \frac{(\phi_{i+1} - \phi_i)^2}{2\Delta L}, \quad (2.7)
$$

where $\Delta C = cd/N$ and $\Delta L = ld/N$. The first term is the sum of the energy stored in each capacitor and the second term is the inductor energy which depends on the flux difference between neighbouring oscillators. In the continuum limit this becomes the integral

$$
L[\phi(x,t), \dot{\phi}(x,t)] = \int_0^d \left( \frac{c \dot{\phi}(x,t)^2}{2} - \frac{1}{2l} \left( \frac{\partial \phi(x,t)}{\partial x} \right)^2 \right) dx. \quad (2.8)
$$

The Euler-Lagrange equation for $\phi(x,t)$ is then
\[ \frac{\partial^2 \phi}{\partial t^2} - v^2 \frac{\partial^2 \phi}{\partial x^2} = 0, \]  

(2.9)

where \( v = 1/\sqrt{lc} \) is the wave velocity. The general solution to this equation is

\[ \phi(x, t) = \sum_{n=1}^{\infty} A_n \cos(k_n x + \alpha_n) \cos(k_n vt + \beta_n), \]  

(2.10)

where \( A_n, k_n, \alpha_n \) and \( \beta_n \) are given by the boundary conditions. Imposing open-circuit boundary conditions at \( x = 0 \) and \( x = d \)

\[ \frac{\partial \phi}{\partial x} \bigg|_{x=0} = \frac{\partial \phi}{\partial x} \bigg|_{x=d} = 0 \]  

(2.11)

gives \( \alpha_n = 0 \) and \( k_n = n\pi/d \). Substituting eqn (2.10) into eqn (2.8) and integrating gives

\[ L(\Phi_1, \dot{\Phi}_1, \ldots) = \sum_{n=1}^{\infty} \left( \frac{C_n \Phi_n^2}{2} - \frac{\Phi_n^2}{2L_n} \right), \]  

(2.12)

where \( \Phi(t) = A_n \cos(k_n vt + \beta_n) \). This is simply an effective Lagrangian for a circuit that consists of uncoupled LC oscillators with effective capacitances \( C_n = cd/2 \) and effective inductances \( L_n = 2dl/n^2\pi^2 \). The quantum Hamiltonian is then

\[ H = \hbar \sum_n \omega_n \left( a_n^\dagger a_n + \frac{1}{2} \right), \]  

(2.13)

with \( \omega_n = n\nu\pi/d \). Generally the modes are well separated and only one mode is able to be excited, usually the fundamental mode, so this simplifies to

\[ H = \hbar \omega_r \left( a_n^\dagger a_n + \frac{1}{2} \right). \]  

(2.14)
2.1. SUPERCONDUCTING QUBITS

Here the \( n = 1 \) subscript has been dropped and \( \omega_r \) is the resonant frequency for the fundamental mode. Thus we have shown that a transmission line can act as a single mode harmonic oscillator.

2.1.3 Nonlinearity - towards a superconducting qubit

As the previous sections have shown, a harmonic oscillator can be constructed using simple circuit elements. It has also been shown how to derive the Hamiltonians of these circuits. As previously mentioned, in order to undertake quantum computing the fundamental building block, the qubit, is required. Qubits are two-level systems where each level can be addressed individually. However, the harmonic levels all share the same energy spacing and cannot be addressed individually. In order to use circuits as qubits some anharmonicity must be introduced into the system to break the degeneracy in the energy separation of the levels.

The Josephson junction is the only known non-linear, dissipationless circuit element; this will allow the harmonic oscillator to become anharmonic. It consists of two pieces of superconductor separated by an insulating barrier [27]. Cooper pairs can tunnel coherently across the insulating barrier, with a supercurrent given by

\[
I(t) = I_c \sin(\phi(t)),
\]

(2.15)

where \( I_c \) is the critical current of the junction and \( \phi(t) \) is the phase difference across the junction [41]. This phase difference evolves in time as

\[
\hbar \frac{d\phi}{dt} = 2eV,
\]

(2.16)

with \( V \) the potential across the junction and the charge of an electron. Taking the time-derivative of eqn. 2.15 gives
\[ \frac{dI}{dt} = (I_c \cos(\phi)) \frac{d\phi}{dt} = \frac{2eV I_c}{\hbar} \cos(\phi). \]  

(2.17)

From Faraday’s law, using \( V = -L \dot{I} \), the Josephson inductance is found to be

\[ L_J = \frac{\Phi_0}{2\pi I_c \cos(\phi)}, \]  

(2.18)

where \( \Phi_0 = h/2e \) is the superconducting flux quantum, which is non-linear. This combined with the intrinsic capacitance of the Josephson junction results in an anharmonic oscillator [28].

### 2.1.4 Charge Qubit Hamiltonian

There are a few different qubit designs depending on the parameter values and what physics dominates the device; the three main kinds are flux, phase and charge qubits [42–52]. Each have their own advantage depending on the operation of the device of interest, but the one of interest here is the charge qubit. In this device the number of Cooper pairs that have crossed the Josephson junction, as counted by the number operator \( n \), acts as a good quantum number for the system.

In order to derive the circuit Hamiltonian for the charge qubit we now replace the linear inductor in the LC circuit with a Josephson junction, and the Hamiltonian in eqn 2.2 becomes

\[ H = \frac{q^2}{2C} - E_J \cos\left( \frac{\Phi}{\Phi_0} \right), \]  

(2.19)

where \( E_J = I_c \Phi_0/2\pi \) is the Josephson energy which characterises the junction, \( \Phi \) is the flux through the junctions, and \( C \) is the total capacitance. Introducing the number operator \( \hat{n} = -q/2e \), which counts the number of Cooper pairs which have been transferred across the
2.1. SUPERCONDUCTING QUBITS

Josephson junction, and the dimensionless phase operator $\varphi = \Phi/\phi_0$, that satisfy $[\hat{n}, e^{i\varphi}] = e^{i\varphi}$, eqn 2.19 can be re-written as

$$H = 4E_C(\hat{n} - n_g)^2 - E_J\cos(\varphi).$$

(2.20)

where $E_C$ is the charging energy and $n_g$ is the effective offset charge of the device induced by an applied electric field. In this circuit the number operator $\hat{n}$ has discrete eigenvalues which correspond to an integer number of Cooper pairs tunneling across the junction. This Hamiltonian can be solved analytically, with the eigenenergies $E_m$ given as

$$E_m(n_g) = E_Ca_2[n_g+k(m,n_g)](-E_J/2E_C),$$

(2.21)

where $a_v(q)$ is the Mathieu’s characteristic value, and $k(m, n_g)$ is a function that orders the eigenvalues [53].

This form of the solution is rather cumbersome; instead the Hamiltonian in eqn 2.20 can be translated into the charge basis by using the relations

$$\hat{n} = i \frac{\partial}{\partial \varphi}$$

(2.22)

$$\hat{n}e^{i\varphi} = e^{i\varphi}(\hat{n} + 1)$$

(2.23)

giving

$$H = 4E_C(\hat{n} - n_g)^2 - \frac{E_J}{2} \sum_n \left( |n\rangle \langle n + 1| + |n + 1\rangle \langle n| \right).$$

(2.24)

In the regime where $E_C \gg 4E_J$, which is deep in the charge regime, the device is known as a Cooper Pair Box. By operating the Cooper Pair Box at a gate charge of $n_g = \pm 1/2$ the system can be reduced to a two-level system with a reduced Hamiltonian
2.1. SUPERCONDUCTING QUBITS

\[ H = 2E_C(1 - n_g)\sigma_z - \frac{E_J}{2}\sigma_x. \]  
(2.25)

2.1.5 Transmon

While operating in the charge regime can be ideal in the view that we effectively have a two-level system, this device is susceptible to charge noise in this regime. Any charge fluctuations cause small changes in \(n_g\) which shifts the qubits transition frequency and causes decoherence of the qubit. Also, even in this two-level regime when operated at the "sweet spot" of \(n_g = 1/2\) the coherence time of the Cooper Pair Box is limited by higher order effects [54].

If, instead, the device was operated in a regime where \(E_J \gg E_C\) the energy levels become insensitive to charge noise [53]. However, the system also becomes less anharmonic and the transition frequencies between higher levels become less distinct. The transmon qubit was designed with such parameters in mind to combat charge noise sensitivity. To see the effect on the energy levels and the anharmonicity when in this regime, first look at the charge dispersion which is defined as

\[ \epsilon_m = E_m(n_g = 0) - E_m(n_g = 1) \]  
(2.26)

for the \(m\)th energy band. In the limit of \(E_J \gg E_C\) this is given as

\[ \epsilon_m = (-1)^m E_C \frac{2^{4m+5}}{m!} \sqrt{\frac{2}{\pi}} \left( \frac{E_J}{2E_C} \right)^{\frac{m+\frac{1}{2}}{2}} e^{-\frac{8E_J}{E_C}}, \]  
(2.27)

which falls off exponentially as \(E_J/E_C \to \infty\) [55].

Since the transmon has weak anharmonicity, it can be treated as a perturbation of a harmonic oscillator. Expanding the cosine in eqn. 2.20 to fourth order gives

\[ H + 4E_Cn^2 - E_J \left( 1 + \frac{\varphi^2}{2} - \frac{\varphi^4}{24} \right). \]  
(2.28)
2.1. SUPERCONDUCTING QUBITS

The offset charge term $n_g$ has been left out as it is exponentially small in the transmon regime. Introducing creation and annihilation operators via

$$n = \frac{i}{2} \sqrt{\frac{E_J}{2E_C}} (c^\dagger - c)$$

$$\varphi = \frac{2E_C}{E_J} (c^\dagger + c),$$

where $c = \sum_j \sqrt{j+1} \langle j | j + 1 \rangle$ is the lowering operator for the transmon, the Hamiltonian can be written in the form of a Duffing oscillator

$$H = \sqrt{8E_CE_J} \left( c^\dagger c + \frac{1}{2} \right) - E_J - \frac{E_C}{12} (c^\dagger + c)^4.$$  

Performing perturbation theory on the last term gives the first-order approximation to the energies

$$E_m \simeq -E_J + \sqrt{8E_CE_J} \left( m + \frac{1}{2} \right) - \frac{E_C}{12} (6m^2 + 6m + 3),$$

which is valid for the lowest few levels. Defining the absolute anharmonicity $\alpha_m$ as the difference of the transition energy between levels $m$ and $m+1$ and the next lowest transition between levels $m$ and $m-1$, we find

$$\alpha_m = E_{m+1,m} - E_{m,m-1} \simeq E_C,$$

where $E_{m,n} = E_m - E_n$.

By comparing this anharmonicity with the ground to first excited state transition $E_{01} \simeq \sqrt{8E_CE_C}$, the relative anharmonicity is then
\[ \alpha_r = \alpha_m / E_{01} = -(8E_J/E_C)^{-1/2}. \] (2.34)

From this it is clear that the anharmonicity falls off algebraically with \( E_J/E_C \). Compare this with the charge dispersion, which falls off exponentially, and we see the advantage of operating in the transmon regime - we can operate far enough in the transmon regime to make the device robust to any charge noise, but still have enough anharmonicity to address two levels individually to operate as a qubit. This has led to devices with coherence times on the order of 10 \( \mu \)s with reduced pure dephasing due to charge noise [53].

Ignoring constant terms, the Hamiltonian in eqn. 2.31 can be rewritten as

\[ H = \sqrt{8E_CE_Jc^\dagger c} + \frac{E_C}{12}(c^\dagger + c)^4, \] (2.35)

Defining \( \hbar \omega \simeq \sqrt{8E_CE_J} + E_C \) and \( \hbar \delta = E_C \), by expanding out the second term in eqn 2.35 and ignoring fast rotating terms via the rotating wave approximation, we obtain

\[ H_{\text{transmon}}/\hbar = \omega c^\dagger c + \frac{\delta}{2} c^\dagger c(c^\dagger c - 1) = \left( \omega - \frac{\alpha}{2} \right) c^\dagger c + \frac{\alpha}{2} (c^\dagger c)^2. \] (2.36)

This can also be written as

\[ H_{\text{transmon}}/\hbar = \sum_j \left( \left( \omega - \frac{\alpha}{2} \right) j + \frac{\alpha}{2} j^2 \right) |j\rangle \langle j| = \sum_j \omega_j |j\rangle \langle j|. \] (2.37)

As \( \alpha \to 0 \) this becomes the equation for a harmonic oscillator, as we would expect and in the large anharmonicity regime the two-level Hamiltonian is recovered.
2.2 Coupling Transmons

In order to perform quantum computing the qubit systems need to be coupled; this can be done in a variety of ways. A common method is to couple the transmons to a common resonator; this can be either a transmission line resonator or a 3D cavity [56, 57]. In either case the transmon will couple to a resonator mode of the cavity depending on where in the cavity it is placed (note: the terms cavity and resonator will be used interchangeably) and will couple strongly with this mode due to its large dipole moment from being a macroscopic object. The cavity also behaves quasi-one-dimensionally and has an extremely small mode volume [25].

The effective Hamiltonian for a single qubit coupled to a resonator is given by

\[ H = 4E_C(n - n_g)^2 - E_J \cos(\phi) + \hbar \omega_r a^\dagger a + 2\beta n e V_0(a^\dagger + a), \]  

(2.38)

where \( \beta \) is the ratio of the gate capacitance to the total capacitance, \( V_0 \) is the zero point root mean-squared voltage and \( 2ne \) is the charge of the transmon. In the basis of the eigenstates of the transmon \(|j\rangle\) this Hamiltonian is given by

\[ \frac{H}{\hbar} = \omega_r a^\dagger a + \sum_j \omega_j |j\rangle \langle j| + \sum_{i,j} g_{i,j} |i\rangle \langle j|(a^\dagger + a), \]  

(2.39)

with \( g_{i,j} = 2\beta V_0 \langle i|n|j\rangle \) are the couplings between the cavity and different transmon transitions. In the asymptotically large \( E_J/E_C \) limit, the matrix elements of this coupling are given by

\[ |\langle j + 1|n|j\rangle| \approx \sqrt{\frac{j + 1}{2}} \left( \frac{E_J}{8E_C} \right)^{1/4}, \quad \langle j + k|n|j\rangle \to 0 \quad \forall |k| > 1. \]  

(2.40)

This implies that in the limit of large \( E_J/E_C \) not only does coupling between non-adjacent levels become negligible, but nearest neighbour couplings become stronger. In the rotating
wave approximation, where terms that excite both the cavity and the transmon simultaneously can be ignored, the Hamiltonian is given by

\[ H/\hbar = \omega_r a^\dagger a + \sum_j \omega_j |j\rangle \langle j| + \sum_j g_{j,j+1} |j\rangle \langle j+1| + |j+1\rangle \langle j| a^\dagger. \tag{2.41} \]

In the regime where there is sufficient anharmonicity that the transmon can be operated as a qubit, the two-level approximation can be taken. Using Pauli spin operators to re-write the Hamiltonian for two-level systems gives

\[ H/\hbar = \omega_r a^\dagger a + \frac{\omega}{2} \sigma_z + g(a\sigma_+ + a^{\dagger}\sigma_-). \tag{2.42} \]

This is the familiar Jaynes-Cummings Hamiltonian from Cavity Quantum Electrodynamics. Thus, superconducting circuits can reproduce the physics of cavity quantum electrodynamics (CQED). With this system otherwise unreachable regimes in CQED are achievable, and so a new research area was formed based on superconducting circuits and CQED called Circuit Quantum Electrodynamics (cQED).

Multiple qubits can be coupled to the same resonator [56]. In this case the Hamiltonian of eqn. 2.41 becomes

\[ H/\hbar = \omega_r a^\dagger a + \sum_{i=1,2} \sum_j \omega_j^{(i)} |j\rangle_i \langle j|_i + \sum_{i=1,2} \sum_j g_{j,j+1}^{(i)} (a^\dagger |j\rangle_i \langle j+1|_i + a |j+1\rangle_i \langle j|_i), \tag{2.43} \]

where the subscript \(i\) denotes the transmon number [58]. In the regime where the qubits are detuned from the resonator, such that \(g_{j,j+1}^{(i)} \ll \omega_{j,j+1}^{(i)} - \omega_r\), the dispersive transformation can be made which is given by

\[ U = \exp \left[ \sum_{i=1,2} \sum_j \lambda_j^{(i)} (a^\dagger |j\rangle_i \langle j+1|_i - a |j+1\rangle_i \langle j|_i) \right]. \tag{2.44} \]
To second order in the parameter $\lambda^{(i)}_j = g^{(i)}_{j,j+1}/(\omega^{(i)}_{j,j+1} - \omega_r)$, the dispersive Hamiltonian is then given by

$$H/\hbar = \omega_r a^\dagger a + \sum_j \left( \omega^{(1)}_j |j\rangle_1 \langle j|_1 + \chi^{(1)}_{j,j+1} |j+1\rangle_1 \langle j+1|_1 \right)$$
$$+ \sum_i \left( \omega^{(2)}_i |i\rangle_2 \langle i|_2 + \chi^{(2)}_{i,i+1} |i+1\rangle_2 \langle i+1|_2 \right)$$
$$- a^\dagger a \left( \chi^{(1)}_{01} |0\rangle_1 \langle 0|_1 + \chi^{(2)}_{01} |0\rangle_2 \langle 0|_2 \right)$$
$$+ a^\dagger a \left[ \sum_{j=1} \left( \chi^{(1)}_{j-1,j} - \chi^{(1)}_{j,j+1} \right) |j\rangle_1 \langle j|_1 + \sum_{i=1} \left( \chi^{(2)}_{i-1,i} - \chi^{(2)}_{i,i+1} \right) |i\rangle_2 \langle i|_2 \right]$$
$$+ \sum_{j,i} \frac{g^{(1)}_{j,j+1} g^{(2)}_{i,i+1} (\Delta^{(1)}_j + \Delta^{(2)}_i)}{2\Delta^{(1)}_j \Delta^{(2)}_i} \left[ |j\rangle_1 \langle j+1|_1 \otimes |i+1\rangle_2 \langle i|_2 + |j+1\rangle_1 \langle j|_1 \otimes |i\rangle_2 \langle i+1|_2 \right].$$

(2.45)

In this Hamiltonian $\chi^{(n)}_{ij}$ is the dispersive coupling for transmon $n$, defined as

$$\chi^{(n)}_{ij} = \frac{(g^{(n)}_{ij})^2}{\omega^{(n)}_{ij} - \omega_r},$$

(2.46)

and $\Delta^{(n)}_j = \omega^{(n)}_{j+1,j} - \omega_r$. In the two level approximation, this Hamiltonian is then

$$H/\hbar = \omega_r a^\dagger a + \frac{1}{2} \left( \omega_1 + 2\chi_1 a^\dagger a \right) \sigma_z^{(1)} + \frac{1}{2} \left( \omega_2 + 2\chi_2 a^\dagger a \right) \sigma_z^{(2)}$$
$$+ \frac{g_1 g_2 (\Delta_1 + \Delta_2)}{2\Delta_1 \Delta_2} \left( \sigma_+^{(1)} \sigma_-^{(2)} + \sigma_-^{(1)} \sigma_+^{(2)} \right).$$

(2.47)

From the Hamiltonians in eqn. 2.45 and eqn. 2.47 it can be seen that, in the dispersive limit, the transmons/qubits and the cavity are effectively uncoupled from one another but the qubits pick up a shift in frequency dependent on the number of photons in the resonator. Additionally the transmon/qubits are effectively coupled to one another due to being coupled to the common mode of the resonator. Thus multiple transmons can be coupled by coupling them to a common cavity mode.
2.3 Quantum Information Processing with Superconducting Qubits

Having outlined the basis for superconducting systems and showing how multiple qubits can be coupled, we now wish to consider how quantum information processing operations may be performed with this system. To perform computations with the qubits we must be able to control them. There are a variety of methods for controlling superconducting qubits, such as flux tuning which is used to dynamically tune the transition frequency of the transmons; this can be used to entangle transmons [59–62]. However, flux-tuning can introduce avenues of decoherence and leakage; one needs to be careful not to tune the transition into resonance with other unwanted interactions or the cavity [63–66]. Another method for control is using microwave drives, where the transition frequency is kept fixed and external microwave drives are used to control interactions [67–70]. This section will introduce some quantum computing operations and show how we can use external microwave drives in order to perform these operations.

2.3.1 External Microwave Driving

To introduce an external microwave drive into the Hamiltonian in eqn. 2.43 an extra term is introduced, given by

\[ H_d = \sum_k \left( a + a^\dagger \right) \left( \epsilon(t)e^{-i\omega_d(k)t} + \epsilon^*(t)e^{i\omega_d(k)t} \right). \]

which represents \( k \) classical time-dependent coherent drives on the cavity; here \( \epsilon \) is the strength and \( \omega_d(k) \) is the frequency of the \( k \)th drive [40, 58]. In the rotating wave approximation, which is valid when the drive strengths are weak compared with \( \omega_r \) and \( g \), the drive term becomes

\[ H_d = \sum_k a\epsilon^*(t)e^{i\omega_d(k)t} + a^\dagger\epsilon(t)e^{-i\omega_d(k)t}. \]

We shall consider a drive that is off-resonant with the cavity, so that only interaction with
the transmons are of interest. To see this a displacement operation is performed, given by
the Glauber displacement transformation

\[ D(\alpha) = \exp[\alpha(t)a^\dagger - \alpha^*(t)a]. \tag{2.50} \]

Focusing, for now, on a single transmon coupled to a cavity with a single coherent drive, this
transformation is applied to eqn. 2.41 to give

\[
H' / \hbar = D^\dagger (H + H_d) / \hbar D - i D^\dagger \dot{D} \\
= \omega_r a^\dagger a + \sum_j \omega_j |j\rangle \langle j| + \left[ g(a^\dagger c + ac^\dagger) + g(\alpha^* c + \alpha c^\dagger) \right] \\
+ (a^\epsilon^*(t)e^{i\omega_d t} + a^\dagger \epsilon(t)e^{-i\omega_d t}) + \omega_r (\alpha a^\dagger + \alpha^* a) - i(\dot{\alpha} a^\dagger + \dot{\alpha}^* a). \tag{2.51}
\]

Choosing \( \alpha(t) \) as a solution of the differential equation

\[
- i \dot{\alpha}(t) + \omega_r \alpha(t) + \epsilon(t)e^{-i\omega_d t} = 0, \tag{2.52}
\]

simplifies the Hamiltonian to

\[
H' / \hbar = \omega_r a^\dagger a + \sum_j \omega_j |j\rangle \langle j| + g(a^\dagger c + ac^\dagger) \\
+ \frac{1}{2} \sum_j \left( \Omega^*(t)e^{i\omega_d t} + \Omega(t)e^{-i\omega_d t} \right), \tag{2.53}
\]

where \( \Omega(t) = 2g\alpha(t) \); for a time-independent drive this is given by \( \Omega = 2\epsilon g / (\omega_r - \omega_d) \). This
now shows the external microwave drive acting on the transmon transitions.

In the dispersive limit this Hamiltonian becomes
2.3. QUANTUM INFORMATION PROCESSING WITH SUPERCONDUCTING QUBITS

\[ H''/\hbar = \omega_r a^\dagger a + \sum_j |j\rangle \langle j| + \sum_j \chi_{j,j+1} |j+1\rangle \langle j+1| - \chi_0 |0\rangle \langle 0| + \sum_j \left( \chi_{j-1,j} - \chi_{j,j+1} \right) a^\dagger a |j\rangle \langle j| + \frac{1}{2} \left( \Omega^* (t) e^{i\omega_d t} + \Omega (t) e^{-i\omega_d t} \right). \] (2.54)

In the qubit limit this becomes

\[ H/\hbar = \omega_r a^\dagger a + \frac{\omega'_a}{2} \sigma_z + \left( \Omega^* (t) \sigma_x e^{i\omega_d t} + \Omega (t) \sigma_+ e^{-i\omega_d t} \right), \] (2.55)

with \( \omega'_a = \omega_a + 2\chi a^\dagger a. \)

2.3.2 Single-qubit gates

One of the most basic operations for a quantum computer is a single qubit operation \[17\]. Generally it is desired to perform a rotation about an axis defined by the Pauli operators \( \sigma_x, \sigma_y, \sigma_z \) given by

\[ R_n(\theta) = e^{-i\theta \sigma_n / 2} = \cos \left( \frac{\theta}{2} \right) - i \sin \left( \frac{\theta}{2} \right) \sigma_n, \] (2.56)

with \( n = x, y, z \), where \( \theta \) is the angle of rotation. If one can generate any of these rotations then these can be combined to form standard single qubit operators such as the Hadamard gate.

In the qubit approximation choosing \( \Omega (t) = \Omega_x (t) + i\Omega_y (t) \) and moving to the rotating frame of the drive gives the Hamiltonian

\[ H/\hbar = \Delta_r a^\dagger a + \frac{\Delta'_r}{2} \sigma_z + \left( \Omega_x (t) \sigma_x + \Omega_y (t) \sigma_y \right). \] (2.57)

By choosing the drive frequency to be resonant with the qubit frequency (and such that it is
2.3. QUANTUM INFORMATION PROCESSING WITH SUPERCONDUCTING QUBITS

far off-resonant with the cavity so there is no appreciable cavity population, giving \( \langle a^\dagger a \rangle \), the above Hamiltonian will generate rotations about the \( x \) and \( y \) axis depending on the choice of the amplitudes. For example, choosing \( \Omega_x = \Omega \pi \) and \( \Omega_y = 0 \) with the drive on for some time \( t_g \) such that \( \int_0^{t_g} \Omega \pi \, dt = \pi \) will generate a \( \pi \) rotation about the \( x \)-axis.

In the case of a transmon, which is really a multi-level system, performing single-qubit rotations is not as straightforward. As the anharmonicity is weak there is the risk of leakage out of the computational state basis, particularly when the bandwidth of the control is comparable to the anharmonicity, as tends to be the case with transmons. The anharmonicity of a transmon is typically around 300MHz, which is close to the bandwidth of the shortest applied microwave pulse of 1 ns. To mitigate against any leakage a proposal was made to use pulses optimized by analytic investigations \[71\textit{-}73\].

To derive the optimal pulse we shall work in the basis that was used in ref \[71\]. In this case the transmon is truncated to three levels, giving the computational basis and one leakage level. For simplicity the cavity is ignored so the Hamiltonian is given by

\[
H/\hbar = \sum_{j=1,2} \left[ \omega_j \, |j\rangle \langle j| + \varepsilon(t) \lambda_j \left( |j\rangle \langle j - 1| + |j - 1\rangle \langle j| \right) \right], \tag{2.58}
\]

where \( \lambda_j \) is a weighting factor. For the sake of the derivation \( \lambda \) is set as \( \lambda_1 = 1 \) and \( \lambda_2 = \lambda \).

Ideally \( \lambda = 0 \) and thus we are simply in the two-level approximation, however this is generally not the case. Allowing two-quadrature control over the drive, the Hamiltonian becomes

\[
H/\hbar = \sum_{j=1,2} \Delta_j |j\rangle \langle j| + \frac{\Omega_x(t)}{2} \left( |0\rangle \langle 1| + |1\rangle \langle 0| \right) + \frac{\lambda \Omega_x(t)}{2} \left( |1\rangle \langle 2| + |2\rangle \langle 1| \right) + \frac{\Omega_y(t)}{2} \left( |0\rangle \langle 1| + i |1\rangle \langle 0| \right) + \frac{\lambda \Omega_y(t)}{2} \left( |1\rangle \langle 2| + i |2\rangle \langle 1| \right), \tag{2.59}
\]

with \( \Omega_x(t) \) the Rabi rate for the \( x \)-quadrature, and \( \Omega_y(t) \) the Rabi rate for the \( y \)-quadrature.

To quantify the leakage to the third level the adiabatic transformation
2.3. QUANTUM INFORMATION PROCESSING WITH SUPERCONDUCTING QUBITS

\[ V = \exp\left[ -i \Omega_x(t) \left( |1\rangle \langle 0| - i |0\rangle \langle 1| + \lambda (|2\rangle \langle 1| - i |1\rangle \langle 2|) \right) / 2\alpha \right], \quad (2.60) \]

can be applied to the Hamiltonian \(2.59\), which becomes

\[
\frac{H}{\hbar} = VHV^\dagger + i \dot{V}V^\dagger \\
= \frac{\Omega_x}{2} \left( |1\rangle \langle 0| + |0\rangle \langle 1| \right) + \frac{\lambda \Omega_x^2}{8\alpha} \left( |2\rangle \langle 0| + |0\rangle \langle 2| \right) \\
+ \left( \Delta_2 + \frac{(\lambda^2 + 2)\Omega_x^2}{4\alpha} \right) |2\rangle \langle 2| \\
+ \left( \Delta_1 - \frac{(\lambda^2 - 4)\Omega_x^2}{4\alpha} \right) |1\rangle \langle 1| \\
+ \left( \Omega_y(t) + \frac{\dot{\Omega}_x}{2\alpha} \right) \left[ (|1\rangle \langle 0| - i |0\rangle \langle 1|) + \lambda (|2\rangle \langle 1| - i |1\rangle \langle 2|) \right]. \quad (2.61) \]

The drive is turned off at \( t = 0 \) and \( t = t_g \) meaning the effect of the applied pulses is the same in both frames.

This Hamiltonian shows that a drive that performs a rotation about the \( x \)-axis will pick up a phase error due to the \( y \)-rotation term (first part of line 3), and also induce some leakage (second term of line 3). However, this term can be removed by setting

\[ \Omega_y(t) = -\frac{\dot{\Omega}_x}{\alpha}. \quad (2.62) \]

One can also remove a phase shift error to the first excited state by setting the detuning of the drive to

\[ \Delta_1 = \frac{(\lambda^2 - 4)\Omega_x^2(t)}{4\alpha}. \quad (2.63) \]

Errors can be removed to higher order, as documented in ref [71], but shall not be documented here.

This technique is termed DRAG (derivative removal by adiabatic gate) [71]. It has been
2.3. QUANTUM INFORMATION PROCESSING WITH SUPERCONDUCTING QUBITS

successfully implemented in experiment to achieve high fidelity single-qubit gates in transmon system and is now used as standard in multi-level single-qubit gates for superconducting circuits \[72\].

2.3.3 Two-qubit gates

The true power offered by quantum computing comes about through the ability to entangle quantum states \[17\]. As entanglement requires at least two qubits we must be able to perform a two-qubit entangling operation. There is currently a rich area of research in how to perform two-qubit entangling gates in superconducting circuits, although it appears that many research groups are settling for some of the best that fit with their architecture and improving these \[74\], \[75\]. Examples of such gates can be found in ref \[26\], these include the geometric phase gate, the 11-02 gate, and the sideband transitions for generating Bell states.

While these gates have been very successful at performing entangling operations with high fidelities, their design procedures can be relatively complex. Another popular two-qubit gate, and the focus of this thesis, is the cross-resonance gate for fixed-frequency off-resonant qubits \[67–69, 74\]. This gate uses only microwave control to perform the entangling operation, with the desired interaction being only single-qubit rotations away from a CNOT gate, thus making it suitable for universal quantum computing.

Cross-Resonance Gate

The original set up for the cross-resonance gate, as implemented by IBM, is two qubits coupled to a common resonator with direct drives on each qubit \[68, 69, 74\]. These qubits are off-resonant with one another and also with the cavity. Therefore starting with the Hamiltonian in eqn. 2.47 and including a single drive term on one of the qubits gives

\[
H/\hbar = \frac{\omega_1(t)}{2} \sigma_z^{(1)} + \frac{\omega_2(t)}{2} \sigma_z^{(2)} + J \left( \sigma_+^{(1)} \sigma_-^{(2)} + \sigma_-^{(1)} \sigma_+^{(2)} \right) + \left( \Omega_1(t) \sigma_-^{(1)} e^{i\omega_1^{(1)} t} + \Omega_1(t) \sigma_+^{(1)} e^{-i\omega_1^{(1)} t} \right),
\]

(2.64)
where \( \omega'_j = \omega_j + 2\chi_j a^\dagger a \), \( J = g_1 g_2 (\Delta_1 + \Delta_2)/(2\Delta_1 \Delta_2) \), the drive is on the first qubit only and we have chosen to ignore the cavity term (since \( \langle a^\dagger a \rangle \approx 0 \)).

In much the same way as with the dispersive transformation, another transformation can be performed based around the qubit-qubit coupling which is weak compared with the detuning of the qubits. In order to do this a Schrieffer-Wolff transformation (see Appendix A) is performed with

\[
S^{(1)} = \frac{J}{\Delta_{12}} (\sigma_+^{(1)} \sigma_-^{(2)} - \sigma_-^{(1)} \sigma_+^{(2)}).
\]  

(2.65)

In the rotating frame of the drive, the Hamiltonian now becomes

\[
H_{\text{eff}}/\hbar = \tilde{\Delta}_1 \sigma_z^{(1)} + \tilde{\Delta}_2 \sigma_z^{(2)} + \Omega(t) \left( \sigma_x^{(1)} - \frac{J}{\Delta_{12}} \sigma_z^{(1)} \sigma_x^{(2)} \right),
\]  

(2.66)

where, for simplicity, we have set \( \Omega^*_1(t) = \Omega_1(t) = \Omega(t) \). Here, we have \( \tilde{\Delta}_j = \tilde{\omega}_j - \omega_d \), where \( \tilde{\omega}_1 = \omega'_1 + J^2/\Delta_{12} \), \( \tilde{\omega}_2 = \omega'_2 - J^2/\Delta_{12} \), and \( \Delta_{12} = \omega'_1 - \omega'_2 \).

Eqn. 2.66 shows that if a microwave drive directly coupled to qubit 1 is driven at the resonant frequency of qubit 2 a two-qubit controlled operation (the \( \sigma_z^{(1)} \sigma_x^{(2)} \) term) can be performed. If we can generate a unitary operation given by

\[
U = \exp \left( -i \frac{\pi}{4} \sigma_z^{(1)} \sigma_x^{(2)} \right),
\]  

(2.67)

then, by performing single qubit operations before and after this, one can generate the CNOT gate as

\[
\text{CNOT} = \exp \left( i \frac{\pi}{4} \sigma_x^{(1)} \right) \exp \left( i \frac{\pi}{4} \sigma_z^{(1)} \sigma_x^{(2)} \right) \exp \left( i \frac{\pi}{4} \sigma_x^{(2)} \right).
\]  

(2.68)

This gate is termed the cross-resonance gate due to the use of the cross-coupling between
the two qubits. It is currently in use in the IBM quantum experience, where the gate fidelities are $\approx 0.95$ with gate times of approximately 200ns [76]. An optimized version of the cross-resonant gate has also been shown to perform the desired operation with a fidelity of $F = 0.991 \pm 0.002$ for a 160 ns gate [74]. This is performed after a tune up procedure determines the optimal gate time, amplitudes and phases of multiple drives on both qubits involved.

So far the cross-resonance gate has not hit the coherence limit allowed by the lifetimes of the qubits and the gate times are still relatively long compared with other two-qubit gates [59–61, 77]. However, it has many advantages as the relative simplicity of its operation is favourable; fundamentally all it requires is a direct microwave drive on one qubit to perform the entangling operation. Therefore, all that is needed to control the cross-resonance is control of the microwave pulse shape, the frequency and the phase, each of which are easily manipulated in experiment. Additionally, it requires fixed-frequency qubits allowing for one to tune the qubits to such a spot as to keep the long lifetimes offered by transmons in cavities. Since it is all-microwave control, perhaps there is a way to use the pulse shaping to achieve the cross-resonance with high-fidelity by using “clever” pulse shapes, rather than the more obvious well known pulse shapes. Optimal control has the power to find such pulse shapes and is the subject of the next chapter.

2.3.4 Fault-tolerant Quantum Computing

Quantum information is inherently fragile and any disturbance can destroy the coherent quantum states; this makes implementing quantum computers an extremely difficult task [78]. To circumvent this, methods have been developed and used to extend the coherence times of the coherent states and suppress any errors that may arise during the operation of the quantum computer. As discussed earlier, engineering tasks have been undertaken to extend the lifetimes of superconducting qubits by designing new types of qubits and protecting them via cavity coupling. However, even with these extended lifetimes, there will still be some other sources of decoherence due to external sources. Additionally, imperfect gate implementation or external disturbances can cause errors during the operation of quantum algorithms that destroy their effectiveness.
2.3 QUANTUM INFORMATION PROCESSING WITH SUPERCONDUCTING QUBITS

Error correction codes have been widely developed for classical computers, but these are based on a digital framework while manipulations of qubits for quantum computing are analogue. Therefore, it was necessary to develop codes specifically for error correction on qubits. Initially, several papers were published that proposed codes appropriate for error correction on quantum data [79–83]. As the field of quantum error correction grew, further progress was made in developing quantum codes and introducing new concepts such as fault-tolerant quantum computation which led to the threshold theorem being developed [84–94].

As mentioned previously, noise is a huge problem in quantum information processing, generally destroying any of the benefits of using quantum states. Ideally, when designing a quantum computer, the system should be isolated as much as possible to protect against noise. However, perfect isolation is not possible and there will inevitably be some errors due to the effects of noise. In classical error correction, the method for protecting against noise is to encode the information in multiple bits, in what is known as redundancy. Therefore, if any of the information is corrupted by noise there should be enough redundancy to recover the encoded information [17]. Unfortunately, the no-cloning theorem prevents quantum information from being copied [95]; however, it is possible to spread the quantum information of one qubit over many qubits by entangling them, thus creating the redundancy and forming a logical qubits [79]. Quantum error correction codes give the encoding and decoding of the quantum information over the many qubits and are generally designed to combat certain errors.

One thing to consider is that in order to entangle the qubits to form the logical qubit, quantum gates must be performed. The issue is that generally the quantum gates are themselves imperfect and likely to cause errors; this is where the theory of fault-tolerance comes in. The essence of fault-tolerant quantum computing is to ensure that any errors that occur do not cascade, i.e. the errors are not propagated throughout the computation to other qubits and degrade the algorithm. More detailed explanations of how errors cascade are beyond the scope of this thesis, but can be found in various references [17, 96]. Essentially, the definition of fault-tolerance is that a single error will cause at most $n$ errors in the output for each logical qubit, where $n$ is the number of errors that can be corrected by any error correction procedure.
that may be implemented. A logical qubit, in this case, is one that is used to perform the quantum operations. Logical qubits are made up of many physical qubits and are encoded using an error-correction code. Generally, the more physical qubits that are used for a logical qubit, the higher the number of errors that can be corrected (for certain schemes).

A consequence of fault-tolerant circuit design and the ability to perform error correction is the threshold theorem. The threshold theorem states that it is possible to perform an arbitrarily large quantum computation as long as the noise in individual quantum gates is below a certain threshold [94]. This threshold varies depending on the architecture used and the quantum error correction protocol used. Initial estimates put the threshold at $10^{-4} - 10^{-6}$, but these did not sufficiently model the physical architectures [94, 97]. More recent estimates that take into account realistic architectures have been estimated, which have shown that the physical architecture has a significant impact on the threshold [98–100].

One fault-tolerant error correction methodology being sought in superconducting quantum computing is the surface code architecture [101–104]; this is a topological error correction code developed from Toric codes [97]. Toric codes used qubits distributed on the surface of a toroid for topological fault-tolerance, but this was found to be somewhat unnecessary and planar versions were eventually developed. The surface codes have a significant tolerance to local errors [105, 106]; the per-operation error rate of surface codes is around 1% [107, 108], which is far less stringent than other quantum computational approaches [99]. These are ideally suited for superconducting qubits, and other solid-state quantum computers, as they only require nearest-neighbour coupling over a simple two-dimensional layout.

One downside to surface codes is the large number of physical qubits required to make one logical qubit. A minimum of thirteen physical qubits is required to implement a single logical qubit, while a reasonably fault-tolerant logical qubit that can be used effectively in surface codes requires around $10^3$-$10^4$ physical qubits [104]. The number of physical qubits required to make a logical qubit depends on the error rate per physical qubit, where error rates just below the threshold will mean more physical qubits are required to make a logical qubit. Clearly, as more than one logical qubit is required to perform quantum algorithms, scaling up this architecture will require thousands or even millions of physical qubits. At this stage of
2.3. QUANTUM INFORMATION PROCESSING WITH SUPERCONDUCTING QUBITS

The development of quantum computing we are not in a position to build one logical qubit out of thousands of physical qubits, but finding manipulations for quantum computing that beat the threshold for surface code error rates is still an interesting challenge. It would ensure that once these large logical qubits could be created, then there are operations in place to use them effectively.

**Noisy Intermediate Scale Quantum Computing**

It appears that the near term outlook for fault tolerant quantum computing is looking rather bleak due to the sheer number of physical qubits required. Additionally, individual quantum gate fidelities are not yet high enough by themselves to perform fault tolerant quantum computing. Recently there have been some published materials suggesting a rather pessimistic outlook to quantum computing [109, 110]; however, these are in a small minority.

While in the near term we may not necessarily have a full working quantum computer, there are currently a number of small imperfect quantum computers being used such as the 16-qubit device offered by IBM on the cloud [76]. Other groups have plans to begin using around 50 qubit quantum computers for proof of principle quantum computing. All these quantum computers will use imperfect gate implementations, with fidelities on the order of $F = 0.96 - 0.99$. Later in the thesis we shall see results that fall within this range of fidelities. While none of these is necessarily large enough, nor perfect enough, to perform ideal quantum computation it is still an interesting time to test the power of quantum computing. Recently there has been an interest in what is termed Noisy Intermediate Scale Quantum (NISQ) technology [111]; these are the imperfectly implemented quantum technologies with on the order of 50-100 qubits performing operations. It is thought that even in these noisy devices we may begin to see tasks performed that surpass today’s classical computers. These devices will be useful tools for exploring many-body quantum physics, as well as many other uses that are discussed in [111], such as quantum annealing and quantum simulation. Thus, even in the near term with small quantum computers, or with gate fidelities around $F = 0.96 - 0.99$, the outlook may not look so bleak and there may be uses yet for these noisy devices. Nonetheless, the aim should still be to achieve the most accurate quantum gates and fault-tolerant quantum
2.3. QUANTUM INFORMATION PROCESSING WITH SUPERCONDUCTING QUBITS

computing.
Chapter 3

Quantum Optimal Control

Since the first realisation of the laser researchers have aimed to use laser fields to coherently control quantum systems. With the creation of femtosecond laser pulses and sophisticated pulse shaping technology this goal was initially achieved; chemists in particular used specifically tailored pulses to control chemical reactions, something that was otherwise unachievable without the shaping ability \[112\text{-}116\]. There are several techniques for finding the required pulse shapes, such as stimulated-Raman-Adiabatic-Passage (STIRAP) \[117\text{-}118\], Brumer-Shapiro coherent control \[119\], among others. One of the more powerful, and widely used, techniques is quantum optimal control theory \[32\text{-}33\text{-}120\].

Optimal control theory is concerned with finding a control law in order to satisfy some optimal cost function for a given system. It is an extension of the calculus of variations, and is widely used to solve many problems in engineering, mathematics and physics \[121\text{-}123\]. In the late 1980s and early 1990s, several papers were published suggesting that it would be possible to steer the evolution of a quantum system by designing laser control fields \[124\text{-}128\]. Further, it was specifically considered that optimal control theory could be used to tailor laser pulse shapes to achieve a desired goal, sparking a field known as quantum optimal control theory (QOCT) \[124\text{-}135\].

Quantum optimal control is becoming more widely used in the realm of quantum computation and information, with many new techniques being developed to design controls for the purpose of quantum computation \[136\text{-}141\text{-}141\text{-}157\]. To perform quantum computation
the operations need to be performed with extreme accuracy since errors will accumulate; in a quantum system any errors are more catastrophic than in a classical system. There is a lot of research into finding new ways of implementing quantum gates with fewer errors and improving the implementation by improving hardware [74, 158]. However, this can be slow and hardware may be fundamentally limited. Instead, pulse shaping techniques to improve the gate implementation can be investigated and by extension quantum optimal control theory can be used to find control solutions to the problem. This is an extremely powerful tool that has seen good results already in practice and may provide more immediate results than attempting to improve hardware.

There are numerous different techniques within quantum optimal control theory to find the optimal solution to a problem. Generally the methods used are ways to search the optimal control landscape by finding maxima and climbing to the top in an effort to find the optimal solution [159]. A powerful subset of QOCT algorithms are the gradient based local search algorithms, which have been shown to converge to optimal solutions rapidly given some good choice of initial conditions [136, 139, 146, 160–164]. In general, the optimal control algorithms are designed to search for the optimal control field to find the desired final solution, often with constraints. However, many times the simulation does not take into account uncertainty in the system parameters or noise within the system, features that are certainly present during experimental implementation. Incorporating these features into the simulation further adds to the desirable output of the optimal control algorithm and ensures the implementation achieves the high fidelity in the presence of realistic uncertainty.

In this chapter we will describe quantum optimal control theory and how it can be used to find shaped pulses for performing desired quantum operations. This chapter introduces the optimal control theory, defining the problem and a general procedure for how to search for the optimal control. The robust optimal control technique is outlined in reference to the work undertaken in this thesis. Additionally the algorithm of choice for this thesis, Sequential Convex Programming (SCP), is described and details of how to include the robustness techniques in this algorithm are laid out. This algorithm is relatively new to the QOCT field but we show the power of SCP and its suitability for robust control compared with other QOCT
algorithms.

3.1 Theory

Generally theoretical work is concerned with one of two problems. First, is the system controllable, i.e. given a certain quantum system can a specified target be reached with a given control? Second, what is the best way of reaching the target? Optimal control theory is concerned with the second problem of finding the best control in order to achieve a certain target. To see how this is done, each part of the problem must be defined.

3.1.1 Optimal Control Problem

The general optimal control problem can be formulated in the following way [120]. Given a set $X$ of state functions $x : \mathbb{R} \to \mathbb{R}^n$, and a set $\mathcal{U}$ of control functions $\varepsilon : \mathbb{R} \to \mathbb{R}^m$, find the functions $x$ and $\varepsilon$ such that the cost function $J : X \times \mathcal{U} \to \mathbb{R}$ is minimized (or maximized) subject to the dynamical constraint

$$\frac{dx}{dt} = f(x, \varepsilon). \quad (3.1)$$

The cost function $J$ varies depending on the type of problem to be solved. Later in the chapter we shall see an example of cost functions for the quantum control setting.

3.1.2 Time Evolution of Quantum Systems

To apply optimal control to the quantum setting, the dynamical constraint must be determined. The time evolution of a quantum system of dimension $N$ without dissipation, in general form, can be described by

$$i\dot{U}(t) = \left( H_0 + \sum_k \varepsilon_k(t) H_k \right) U(t), \quad t \in [0, T], \quad U(0) = I, \quad (3.2)$$

where $U(t)$ is the time evolution of the system at time $t$, $H_0$ is the free Hamiltonian, $\varepsilon_k(t)$
is the $k$th control function at time $t$, and $H_k$ is the $k$th control Hamiltonian. The free Hamiltonian, $H_0$ describes the dynamics of the quantum system without the control, while the control Hamiltonians $H_K$ describe the coupling of the quantum system to the control field and the dynamics the system goes through due to the drive.

Taking the time integral of eqn 3.2 from time $t = 0$ to $t = T$ gives the time evolution operator

$$U(T, 0) = \mathbb{T} \exp \left( -\frac{i}{\hbar} \int_0^T \left( H_0 + \sum_k \varepsilon_k(t) H_k \right) dt \right).$$

Here, $\mathbb{T}$ denotes the time evolution operator. This time ordering operator fully describes the dynamics of the quantum system from $t = 0$ to $t = T$ and can be applied to some quantum state $|\psi(0)\rangle$ to find the state at time $t = T$ via $|\psi(T)\rangle = U(T, 0) |\psi(0)\rangle$.

It should be noted that eqn 3.2 is in the form of the dynamic constraint of equation 3.1. Relating the forms, the $x$ variable in eqn. 3.1 is given by $U(T)$ in eqn. 3.2 and the $\varepsilon$ variable is given by $\varepsilon(t)$. This gives

$$f(x, \varepsilon) = -i(H_0 + \sum_k \varepsilon_k(t) H_k) U(t).$$

Therefore, quantum systems have an equivalent equation describing the dynamic constraint in optimal control theory and it could be possible to apply optimal control techniques to quantum systems. The next sections define the optimal control problem for quantum systems and how to find optimal solutions.

### 3.1.3 Cost Functions

As the dynamics of a quantum system have been defined in a way that is suitable for optimal control theory, the next step is to determine cost functions $J$ to measure the effectiveness of the controls. All cost functions can be defined in the general form
which are the general class of control objective functionals with $F$ being a continuously differentiable function on $U(N)$ and $G$ a continuously differentiable function on $U(N) \times \mathbb{R}$. The first term defines a cost function that depends on the evolution at final time $T$, while the second term accumulates with time. Generally the first term is the definition of some functional that determines how close the system evolution is to some target operator. The types of problems with just the first term as the cost function are known as Mayer problems. The second term generally defines constraints on the system. Problems with just the second term for the cost function are known as Lagrange problems. When both cost function are present it is known as a problem of Bolza \[33, 120\].

The cost functions take a variety of forms depending on what the problem is. For example, if the problem is to generate some time evolution operator $U(T)$ that is as close as possible to some desired unitary $W$, the Mayer-type cost function could take the general form

$$F(U(T)) = 1 - ||W - U(T)||, \quad (3.6)$$

where $||.||$ is some normalized matrix norm. This cost function is maximized as $U(T)$ gets closer to $W$. If the problem is to steer an initial state $\rho_0$ to some desired final state $\rho_f$, the cost function may take the form

$$F(U(T)) = 1 - ||U(T)\rho_0U^\dagger(T) - \rho_f||. \quad (3.7)$$

Another goal is to maximize the expectation value of a target quantum observable $\Theta$, as is the case for observable control. In this case, the cost function is given by

$$F(U(T)) = \text{Tr}(U(T)\rho_0U^\dagger(T)\Theta). \quad (3.8)$$
This type of cost functional may be more useful in experiment as the expectation value is easier to measure than the final state of the quantum system.

In quantum computation, the goal is to implement logical qubit operations, generally as single- and two-qubit gates; these are usually unitary operators. As such, the goal is to design control fields such that the time evolution of a quantum system resembles the unitary operator for the quantum gate being undertaken. Therefore, the cost function of interest is that given in eqn. 3.6. This cost function can generally be defined as the fidelity and can take many different forms. One such popular choice of this cost functions is given as

$$\mathcal{F} = \left| \frac{1}{n_s} \text{tr}(W^{\dagger} \hat{O} U(T) \hat{O}) \right|^2.$$  \hspace{1cm} (3.9)

Here $W$ is the desired final state and $\hat{O}$ is the projection operator from the $N \times N$ space to the subspace of interest which is of size $n_s \times n_s$. In this definition $\mathcal{F} \in [0, 1]$, with $\mathcal{F} = 1$ when there is no measurable distinction between $W$ and $U(T)$, and no leakage out of the relevant subspace.

Another form of the fidelity function which is more applicable to experiment is the average fidelity, defined as the average fidelity between the actual output state and the ideal output state over all possible input states \[165\]. This fidelity function is given by

$$\mathcal{F}(\xi, W) \frac{\sum_j \text{tr}(W A_j^\dagger W^{\dagger} \xi(A_j))}{d^2(d+1)}.$$  \hspace{1cm} (3.10)

In this equation, $W$ denotes the ideal unitary operation, $A_j$ denote the set of input operators such as the 16 two-qubit Pauli matrices, $\xi$ maps the input state to an output state via the dynamics of the quantum system, and $d$ is the dimension of the Hilbert space. In general, $\xi$ is determined via quantum process tomography which is carried out in experiment. This fidelity function is used in Chapter 6, where a short review of quantum process tomography is also given.
3.1. THEORY

In the later parts of this chapter we shall define some constraints that may be on the systems and in these constraints we shall define some cost functions of the Lagrange type if they are required.

3.1.4 Quantum Control Landscape

The previous section defined a metric to indicate how close an output is to its ideal output. Following this there are a couple of questions to be asked: 1) given a certain problem, does an optimal solution exist? 2) How does one search for an optimal solution? Initially, a few studies described conditions under which optimal solutions exist, but did not explore the complexities in searching for the optimal solutions [166–168].

A relation exists between the control variables and the cost function, whereby the cost function changes depending on the control variables; this relation defines the control landscape [33, 169, 170]. Analysis of the control landscape can establish whether optimal control solutions exist and what kind of solution it is, whether it is a global optimal solution or a local. By moving through this landscape, searches can be carried out to find the optimal solution and determine whether it is a globally optimal solution or a locally optimal one by further analysis of the landscape [170]. There has been much work looking into the analysis of quantum control landscapes for a variety of problems and defining conditions under which the optimisation search converges on the optimal solutions [171–177].

The formal definition of a quantum control landscape requires a reforming of the cost functional. Following [33], consider a control problem for a closed quantum system with unitary evolution, where the evolution is over some fixed time $T$. The endpoint map $V_T : \mathcal{C} \mapsto \mathcal{U}(T)$ from the space of control functions to the space of unitary evolution operators is generated by the Schrödinger equation, given by eqn. 3.2, so that $U(T) = V_T(\varepsilon(.))$. Further, a Mayer-type cost function $F(U(T))$ defines a map $F$ from the space of evolution operators to the space of real-valued costs. Therefore, the composition of these two maps $J = F \circ V_T : \mathcal{U} \mapsto \mathbb{R}$ is a map from the space of control functions to the space of real-valued costs, which generates the functional $J[\varepsilon(.)] = F(V_T(\varepsilon(.)))$. The functional $J[\varepsilon(.)]$ is referred to as the control landscape. In this case, the control problem can be expressed as
the unconstrained search for

\[ J_{\text{opt}} = \max_{\varepsilon(.)} J[\varepsilon(.)]. \]  \hspace{1cm} (3.11)

The critical points of the landscape areas where the first-order functional derivative of \( J[\varepsilon(.)] \) with respect to the control field is zero for all time

\[ \frac{\delta J[\varepsilon(.)]}{\delta \varepsilon(t)} = 0, \quad \forall t \in [0, T]. \]  \hspace{1cm} (3.12)

By using the gradient of the control landscape with respect to the control field, searches of the control landscape can be made to find the optimal solutions which should exhibit the relation given in eqn. \[ \text{3.12} \]. This defines a method for searching for optimal solutions to quantum optimal control problems. Many popular and efficient search methods use the gradient of the landscape to find optimal control solutions, later in the chapter we shall describe one such method.

One pitfall of using eqn. \[ \text{3.12} \] as an identifier of an optimal solution is that this relation does not distinguish between saddle-points, minima, or maxima \[ 33 \]. Generally, if the search demands that the cost functional \( J[\varepsilon(.)] \) always increases then it is unlikely the search will stop in a minima. However, this does not stop the search from becoming stuck in a saddle-point \[ 176 \]. Additionally, there is much speculation as to the structure of quantum control landscapes and the existence of local maxima that may trap a search from finding the global maxima. A variety of papers have been published stating that under certain conditions the landscape is trap-free and, further, that all local optimal solutions are also global solutions \[ 178,182 \]; but there has also been a rebuttal to this claim \[ 183 \]. Nevertheless, studies of quantum control landscape topologies are still a very active research field and will certainly help with finding optimal solutions and determining their type \[ 170, 176, 179, 182, 184, 189 \]. One thing is also certain, if the search is constrained in any way this can introduce artificial local traps that make exploring the landscape more difficult \[ 190 \]. Constraints may have to
be implemented in the search to find realistic and implementable solutions, causing the search to be more complex. Later in this chapter, some examples of such constraints will be given.

### 3.1.5 Robust Control Technique

Quantum information processing requires precise control of the system to steer it to the desired final state; this can be very difficult due to potential sources of uncertainty in the system such as noise in the system, inaccuracies in the measurement of the system parameters, and fluctuations in the fields \[153, 190, 191\]. Ideally one would have a control system that was robust to these types of uncertainties.

There are a variety of techniques in order to overcome the uncertainty in the system \[192-195\]; one such example is feedback control where designed control fields are implemented and the readout is fed back in order to re-optimise if necessary \[33, 191, 195-197\]. This is known as closed-loop quantum control. While this method can be very effective, it is difficult to implement in quantum systems as the time scales of the operations are extremely small and any measurement of the system produces some back action which will affect the results \[17\]. Robust techniques can also be implemented in open-loop quantum control, where no feedback signal is necessary \[33\]. Examples of open loop in experiment are dynamical decoupling \[198-200\] and noise filtering \[201\], which have both been used to enhance robustness in quantum information processing. Optimal control techniques can also be used in the open-loop format to design control fields that are robust to defined uncertainties and fluctuations \[153, 190, 191\].

One method to design control fields that are robust to uncertainties is to implement the robust technique known as sampling-based learning control. In this method, uncertainty parameters \(\delta \in \Delta\) are sampled, where \(\Delta\) is the full range of the uncertainty and \(\delta\) are the sampled parameters. The fidelity is calculated for the system with the different sampled parameters, creating a vector of fidelity values. With this output optimal control techniques can be used to find controls, \(\varepsilon \in E\), that maximise the worst-case fidelity (\(E\) is the allowed set of controls). Other sampling-based control methods try to maximise the average fidelity \[153, 191\], but this is generally not a stringent enough requirement for quantum systems as we require high-fidelity controls for quantum information processing \[190\]. By demanding
the maximisation of the worst-case fidelity it is ensured that all values of fidelity are better than the worst-case thus ensuring that there are no low values. If instead the average were maximised it may be that certain fidelity values in the uncertainty range perform significantly lower than the average fidelity and are counterbalanced by the higher fidelity values in the rest of the range. During the operation of the designed pulse the parameters may drift to these detrimental values, which will reduce the fidelity of the desired operation even though the final reported average fidelity may be much higher.

### 3.2 Numerical Optimisation

Generally the problem of finding the optimal control for quantum systems cannot be performed analytically as the systems become extremely complex and large; in this case we can use numerical methods to find the optimal control. Numerical optimal control algorithms are split into two classes [202]: 1) gradient ascent algorithms [136, 203], and 2) Krotov-type algorithms [161, 204, 205]. The two classes of algorithms differ by the method of updating the control; gradient ascent algorithms update the controls for all times simultaneously, while the Krotov-type algorithms update the controls for all times sequentially. A comparison has previously been made of the two types of numerical optimal control algorithm and found that gradient ascent type algorithms can be more successful in finding high fidelity controls, while the Krotov type algorithms can be more successful in optimising for robustness [146]. For quantum gates, high fidelity is of paramount importance, which suggests that gradient based algorithms will be more suited to finding controls for gates. Robust techniques can be combined with gradient based algorithms to find robust pulses with high fidelity.

#### 3.2.1 Parameterisation of the Problem

To perform numerical optimisation, a method of parameterising the problem must be chosen. The method most widely chosen is a piece-wise constant approximation whereby the control field is split into $M$ constant amplitudes of length $\Delta t = T/M$. The $j$th Hamiltonian is then given by
3.2. NUMERICAL OPTIMISATION

\[ H^{(j)} = H_0 + \sum_k \varepsilon_k^{(j)} H_k. \quad (3.13) \]

As this is now constant over each \( \Delta t \), the dynamical constraint equation 3.2 can be integrated directly with \( U(0) = I \) to give

\[ U(T) = U_M U_{M-1} \ldots U_2 U_1, \quad (3.14) \]

with

\[ U_j = \exp \left[ -i \Delta t H^{(j)} \right] = \exp \left[ -i \Delta t \left( H_0 + \sum_k \varepsilon_k^{(j)} H_k \right) \right]. \quad (3.15) \]

This now ensures that the simulation of the time evolution of the system is manageable computationally and that the gradient can be calculated as a vector of each of the individual control pixels defined as the piecewise constant amplitude.

3.2.2 Sequential Convex Programming

Finding an optimal control using the above formalism requires an algorithm that can search the control landscape based on the parameterisation. To implement the robust control techniques we also require an algorithm that can meet the requirements of the maximizing the minimum fidelity across the range of sampled parameters - one such algorithm is sequential convex programming (SCP) [190, 206].

SCP is a gradient based optimal control algorithm, falling within category 1) of numerical optimal control algorithms. In this algorithm we initialize the problem with a control from the feasible set, \( E \), which is assumed to be convex. If we are interested in robust control we also take samples, \( \delta_i, i = 1, \ldots, L \) from the uncertainty set \( \Delta \), which is not necessarily convex. A convex trust region, \( \tilde{E}_{\text{trust}} \), is also initialised which is chosen so that the linearised fidelity

\[ \mathcal{F}(\varepsilon, \delta_i) + \varepsilon^T \nabla_{\varepsilon} \mathcal{F}(\varepsilon, \delta_i), \quad (3.16) \]
where $\tilde{\epsilon} \in \tilde{E}_{\text{trust}}$, used in the optimization step retains sufficient accuracy. Each iteration returns the optimal $\tilde{\epsilon}$ to improve the fidelity (or the worst case fidelity if undertaking robust control). This optimization step, using the linearized fidelity, is gradient based and results in $L$ affine constraints in $\tilde{\epsilon}$. This is then a convex optimization problem.

The full algorithm goes as such:

1. • Guess some initial control $\epsilon \in E$.
   • Set the trust region size $\tilde{\epsilon}_{\text{trust}}$.
   • For robust control, select a sample of uncertain parameters $\delta_i \in \Delta$, $i \in [1, L]$ where $L$ is the number of samples.

2. Calculate the fidelities $F(\epsilon, \delta_i)$ and the gradients $\nabla_\epsilon F(\epsilon, \delta_i)$ with respect to $\epsilon$ at each uncertainty sample.

3. Using the linearized fidelity $F(\epsilon, \delta_i) + \tilde{\epsilon}^T \nabla_\epsilon F(\epsilon, \delta_i)$, solve for the increment $\tilde{\epsilon}$ from the convex optimization:
   
   \begin{align*}
   \text{maximize} & \ min_i [F(\epsilon, \delta_i) + \tilde{\epsilon}^T \nabla_\epsilon F(\epsilon, \delta_i)] \\
   \text{subject to} & \ \epsilon \in E, \ \tilde{\epsilon} \in \tilde{E}_{\text{trust}}.
   \end{align*}

4. Calculate the fidelities with new control $F(\epsilon + \tilde{\epsilon}, \delta_i)$.
   • If $\min_i F(\epsilon + \tilde{\epsilon}, \delta_i) > \min_i F(\epsilon, \delta_i)$ then update the initial control, increase the trust-region $\tilde{E}_{\text{trust}}$.
   • Otherwise, decrease trust-region.

5. Run algorithm from step 2 and continue until some stopping criteria is satisfied.

**Stopping Criteria**

There are a variety of criteria for which the algorithm can stop, all of which can be set by the user:
3.2. NUMERICAL OPTIMISATION

- **Maximum number of iterations reached.** In this work this is generally set to be 1000 which we have seen to be sufficient to find a good control while keeping the algorithm run time reasonable.

- **Fidelity change tolerance.** This is the difference in fidelity between each iteration, if the change is below some threshold the optimizer stops. For much of this work this is set to $\Delta F = 10^{-12}$.

- **Trust-region tolerance.** This is the minimum size the trust-region can be, if it goes below this figure the optimizer exits. This is generally set to $\min(\tilde{E}_{\text{trust}}) = 10^{-8}$.

- **Elapsed Time/CPU Time** We can set maximums on the computational time for the optimization. In this work this is set to infinity as it was found that the algorithm converged in reasonable time.

**Comparison with GRAPE**

One of the most well known quantum optimal control algorithms is GRAPE (GRadient Ascent by Pulse Engineering) [136]. It is also a gradient-based local search algorithm and has been used to great success in theoretical optimal control research as it is generally quick to converge to a solution [139, 203, 207].

The GRAPE methodology is similar to SCP. To do a search in GRAPE a starting pulse must be chosen, as with SCP, and the cost function is calculated using this initial pulse guess. The gradient of the cost function with respect to the control function is calculated. The difference in the two algorithms is that for GRAPE the gradient is used to directly update the control via

$$
\varepsilon_k^{(j)} \rightarrow \varepsilon_k^{(j)} + s \frac{\partial J}{\partial \varepsilon_k^{(j)}},
$$

where $s$ is some step size that is either predefined or can be chosen during the search. This step guarantees an increase in the cost function at every step.
3.2. NUMERICAL OPTIMISATION

While GRAPE has proven to be a powerful local search algorithm, it is unable to accommodate maximising the worst-case fidelity that is desired for the robust control of this thesis. For the robust search with SCP, multiple instances of the linearised fidelity in eqn. 3.16 are calculated for each sampled parameter $\delta_i$. With these multiple instances, the optimal increment $\tilde{\epsilon}$ is determined so that all linearised fidelities for each uncertain parameter increase. This optimal increment is then inserted into the methodology defined above to determine if the new worst-case fidelity is greater than the previous. For GRAPE, as the control is directly updated via the gradient, the only way to include robustness is to maximise the average fidelity and calculate the fidelity with respect to the average fidelity [153, 191]. The update step then guarantees an increase in the average fidelity and not the worst-case fidelity.

3.2.3 Constraints

In order to keep the results more experimentally relevant we can impose constraints on the optimization [32]. If these constraints are not imposed, much of the time the optimizer may return a result that is physically unfeasible, particularly if assumptions are made in the construction of the system, or the parameterisation of the problem allows these unphysical results. The constraints can either be hard-coded so that the search cannot break them, or they can be included in the cost function as something to minimize over. Here we shall go over a few examples, some of which are included in this work.

**Maximum/Minimum Amplitudes**

One simple such constraint that is most commonly used is a constraint on the maximum and minimum amplitudes [190]. If this is not set, the optimizer has been known to return results with amplitudes in the 10’s of GHz, which would be detrimental in experiments due to the large bandwidth of such a pulse. In this optimizer, the way this is included is to hard-code in the maximum and minimum. If during the search, a pulse is produced in the optimization process with amplitudes outside of this constraint, then the optimizer resets the amplitude to be at the maximum/minimum for this point.
3.2. NUMERICAL OPTIMISATION

Filtered Pulse

A piece-wise constant approximation to a pulse has many constant amplitude parts. The changes between each piece-wise constant amplitude happen infinitesimally quickly, with no rise time. In reality, when this pulse is input into the device for control of the qubit, there will be some finite rise time and the piece-wise constant amplitudes will be smoothed out. Additionally, when the pulse is applied to the device it must go through some attenuation and filtering as it enters the dilution refrigerator that holds the device. This will also lead to some smoothing and filtering of the pulse. It would be desirable to simulate this and ensure it is accounted for in the search to produce the most realistic result [190, 208]. Later in this thesis a filter function is defined and applied during the search. Much like the amplitude constraint, rather than applying a cost function to penalise the fast rise time of the pulse the filter is applied during the search as a hard coded constraint.

Operation Time

By virtue of choosing the time evolution over a specific time the problem is constrained to operate in this time, as opposed to finding the optimal time for the operation. This in itself is a constraint. However, it may also be sought to find a solution that occurs in a time faster than the predefined evolution time. In this case it may be desired to include a cost function that penalises longer operation times and constrains the pulse to earlier operation times [120, 157]. An example of such a cost function is

$$J = 1 - \frac{1}{N} \sum_{j=1}^{N} \left| \text{tr}(K_j^T K_j) / n_s \right|^2,$$

(3.18)

where $K_j = U_j U_{j-1} \ldots U_1 U_0$. This cost function accumulates size with time and is therefore minimised if the time is minimised. This is an example of a Lagrange type cost functional where the integral has been replaced by a summation.
3.3 Minimal Time Quantum Control

An important goal in quantum control is to perform gates in short times such that incoherent errors do not degrade the performance of the gate. This leads naturally to a question of how to find controls that perform the gate in the shortest time possible (ideally while still being realistic controls) and what is the shortest time possible for the quantum gates. As mentioned in the previous section, we can include a cost function in the search that penalises longer gate operation times during the search algorithm to help find shorter gate times. Along with this method, there are also other methods to design these short gate times.

Ultimately, the minimum time to perform some quantum operation has a lower bound due to the finite energy constraint on controls. This lower bound is closely related to the time-energy uncertainty relation and is termed the quantum speed limit [209]. Initially, a time-energy uncertainty relation was derived that bounded the speed of quantum state evolution in terms of the energy dispersion [210]. Since then there has been much work in determining quantum speed limits for a variety quantum operations [211–216]. An area relevant to quantum computing is the derivation of quantum speed limits for which a quantum system can evolve to some target unitary operator [217]. This has seen a lot of activity in recent years and papers have been published detailing the quantum speed limits on unitary evolution for two-level systems and even multi-level systems [218–223].

While many studies have been published detailing proofs of quantum speed limits for unitary evolution, finding controls that achieve these speed limits has proved to be more challenging. In certain cases, analytical methods can be used to derive controls. Examples of such methods are the quantum brachistochrone problem [224–227], as well as other methods [218, 219, 228–231]. In reality, however, the quantum system Hamiltonians of use will not generally be so simple as there are many dynamics in play. Additionally, the implementations of certain devices for qubits exhibit multi-level structure rather than being restricted to two-level systems. In superconducting qubits, the weak anharmonicity of the transmon qubits means these devices are certainly not limited to two-levels, and there are also the different coupling schemes to take into account plus spurious couplings to unwanted transitions and decoherence effects. Numerical methods for finding minimal time controls amounts to a brute-
force method whereby optimal control algorithms are run multiple times for many different start points for each time point [223, 232–234]. Using the results, the minimal time achievable by these methods is then extrapolated. These methods, while perhaps less appealing than the analytical methods, have shown improving effectiveness in finding minimal time controls. While the numerical methods have not necessarily achieved the theoretical quantum speed limits [223], they have shown improvements over the experimental implementations of certain gates where time optimality has not been taken into account [233]. In Chapter 5, we use the numerical technique to find improved gate times when compared with the experimental implementation.
Part II

Novel Contributions
Chapter 4

Optimal Control of Two Qubits via a Single Cavity Drive in Circuit Quantum Electrodynamics

When designing a quantum computer one of the key considerations is the lifetime of the qubit and how this can be affected by design and control. For a quantum system to behave as a qubit, and be able to perform the many quantum operations required to perform quantum algorithms, the lifetime of the qubit must be long enough that the quantum state does not degrade past some threshold during the operations [17]. To keep the lifetime of the qubit as long as possible one can isolate the system from the environment to try and mitigate any unwanted interactions that can cause dephasing and decoherence. For example, the state-of-the-art lifetime of a superconducting qubit is a transmon embedded in a 3D cavity, which is of the order of $\approx 0.1 \text{ ms}$ [235]. This is specially designed to exhibit extremely long lifetimes.

To perform quantum operations the qubits must be addressable via some kind of probe. In superconducting circuits, the method for achieving this is to input a control line to the system so that the qubits can be driven; this can be either by flux biasing or by microwave control. Seemingly the more control lines the better as this means there are more control "knobs" to tune. However, as more control lines are added the more avenues for decoherence open up. Any control input to the cavity carries with it some loss mechanism; for example,
dielectric loss coming from flux-bias line \[53, 236-238\]. There is therefore a trade-off between the longest lifetime a system can have versus how controllable the system can be.

In this chapter we investigate the use of a single microwave drive applied to a superconducting resonator embedded with two transmons to implement the cross-resonance gate; this is done to reduce the number of controls needed to perform quantum gates and thus keep the avenues of decoherence down. This is applicable to 3D systems, where the transmons are embedded in a 3D cavity. In this case it will ideally take advantage of the long lifetimes offered by the combination of transmons in 3D cavities. Additionally, this is applicable to 2D superconducting system where the transmons are coupled to a common resonator. Here, the reduction in control lines will aide in reducing decoherence. We find that for both the two-level approximation, and the multi-level situation, it is possible to find pulses that are able to perform the "cross-resonance" gate with a single, global drive.

Robustness is also a key factor considered in this chapter and we show good results when including robustness in the simulation versus not including it. The results show that we are able to find pulses that are robust to $\pm1\%$ error in one of the qubit frequency parameters. However, when increasing this to both qubit frequency parameters the algorithm does not perform as well; in this case we consider how this could be made better.

4.1 “Cross-Resonance” with global cavity driving

As was shown in chapter 2, the cross-resonance gate is an all-microwave gate that utilises the coupling between two qubits to generate a two-qubit operation. In general this is performed in a system where the qubits have individual local drives \[68, 69, 74\]; this is to ensure that the cross-resonance drive, which is on-resonance with the target qubit but applied to the control qubit, does not induce any unwanted rotations in the target qubit during the operation. However, including more drives in the system opens up more avenues for decoherence. It is possible to control the qubits by driving the common cavity that they are coupled to; single-qubit operations require the drives to be on resonance with the target qubit, if the qubits are far detuned this will not drive single-qubit rotations in the other qubit. In the case of a
3D cavity system it is currently\(^1\) not possible to include local drives on the qubits without destroying any of the coherence time advantages offered by embedding the qubits in the cavity in the first place. This section will show how a cross-resonance interaction can be performed by driving via the common cavity.

The system is driven using a “global” drive; this is a microwave drive coupled to a cavity mode \([40, 58, 145]\). In this case it is coupled to the same cavity mode as the qubits, thus any drive on the cavity is also “felt” by the qubits. If all the components of the system are detuned from one another, then by choosing the correct drive frequency one can choose which component to address. This is explicitly shown by considering the Hamiltonian of the system in this case. For the case of two transmons coupled to a common cavity with a cavity drive, the Hamiltonian is \([40, 58]\):

\[
H = \omega_r a^\dagger a + \sum_{i=1,2} \omega_{ji} |j_i\rangle \langle j_i| + \sum_{i=1,2} g_i (a^\dagger c_i + a c_i^\dagger) + (\varepsilon(t)a^\dagger e^{-i\omega_d t} + \varepsilon^*(t)a e^{i\omega_d t}), \tag{4.1}
\]

where \(\omega_r\) is the cavity resonance frequency, \(i\) denotes transmon \(i\), \(\omega_{ji}\) is the frequency of the \(j^{\text{th}}\) level of the \(i^{\text{th}}\) transmon \(|j_i\rangle\), \(g_i\) is the coupling between transmon \(i\) and the cavity, \(\varepsilon(t)\) is the time-dependent pulse envelope of the microwave drive, \(\omega_d\) is the drive frequency, \(a^{(\dagger)}\) is the annihilation (creation) operator of the cavity mode photon, and \(c^{(\dagger)}\) is the annihilation (creation) operator of the transmon excitation. For convenience, the \(\hbar\) term has been dropped from this equation and will be dropped for all equations for the rest of the thesis.

In order to highlight the difference between this Hamiltonian in the 3D case, and the usual one derived in the 2D case, the two-level approximation will be made. In this case the Hamiltonian in equation (4.1) now looks like:

\[
H = \omega_r a^\dagger a + \sum_{i=1,2} \frac{\omega_{\alpha}^{(i)}}{2} \sigma_z^{(i)} + \sum_{i=1,2} g_i \sigma_x^{(i)} (a^\dagger + a) + (\varepsilon(t)a^\dagger e^{-i\omega_d t} + \varepsilon^*(t)a e^{i\omega_d t}), \tag{4.2}
\]

\(^1\)as of October 2017
4.1. “CROSS-RESONANCE” WITH GLOBAL CAVITY DRIVING

where $\omega_a^{(i)}$ is qubit $i$ transition frequency, and $\sigma_{x/z}^{(i)}$ are the Pauli spin matrices for qubit $i$. Taking the qubits to be far detuned from the cavity, with $g_i \ll |\Delta_i| = |\omega_a^{(i)} - \omega_r|$, the standard two-qubit dispersive transformation can be applied \cite{26}:

$$ U = \exp \left[ \frac{g_1}{\Delta_1} (a^\dagger \sigma_+^{(1)} - a \sigma_-^{(1)}) + \frac{g_2}{\Delta_2} (a^\dagger \sigma_+^{(2)} - a \sigma_-^{(2)}) \right]. \quad (4.3) $$

Expanding to second order in the small parameter $g_i/\Delta_i$ and dropping fast oscillating terms gives the effective Hamiltonian:

$$ H'' = \omega_r a^\dagger a + \sum_{i=1,2} \frac{\omega_a^{(i)} }{2} \sigma_x^{(i)} + \frac{g_1 g_2 (\Delta_1 + \Delta_2) }{2\Delta_1 \Delta_2} (\sigma_+^{(1)} \sigma_-^{(2)} + \sigma_-^{(1)} \sigma_+^{(2)}) $$

$$ + (\varepsilon(t) a^\dagger e^{-i\omega_dt} + \varepsilon^*(t) a e^{i\omega_dt}) + \sum_{i=1,2} \left( \Omega_R^{(i)} \sigma_+^{(i)} e^{-i\omega_dt} + \Omega_R^{(i)*} \sigma_-^{(i)} e^{i\omega_dt} \right), \quad (4.4) $$

where $\omega_a^{(i)}$ is the shifted qubit frequency given by:

$$ \omega_a^{(j)} = \omega_a^{(j)} + 2 \frac{g_j^2}{\Delta_j} \left( a^\dagger a + \frac{1}{2} \right), \quad (4.5) $$

and $\Omega_R^{(i)} = 2g_i/(\omega_r - \omega_d)$.

In this dispersive limit, as was seen before in chapter \cite{2}, the qubits and cavity are effectively decoupled with the qubit frequencies shifted by some amount depending on the size of the coupling and the photon number inside the cavity (given by terms 1 and 2 in eqn. 4.4). The standard qubit-qubit coupling arises due to the qubits being off-resonance from the cavity but being coupled to the same mode (term 3 of eqn. 4.4). Additionally, the microwave drive contains terms that include the original cavity drive term (term 4 in eqn. 4.4) and one that directly drives the qubits with some reduced amplitude due to the dispersive coupling (term 5 in eqn. 4.4) are given. Thus the qubits can be controlled by driving the same cavity mode.
4.1. “CROSS-RESONANCE” WITH GLOBAL CAVITY DRIVING

they are coupled to.

Eqn. 4.4 shows how the drive can perform single qubit rotation by driving via the cavity. However, it is not clear how entangling operations can be explicitly driven; for this a further transformation is required. If the device is designed so the detuning between the qubits is much larger than the qubit-qubit coupling, i.e. \( J = g_1 g_2 (\Delta_1 + \Delta_2)/2 \Delta_1 \Delta_2 \ll \Delta_{12} = \omega'_{a_1} - \omega'_{a_2} \), then a Schrieffer-Wolff transformation can be made (see Appendix A), with \( s^{(1)} \) given by:

\[
s^{(1)} = -\frac{J}{\Delta_{12}} (\sigma_+^{(1)} \sigma_-^{(2)} - \sigma_-^{(1)} \sigma_+^{(2)}).
\] (4.6)

Performing the Schrieffer-Wolff transformation, the transformed Hamiltonian is given by:

\[
H_{\text{eff}} = \omega_r a^\dagger a + \sum_{j=1,2} \frac{\tilde{\omega}_a^{(j)}}{2} \sigma_z^{(j)} + \Omega_1^{(1)} \left( \sigma_z^{(1)} + \frac{J}{\Delta_{12}} \sigma_z^{(1)} \sigma_x^{(2)} \right) \cos(\omega_c t) + \Omega_1^{(2)} \left( \sigma_z^{(2)} - \frac{J}{\Delta_{12}} \sigma_z^{(1)} \sigma_x^{(2)} \right) \cos(\omega_c t),
\] (4.7)

where \( \tilde{\omega}_a^{(1)} = \omega_a^{(1)} + J^2/\Delta_{12} \), and \( \tilde{\omega}_a^{(2)} = \omega_a^{(2)} - J^2/\Delta_{12} \). This Hamiltonian contains two two-qubit terms \( \sigma_z^{(1)} \sigma_x^{(2)} \) and \( \sigma_z^{(1)} \sigma_z^{(2)} \), which are two-qubit controlled entangling operations. This Hamiltonian is a key result from the derivations; although this set of transformations has been performed for the 2D superconducting system, it has not previously been performed for the 3D case.

Eqn. 4.7 shows that the standard single- and two-qubit terms derived in [68] are still in the effective Hamiltonian, but they occur for both qubits due to the global drive of the cavity. In order to select the operation of choice the drive frequency must be chosen accordingly. As was shown in chapter 2 in the direct driving case, to drive the entangling operation the control qubit must be driven at the target qubits frequency. This has the effect that almost no direct single-qubit operations are performed on the target qubit due to the weak coupling between the qubits (excluding any direct driving from potential crosstalk). However, in the global drive case, eqn. 4.7 demands that to drive the entangling operation will also drive a
4.2 RELEVANT EXPERIMENTAL CONSTRAINTS

single-qubit rotation on the target qubit; this is interesting as it shows that during single-qubit driving an entangling operation is also driven. In general though, the term $J/\Delta_{12} \ll 1$ and the entangling operation performed is negligible when performing the single-qubit operation. For this work, we are interested in driving the two-qubit interaction to perform the entangling operation while mitigating the unwanted single-qubit rotations. In this case, the gate is no longer strictly the cross-resonance gate as both qubits are globally driven, but the target operation is still the same as for the cross-resonance gate.

4.2 Relevant experimental constraints

As previously mentioned in chapter 3 to accurately represent a realistic system in simulation, experimentally realistic constraints must be taken into account. In general, if left unconstrained, the simulation may produce unfeasible solutions as it will not take into account certain effects that would be present in reality. How one includes the constraints depends on its type. There are a variety of constraints that it may be desired to include which shall be discussed in this section.

The first constraint is one of maximum and minimum amplitude of the pulses [190]. Generally, if this is left unconstrained the optimizer could produce pulses with extremely large amplitudes, in the GHz for example. This would cause problems in the experiment as these amplitudes may not be accessible to the microwave generator [239]. Such large amplitude pulses would also open up decoherence in the system and potentially drive unwanted interactions. To simulate the quantum system simplifications must be made in order to keep the computational complexity down; for example, the system is simulated as closed to keep the matrix sizes down. This is considered valid as long as the operations time is not comparable to the lifetime of the qubits. However, this means decoherence is not taken into account; thus when driving with large amplitude pulses, the decoherence effect is neglected in the simulations. A good maximum amplitude can be applied based on discussion with experimentalists and incorporated into the simulation by simply setting it as a hard maximum as described in chapter 3. Any time one part of the pulse goes above the set maximum this
4.2. **RELEVANT EXPERIMENTAL CONSTRAINTS**

is reset to the maximum amplitude, thus constraining the search.

The other constraint relevant to this work is the finite rise times of the real pulses [32, 71]. In the piece-wise constant approximation it is effectively assumed that the rise time between each piece-wise constant part is zero and the change is immediate; of course this is not the case in reality and should be taken into account. Additionally, with zero rise times comes high-frequency components in the Fourier transform of the pulse which could drive unwanted interactions which have not been included in the simulation. To include finite rise times in the simulation we follow the procedure in ref [208] where a filter function is included on the pulse; this is the included in the optimization during the simulation.

The filter is included via a transfer function

\[
s_{k,l} = \sum_{j=0}^{N-1} T_{k,l,j} u_{k,j},
\]

where \(T_{k,l,j}\) is the transfer function, \(u_{k,j}\) is the piece-wise constant amplitude for time slot \(j\) and control channel \(k\), while \(s_{k,l}\) is the new piece-wise constant amplitude for new time slot \(l\). The filter function in this work is the Gaussian filter function given by

\[
T_{k,l,j} = \frac{1}{2} \left\{ \text{erf} \left[ \omega_0 \left( \frac{l \delta t - j \Delta t}{2} \right) \right] - \text{erf} \left[ \omega_0 \left( \frac{l \delta t - (j + 1) \Delta t}{2} \right) \right] \right\},
\]

where \(\delta t\) is the width of the new piecewise constant amplitudes, \(\Delta t\) is the original width, and \(\omega_0\) is the reference frequency for the \(k\)th control.

These filters are a good approximation of the hardware filtering typically found in experiments [208]. These are usually parameterised by their bandwidth \(\omega_B\), which is the frequency of 3dB attenuation. For a Gaussian, 3dB attenuation gives \(\omega_B = 0.5887 \omega_0\). Figure 4.1 shows some examples of applying the Gaussian filter to pulses with different \(\Delta t\). This shows the smaller the width of the piece-wise constant parts, the more extreme the filter effect is. Thus this should filter out some high-frequency components from the pulse as the rise time is more smoothed.
4.3 Two-level Optimal Control

As it is desired to see whether it is possible to perform the desired gate when there is a global drive it is instructive to start with the two-level approximation. Therefore the Hamiltonian in equation 4.7 needs to be adapted to the control problem so that it may be simulated for optimal control. To do this it will be made time-independent and split into a control part and a drift part. In the rotating frame of the drive the drift Hamiltonian is given by

\[ H_0 = \Delta_r a^\dagger a + \sum_{j=1,2} \frac{\tilde{\Delta}_a^{(j)}}{2} \sigma_z^{(j)}, \]

(4.10)

where \( \Delta_r = \omega_r - \omega_d \) and \( \tilde{\Delta}_a^{(j)} = \tilde{\omega}_a^{(j)} - \omega_d \). The control Hamiltonian in the drive frame is given by

\[ H_c = \frac{2g_1}{\Delta_r} \left( \sigma_x^{(1)} + \frac{J}{\Delta_{12}} \sigma_z^{(1)} \sigma_z^{(2)} \right) + \frac{2g_2}{\Delta_r} \left( \sigma_x^{(2)} - \frac{J}{\Delta_{12}} \sigma_z^{(1)} \sigma_z^{(2)} \right), \]

(4.11)

where \( c(t) \) has been set as \( c(t) = \varepsilon(t) \). The control has been set as single quadrature for initial simplicity and there will be no leakage out of the control subspace in the two-level approximation. For the simulations in this chapter the parameters are set as \( \omega_r/2\pi = 6.44 \text{GHz}, \omega_a^{(1)}/2\pi = 4.50 \text{GHz}, \omega_a^{(2)}/2\pi = 4.85 \text{GHz}, g_1/2\pi = g_2/2\pi = 133 \text{MHz} \). These have been chosen as they are relevant superconducting qubit parameters used in a previous work.
The desired unitary is the one given in eqn. 2.67.

Initially, when performing the simulations, only constraints on the amplitude have been included. As discussed in Chapter 3, this fragments the control space whereby certain areas of the control space become inaccessible due to the need for larger amplitudes. This makes the search more difficult as it opens up potential traps for the optimizer to become stuck in, particularly as the optimizer is sensitive to initial conditions due to being a local search optimizer.

The initial pulse for this optimization was chosen to be of the form of a flat-top Gaussian; this is the pulse of choice for the experiments at IBM and has proven to be very effective. In this case, however, it is desired keep the number of piece-wise constant amplitudes low in order to keep the computation time down and see whether high fidelity can be achieved with low dimensional control space. It was found that 16 piecewise constant control amplitudes for the control was the minimum number of pixels that still achieved high fidelity results. The initial pulse using 16 piecewise constant amplitudes is shown in figure 4.2.

Figure 4.2: An example of the flat-top Gaussian-like pulse used as the initial pulse guess in the optimisation for the two-level approximation, where the aim is to achieve the cross-resonance gate. In this pulse the piecewise constant parts are 12.5ns long, with a total pulse time of 200ns. \( c(t) = \frac{\varepsilon(2)}{2\pi} \) gives the pulse amplitude in GHz. Each separate part can be varied to optimize over the problem at hand. This initial pulse gives a fidelity of \( \mathcal{F} = 0.1461 \). (Reproduced from [241])

From these initial conditions, the fidelity produced before optimisation is \( \mathcal{F}_i = 0.1461 \). Upon optimising for the desired operation, given the input constraints, a pulse is found that
generates a two-qubit operation with fidelity $F_j = 0.9945$. The new pulse shape is shown in Figure 4.3 as the outlined area, which is compared with the original pulse, shown in the shaded area. Due to a good choice of initial guess it can be seen that the optimizer has hugged the shape and rapidly found a solution with high fidelity, even with the maximum/minimum constraints and few pulse pixels to optimise over.

Figure 4.3: The initial pulse sequence for the SCP algorithm (coloured area), with $F = 0.1461$, and the optimal pulse sequence (outlined area) showing the variation from initial to final. As is shown, the solution tends to stay close to the initial solution if a good initial guess is chosen. Here $c(t) = \varepsilon(t)/2\pi$ is given in GHz while $t$ is given in ns. This optimal pulse sequence generates the desired unitary with $F = 0.9945$. (Reproduced from [241])

Figure 4.4 shows how the entanglement (given by $2|ab - bc|$ for an arbitrary two-qubit state $|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$) and the fidelity (given by $F = \left|\langle\Phi^-|\hat{U}_m|+y\rangle|+y\rangle\right|^2$, with respect to the state

$$\hat{U}^m|+y\rangle|+y\rangle = \prod_{k=1}^{m} \exp(-iH(t_k\tau)|+y\rangle|+y\rangle);$$

changes with each successive $c(t_k)$. The states $|+y\rangle = (|0\rangle + i|1\rangle)/\sqrt{2}$ are chosen since, when the desired unitary is applied $U_{des}|+y\rangle|+y\rangle = (|00\rangle - |11\rangle)/\sqrt{2}$ which is a maximally entangled Bell state. Figure 4.4 shows that although the fidelity fluctuates, the entanglement monotonically increases with each pulse. This suggests that the pulse shape continually performs the desired two-qubit operations, but has optimized to produce single-qubit rotations

\footnote{This figure and the related fidelity and entanglement calculation were produced by Dr. Jaewoo Joo for the publication [241]}. 

61
at each step such that at the end the qubits will be rotated into the correct basis and that the function performed at the end is effectively just the desired two-qubit operation.

Figure 4.4: Entanglement versus pulse number for the optimized pulse with 16 piecewise constant amplitudes, each amplitude is applied for $\tau = 12.5$ ns. The entanglement $E$ of a pure state is given by $2|ad - bc|$ for an arbitrary two-qubit state $|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$. The fidelity curve is given by $F = |\langle \Phi^{-}\tilde{U}_{m} |+y \rangle + y \rangle |^{2}$ where $\tilde{U}_{m} |+y \rangle + y \rangle = \prod_{k=1}^{m} \exp(-iH(t_{k}\tau) |+y \rangle + y \rangle$. (Reproduced from [241])

Optimal Pulses with Filtering Effects

As mentioned in the previous section, the pulses as shown in figures 4.2 and 4.3 will not be the pulses that reach the cavity and qubits. The microwave pulse will be (mostly low-pass) filtered by control hardware. To model this we use the transfer function method mentioned above and assume the Gaussian filter transfer function. If this were simply added at the end, after optimising without including it, the fidelity of the final pulse drops from $F = 0.9945$ to $F = 0.8303$. However, re-optimizing including the filter function in the simulation gives a new pulse that achieves $F = 0.9947$. Figure 4.5 shows the optimal pulse before re-optimising (coloured area) and the new pulse generated after the filter effect is taken into account in the optimization (outlined area).

Robust Pulses for Errors in System Parameters

The previous results have been obtained for no uncertainty in the system parameters, but as mentioned in chapter 3 this is not truly the case. When simulating the system the uncertainties should be taken into account in order to produce a pulse that is capable of producing high fidelity across the whole uncertain range; therefore, we use the procedure of robust optimal control.
4.3. TWO-LEVEL OPTIMAL CONTROL

Figure 4.5: The optimal pulse when there is no filtering (coloured area) gives a fidelity of $F = 0.8303$ when the simulations takes into account filtering. Upon reoptimising a new pulse is generated (outlined area) which generates the desired unitary with $F = 0.9947$. (Reproduced from [241])

In the first instance optimisation for a single uncertainty in the Hamiltonian with a $\pm 1\%$ error in the transition frequency of qubit 2 $\omega_2 = 4.85 \pm 0.05\,\text{GHz}$ is considered. To perform the robust procedure 11 points are sampled from this range; this number has been shown to be more than adequate to cover the range [153]. Figure 4.6 gives the fidelities for each point sampled from the error range $\omega_2$ after robust optimisation has been undertaken for the system. In the presence of uncertainty in one parameter a solution that can produce the desired unitary with $F > 0.986$ for the whole range has been achieved. Excluding the lowest points, the pulse can produce the gate with fidelities $F > 0.99$ if the uncertain parameter does not fall in the lower range. This is a promising first step as pulses specifically designed to be robust to system uncertainties have not previously been developed. Further, the fidelities produced are comparable to previous state-of-the-art experimental values [68] and values currently in commercial use [76].

The following step was to include the filtering into the single parameter uncertainty. In this case the search becomes much slower as calculating the time evolution operator becomes computationally more expensive due to there being more matrix exponential calculations. Nonetheless, when including the filtering effect to achieve a more experimentally realistic pulse the fidelities shown in the figure 4.7 are achieved. This has improved the previous result as all fidelity values are $F > 0.992$. 

63
4.3. TWO-LEVEL OPTIMAL CONTROL

Figure 4.6: Fidelity against $\omega_a^{(2)}/2\pi$ when there is no filter in the simulation. It can be seen that the fidelity, $\mathcal{F} > 0.986$, and that in the range $4.83\text{GHz} < \omega_a^{(2)}/2\pi < 4.88\text{GHz}$ the fidelities are all $\mathcal{F} > 0.995$. Therefore a robust pulse has been generated for the range of qubit 2 values $\omega_a^{(2)} = 4.85 \pm 0.05\text{GHz}$. (Reproduced from [241])

Figure 4.7: Fidelity against $\omega_a^{(2)}/2\pi$ when the filter effect has been included in the simulation. In this case a robust pulse has been generated that gives $\mathcal{F} > 0.992$ for the whole range $\omega_a^{(2)}/2\pi$. (Reproduced from [241])

As there are two qubits, potential errors in both of the qubit parameters, $\omega_a^{(1)}$ and $\omega_a^{(2)}$, should be accounted for. This proves to be a greater challenge as the drive is on-resonance with the dressed qubit 1 transition frequency and thus will cause the drive to be slightly off-resonance if there are errors. Initially the simulations attempted to find a pulse for $\pm 1\%$ errors in both qubit frequencies: $\omega_a^{(1)}/2\pi = 4.50 \pm 0.05\text{GHz}$ and $\omega_a^{(2)}/2\pi = 4.85 \pm 0.05\text{GHz}$. This was unsuccessful, however, given the initial start point of the previous problem. It was then chosen to reduce the error sampling range for qubit 1 to $\omega_a^{(1)}/2\pi = 4.50 \pm 0.005\text{GHz}$ to find a robust pulse from the same starting control. Figure 4.8 shows the fidelity range. In
this reduced range the optimizer has found a solution that produces all fidelities $F > 0.9875$, with parts of the range achieving $F > 0.99$. This is closer to producing robust pulses with the required fidelity for noisy intermediate-scale quantum computing [111]. In both of these cases the filter effect was included in the simulation as it was previously shown to produce higher fidelity results and is a more realistic implementation of the pulse.

Using the robustness method can be effective at designing a pulse to be robust to errors in some range, but clearly it becomes more difficult as more error parameters are introduced. This can perhaps be solved by choosing different start points for the optimizer, but thus far the flat-top Gaussian has proven to be a good start point for the Hamiltonian and desired unitary of interest.

4.4 Multilevel transmon model

As most charge-based superconducting qubit systems use transmons [53], the system should be simulated as a multi-level system with higher levels to truly simulate the transmon. This is more computationally expensive to calculate but is important for capturing leakage out of the two-level logical basis. In the deep transmon limit, with $E_J/E_C = 100$, the anharmonicities for the transmons are $\delta_1/2\pi = -160\text{MHz}$ for transmon 1 and $\delta_2/2\pi = -170\text{MHz}$ for transmon 2. In this limit, the transmons can be approximated as Duffing oscillators [145, 155].
4.4. MULTILEVEL TRANSMON MODEL

Hamiltonian for two Duffing oscillators coupled to a common cavity mode with a single drive is given by

\[
H = \omega_r a^\dagger a + \sum_{j=1,2} \left( \omega_r^{(j)} c_{j}^\dagger c_{j} + \frac{\delta}{2} c_{j}^\dagger c_{j} (c_{j}^\dagger c_{j} - 1) \right) + \sum_{j=1,2} g_{j} (a^\dagger c_{j} + ac_{j})
\]

\[+ (\epsilon(t)a^\dagger e^{-i\omega dt} + \epsilon^*(t)ae^{+i\omega dt}). \tag{4.13} \]

The first line of the Hamiltonian can be diagonalised to find the Hamiltonian for the cavity + two transmons in the dressed basis, where the frequencies of each component will now include dependencies on all the other parts. For the purposes of optimal control this will form the drift Hamiltonian. The drive term is then transformed to form new operators in the dressed basis and can be used as the new drive term \( H_C \) for the simulations.

For the multi-level simulations, the drive term has been cast into two parts to include complex control as it has been shown that using both quadratures can suppress leakage via the DRAG method outlined in chapter \([71,73]\). The drive term in this case becomes

\[
H_d = \epsilon_a(t) (a^\dagger e^{-i\omega dt} + ae^{+i\omega dt}) + i\epsilon_y(t) (a^\dagger e^{-i\omega dt} - ae^{+i\omega dt}). \tag{4.14} \]

In this new transmon limit the control dimension must be increased in order to reach a good fidelity, as it was found that using the same control dimension as the two-level case was unable to find good fidelity pulses. For these simulations using transmons each piece-wise constant control amplitude is now 2 ns long, which is well within the capabilities of current AWGs. To ensure the computation is not overly complex the Hamiltonian has been truncated to include just a third level to represent a leakage channel. Starting in the case where there are no errors in the system there are many points in time that perform well with fidelities \( \mathcal{F} > 0.9999 \) due to the extra discretisation of the control. Figure \(4.9\) shows the fidelity of the optimized pulses, where each initial pulse has taken the form of a flat-top Gaussian with \( dt = 2 \text{ns} \) for each piece-wise constant amplitude, against time. The fidelities converge to \( \mathcal{F} > 0.999 \) for all times \( T > 100 \text{ns} \).
4.4. MULTILEVEL TRANSMON MODEL

Figure 4.9: Fidelity of optimized pulses using a multilevel system Hamiltonian comprised of two Duffing oscillators each coupled to a common cavity mode with a single cavity drive. The initial pulse had the form of a flat-top Gaussian with each piece-wise constant part being 2 ns long, for different total times ranging from 2 to 200 ns. For $T < 100$ ns the optimized pulses perform poorly, however for all time $T > 100$ ns the fidelity converges to $F > 0.999$ and even to $F > 0.9999$ for certain times in this range.

Robust Pulses

As in the previous section we now investigate the robustness method for a multi-level transmon system, where we look at the same parameter uncertainties as in the two-level approximation. Initially it was chosen to use a pulse designed without robustness and find the fidelity across the range for some uncertainty in $\omega_a^{(2)}$. Figure 4.10 shows a plot of the pulse fidelity $F$ against $\omega_a^{(2)}$ for a pulse that did not take into account uncertainty in the simulation. As is clear, the pulse performs extremely well for the specific parameters used in the simulation, where the fidelity at $\omega_a^{(2)}/2\pi = 4.85$ GHz is $F > 0.9999$. Away from this value the fidelity drops away sharply, thus showing how the fidelity is highly dependent on the parameters chosen.

Following the the previous section we first use the robust methods to find a pulse that is robust to errors in $\omega_a^{(2)}$. In this case the algorithm finds a solution that gives a result of $F \approx 0.9937$ for all values in the range $\omega_a^{(2)}/2\pi \in [4.80, 4.90]$ GHz, shown in figure 4.11a, for a time of 199 ns. This time all the values in the range give the same fidelity value compared with the fluctuating fidelity values in the range for the two-level case. This is likely due to the larger number of degrees of freedom in the control space due to using more piece-wise constant amplitudes for the control.

For the two parameter case the same situation occurs as with the two-level case; for
4.4. MULTILEVEL TRANSMON MODEL

Figure 4.10: Variation in the fidelity $\mathcal{F}$ with changing $\omega_a^{(2)}$ for a pulse given without taking into account an error in this parameters during optimisation. The area of interest is highlighted by the red rectangle: at the ideal parameter, with $\omega_a^{(2)}/2\pi = 4.85$GHz, $\mathcal{F} > 0.9999$, but the fidelity rapidly decreases as the parameter value moves away from the optimal. (Reproduced from [241])

uncertainties of approximately equal size in both qubit frequency parameters the optimizer is unable to find a pulse that produces good robust fidelity. However, in the case that the parameter ranges are $\omega_a^{(2)}/2\pi \in [4.80, 4.90]$GHz and $\omega_a^{(1)}/2\pi \in [4.495, 4.505]$GHz a robust fidelity of $\mathcal{F} \approx 0.9639$ for a gate time of 199 ns is found.

Figure 4.11: Fidelity versus the sampled parameter range for optimized pulses using the robust method on a multilevel system comprised of two Duffing oscillators each coupled to a common cavity mode with a single cavity drive. (a) For the sampled parameter range of $\omega_a^{(2)}/2\pi = 4.85 \pm 0.05$GHz all fidelity values $\mathcal{F} = 0.9937$, outside of this range it can be seen that the fidelity rapidly drops off. (b) For the sampled parameter ranges of $\omega_a^{(2)}/2\pi = 4.85 \pm 0.05$GHz and $\omega_a^{(1)}/2\pi = 4.50 \pm 0.005$GHz, all fidelity values $\mathcal{F} = 0.9639$. Outside of this range it can be seen that the fidelity rapidly drops off. (Reproduced from [241])
4.5 Discussion

In both the two-level case and the multi-level case when finding a robust solution for the single parameter case of just $\omega_a^{(2)}$, the solver is able to achieve solutions with $\mathcal{F} > 0.99$. However, in the case that uncertainty in $\omega_a^{(1)}$ is also included the solver has a much harder time finding a good solution with high fidelity across the whole range. Nonetheless, a pulse is found that achieves $\mathcal{F} > 0.96$ in both cases when considering a smaller uncertainty size in $\omega_a^{(1)}$ compared with $\omega_a^{(2)}$. This is a value that has been discussed as applicable for NISQ devices and is therefore promising for more near-term implementations of quantum information processing.

One of the causes of the discrepancy between the fidelities of the two-level case and the multi-level case is the anharmonicity of the transmons we have simulated. Currently we are operating deep in the transmon regime with $E_J/E_C = 100$ and so one of the limiting factors is down to leakage from the computational subspace as fluctuations in the qubits $\omega_{01}$ transition brings it even closer to the $\omega_{12}$ transition. However, to account for this the number of control dimensions was increased in the multi-level simulations; this has led to better performing controls and more robust solutions. For the multi-level simulations it is clear from Fig 4.11 that the solutions lead to equal fidelities across the optimised uncertain range, whereas for the two-level case the fidelities within the range vary more, as seen in Figures 4.6, 4.7 & 4.8. It would be interesting in future work to reduce the number of control dimensions are determine what the minimum number of dimensions is needed to find a high fidelity robust pulse.

For this work we have chosen not to include errors in the coupling strengths, $g_j$ between the transmons and the cavity. Tests with errors in coupling strengths have shown minimal effect on the output given without including these errors up to 10%. While this range is feasible in experiments this would merely add to the parameter range selection in the simulations, which can be included when performing simulations for real experimental demonstrations. Errors in the cavity frequency have also not been included as the drive and qubit frequencies are far off resonant from the cavity, therefore the cavity frequency effectively plays no part in the dynamics of the system.

This work focused on achieving high-fidelity controls on time scales shorter than decoherence times and, therefore, we did not include decoherence in the simulations. It is important
4.6 CONCLUSION

to correct control errors in this regime if they represent the largest source of infidelity. For example, a state-of-the-art circuit with two transmons with 50 µs coherence times acted on with an entangling unitary operation that requires 200 ns will see a probability of corruption of the operation due to decoherence estimated at 0.4%. Since the typical operations errors due to unoptimised controls will be larger than this, we can focus on optimizing without including decoherence; usually this is the only relevant regime in which we will gain by optimising. However, since some forms of decoherence can be tackled actively with dynamical decoupling schemes [198, 243], it would be interesting to consider optimizing for Hamiltonian control errors and external decoherence in the future.

4.6 Conclusion

We have shown that robust quantum control can produce pulse shapes that achieve a desired unitary with high fidelity for a realistic quantum system. In particular, we have shown that in a system where a single-microwave drive coupled to a cavity containing two transmon qubits is chosen on resonance with a qubit, modifying the shape of the driving microwave pulse can produce a desired unitary two-qubit interaction while mitigating the unwanted rotation of the qubit that is on-resonance with the drive. This can be done while considering filtering on the control and errors in the system parameters with a modest amount of resource and can be achieved even when realistic constraints are placed on the pulses.

The two-level results have indicated that including constraints on the pulse may open up more areas of local maxima in the control space. These “traps” could be what is limiting the range of robustness in the two-qubit frequencies. However, it could be that the algorithm is becoming stuck in areas due to the search parameters such as the trust region size change. This can have a detrimental effect if features like saddle-points appear in the control landscape [176], leading to the false traps in the landscape where the optimiser assumes it has reached a maxima. Future work will look at how to make the error range for \( \omega^{(1)}_s \) larger, potentially by combining these methods with a non-local optimizer in order to circumvent local traps and escape saddle-points.
4.6. **CONCLUSION**

We have shown that it is still possible to achieve good fidelity control with reduced circuit complexity, by increasing the complexity of the control pulse. This shows a trade-off between the circuit complexity and pulse complexity and that as quantum computers grow we are likely to require more complex pulse shapes if it is desired to keep the circuit complexity down.
High fidelity quantum gates are one of the biggest goals in quantum computing [17]. The ability to perform extremely accurate gates means that the many operations required to run a quantum algorithm can be implemented without building up error. Currently single-qubit operations are on the order of 99.9% fidelity [76], while two-qubit operations have begun to reach the order of 99% [64, 74, 77, 244]. There are a variety of factors that are limiting the fidelity of quantum operations including coherent and incoherent errors, and uncertainties [77].

Dominant sources of error come from incoherent errors, characterised by $T_1$ and $T_2$ time constants, particularly given the length of gate times in superconducting systems, as well as unitary errors from imperfect control implementations. Currently gate times are on the order of 100’s of ns, while the average lifetimes are on the order of $\mu$s. One example, the state-of-the-art cross-resonance gate, is performed in a time of 160 ns, with the $T_1$, $T_2$ times on the order of 10’s of ns [74]. With these lifetimes the fidelity of the operation is limited to 99.6%. Two ways to counteract this are to increase the lifetimes of the qubits or to decrease the gate times. Currently the state-of-the-art lifetime for superconducting qubits is of the order of 0.1 ms, but this has been specially designed to exhibit this long lifetimes and is more difficult to control due to its isolation [235]. However, there is still scope to decrease the gate
time to ensure incoherent errors become negligible. Ultimately, there is a speed limit for the
gate time operation \[234, 245, 246\], but this has not yet been reached in practice.

In order to find a way of decreasing gate time, optimal control theory can be used to find
minimal time pulses \[120, 157, 233\]. This will ensure incoherent error degradation of the gate
will be minimised. Additionally, using the robust optimal control approach will ensure that
the pulses are further robust to uncertainty error. The combination of the two makes for a
powerful search to find the minimal time optimal gates that are robust to uncertainty in the
system. In this chapter we combine the two approaches by using the sampling-based robust
methodology with iterations over gate time operation to find optimal high fidelity pulses that
reduce the gate times to under 100 ns; this is while ensuring the pulses are robust to errors
up to 10% in the coupling strength between the qubits. This is considered one of the biggest
sources of uncertainty in the system parameters due to the method by which it is estimated.

Three cases relevant to superconducting qubits are considered: (1) two directly coupled three-
level qubits with direct drives and no classical crosstalk, (2) two directly coupled three-level
qubits with direct drives with classical crosstalk from the drives, (3) two directly coupled
two-level qubits qubits with direct drives. In each case, uncertainty sizes from 1% to 10% are
studied and it is further shown the maximum size of uncertainty that should be allowable to
find the highest fidelity pulses.

5.1 Coupled Multi-Level Systems with Direct Drives

For this work we are interested in the more conventional setup for the cross-resonance gate,
in which two superconducting qubits are coupled via some chosen method and have direct
microwave drives to control them \[68, 69, 74, 233\]. This has the advantage of having more
control of the qubits with lower potential crosstalk between the drives. While, in practice,
this could increase avenues of decoherence, finding pulses that perform gate operations that
are extremely short in time compared with the coherence times would ideally circumvent the
issue.

Whether the qubits are coupled via a common cavity that is far off-resonant from the qubit
transition frequencies, or whether they are directly coupled, the same Hamiltonian can be used to describe either case. Starting with the multi-level description for two transmons coupled with direct microwave drives exhibiting some classical control crosstalk, the Hamiltonian in this case is

\[
H = \sum_{j=1,2} \left( \omega_j c_j^+ c_j + \frac{\delta_j}{2} c_j^+ c_j (c_j^+ c_j - 1) \right) + J (c_1^+ c_2 + c_1 c_2^+) \\
+ \sum_{j,l=1,2}^{K} \sum_{k=1}^{\infty} \varepsilon_j^k(t) \cos(\omega_j^k t + \phi_j^k) \left( (c_j^+ + c_j) + \lambda_j (c_l^+ + c_l) \right).
\]

Here, \( \omega_j \) is the frequency of transmon \( j \), \( \delta_j \) is the anharmonicity of transmon \( j \), \( J \) is the coupling between the two transmons, \( \lambda_j \) gives the amount of classical crosstalk from the control line to qubit \( j \) on qubit \( l \), and \( \varepsilon_j^k(t) \) is the time-dependent pulse envelope of drive \( k \) on transmon \( j \) with carrier frequency \( \omega_j^k \) and phase offset \( \phi_j^k \). In general, the idealised case for the drive term would have no classical crosstalk. However, in reality there may be some amount of classical cross-talk due to the way in which the control drives are brought in to the circuit. This classical cross-talk manifests itself as the drive of one qubit directly driving the other qubit with some weighting dependent on the coupling of the drive with the other qubit [68], as shown in the second line of eqn. 5.1.

The state-of-the-art implementation for the cross-resonance gate uses two quadrature control on both qubits, with each individual drive using the same carrier-frequency, that of the target qubit [74]. To perform the cross-resonance gate, one must drive the control qubit and the qubit transition frequency of the target qubit; for the target qubit, the drive at it’s own frequency is to correct to any unwanted rotations caused by cross-talk from the cross-resonance drive. In particular, in [74], the direct drive on the target qubit was to correct for unwanted rotations about the y-axis. Therefore in this work we use two quadrature control for each qubit, with both drive carrier frequencies being the same as the target qubit. In the rotating frame of the target qubit, equation 5.1 becomes
5.2 Cross-resonance Simulation and Optimal Control

In this work we are interested in using robust optimal control to find the minimal time in which we can perform a cross-resonance operation that is robust to uncertainty in a measured system parameter. In particular it is desired to find solutions that can be performed in the laboratory. This section defines the problem parameters and the methods to be used for finding minimal time solutions.

5.2.1 Desired Operation

In the two-qubit definition of the cross-resonance gate, the cross-resonance interaction is given by the term $\sigma_z^{(1)}\sigma_x^{(2)}$ when the second qubit is the target qubit. To perform entanglement using this operation the desired unitary is generally given by

$$U_{\text{des}} = \exp\left(-i\frac{\pi}{4}ZX\right),$$  \hspace{1cm} (5.3)$$

where $Z = \sigma_z$ and $X = \sigma_x$ \cite{241}. This is known to define an entanglement operation as it is related to the CNOT gate by single-qubit rotations before and after it, as shown in Chapter 2 and local qubit gates do not affect the entanglement of the operations being performed.
As the desired unitary is a two-qubit operation, it must contain qubit terms. However, to be suitable for the multi-level description of transmons the desired unitary must be extended to include the higher levels. Generally we are only concerned with the dynamics within the two-qubit subspace and ensuring there is no leakage out of this space; any dynamics in the higher levels subspace does not effect the operation as long as there is no interaction between the two subspaces. Based on this, we define the desired unitary to be

\[ U_{\text{des}} = \hat{O}_{\text{qubit}} \exp\left(-i\frac{\pi}{4} \sum_{(1)} \sum_{(2)} \right) \hat{O}_{\text{qubit}}, \tag{5.4} \]

where \( \hat{O}_{\text{qubit}} \) is the projection operator into the two-qubit subspace, \( \sum_{z} \) is the Pauli \( z \) operator extended to the multi-level system, and \( \sum_{x} \) is the Pauli \( x \) operators extended to the multi-level system. For our definition, these operators are given as:

\[
\hat{O} = \begin{pmatrix}
1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 0
\end{pmatrix} \otimes \begin{pmatrix}
1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 0
\end{pmatrix},
\]

\[
\sum_{x} = \begin{pmatrix}
0 & 1 & 0 & \cdots & 0 \\
1 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 0
\end{pmatrix}, \quad \sum_{z} = \begin{pmatrix}
1 & 0 & 0 & \cdots & 0 \\
0 & -1 & 0 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 0
\end{pmatrix}.
\]

These operators are suitable for multi-level implementation and the act of using the projection operators ensures only the desired interaction within the two-qubit computational space is relevant to the final result. For the simulations of this work, the multi-level operators are truncated to include the first three levels of the qubits to simulate the computational subspace and one extra leakage level.
5.2. CROSS-RESONANCE SIMULATION AND OPTIMAL CONTROL

5.2.2 Dressed Frame for Hamiltonian

As seen in section 2.3.3, the cross-resonance gate is implemented by making use of the weak coupling between the two qubits and a driving field. As the qubits are far off resonant from one another and the coupling cavity (if one exists), and are weakly coupled, then one can define a frame in which the qubits are effectively decoupled. In this frame, when a drive is applied to the control qubit (e.g. qubit 1) at the transition frequency of the target qubit (e.g. qubit 2), then the two-qubit term $\sigma_z \sigma_x$ is revealed in the control term in this new frame.

In previous derivations of the cross-resonance Hamiltonian given in equation 2.66, approximations are made to remove small, unwanted terms [68]. However, these approximations mean the final Hamiltonian is not effectively replicating the physical system. Performing the cross-resonance gate becomes more difficult when including a multi-level system such as the transmon. If we wish to derive an effective Hamiltonian for the cross-resonance gate in the two transmon case, we must necessarily make approximations and simplifications, which has been done previously. However, to simulate the system close to the real case then an effective Hamiltonian must not be used. Instead the process in chapter 4 is undertaken where the first line of equation 5.2 is diagonalised. This can be performed provided the parameters have the two qubit transition frequencies far detuned from one another and the coupling between the two transmons much smaller than the detuning between the qubits, i.e. $J \ll |\omega_1 - \omega_2|$. This diagonalisation then puts the transmons into a new frame in which they are effectively two distinct (dressed) transmons, uncoupled from one another, with new transition frequencies shifted by terms related to the original weak coupling (see [250] for examples of the shifting terms in this multi-level case). With the eigenvectors and eigenvalues defined for this new system, we can then transform the second line of equation 5.2 into this same basis. As in Chapter 4, this then produces an entangling operation in the drive terms.

5.2.3 Searching for the minimal time

In the literature of optimal control there are a variety of ways to find minimal time optimal controls, such as including the operation time of the gate as a cost function to be minimised [120, 157]. One straightforward method that is easily implementable in piece-wise constant
approximation optimal control is to run searches at different time points with many different random initial starting conditions for the same time values [233], as described in Chapter 3. This is effectively using one method for searching for global optimal control, namely the multi-start method that starts many different searches in different parts of the landscape in order to find the global maximum. This “global” search is performed for all different time values and should then give an indication as to the minimal time of the desired operation.

5.2.4 Controls for optimization

In order to use optimal control to solve the problem, one must first parameterise the problem and define the controls. For this problem the piecewise constant approximation is chosen to use the SCP algorithm to find pulses robust to the uncertainty of interest. The current state-of-the-art AWGs have a resolution of 0.5 ns for changes in the amplitude of the control pulse\(^1\), therefore each of the control pulses we optimize has piecewise constant amplitudes of length 0.5 ns. This means that the number of dimensions of the control space will be dictated by the full length of the pulse; the shorter the time the smaller the dimension of the control space and vice versa. While this seems to limit the search for the theoretical minimal time for the cross-resonance operation, this will keep the results relevant to experimental exploration as the sampling rate will ensure that the results can be performed in the laboratory. Therefore, the time limit that will come out of these results will be the experimental minimal time for robust piece-wise constant controls.

5.3 Minimal Time Searches

This section will now present the results of the searches for each of the three cases described in the introduction: (1) two directly coupled three-level qubits with direct drives and no classical crosstalk, (2) two directly coupled three-level qubits with direct drives with classical crosstalk from the drives, (3) two directly coupled two-level qubits with direct drives. In each case it is instructive to find the minimum operation time for the cross-resonance operation without any

\(^1\)According to discussions with experimental collaborators
5.3. MINIMAL TIME SEARCHES

errors in the system to set a benchmark against which to test the results. Naturally this search
will be limited due to the nature of the search operation being used, i.e. the use of a local
gradient search algorithm necessarily dictates that wherever the search is started, unless there
is a single global maximum, the search will be confined to the space close to the initial starting
point. For specific problems with no constraints, this would not necessarily cause a limiting
search as any maximum found by the algorithm is necessarily a global maximum, however in
the more complicated case of interacting quantum systems with leakage and constraints, any
maximum reached is not necessarily the global maximum. Nonetheless by starting with many
random points we aim to get over this constriction.

5.3.1 Two Three-level Qubits with No Crosstalk

For the idealised simulation of two three-level qubits with no crosstalk, eqn. 5.2 is used with
\( \lambda_j = 0 \) for both drives. The initial benchmarking test begins with 20 random start points for
each time point, exploring from 1 ns to 100 ns. The SCP algorithm then runs until either the
maximum number of iterations is reached or the maximum fidelity for that search is reached.
Figure 5.1 displays a logarithmic plot of the maximum and average infidelity of the 20 random
runs against the operation time of the gate.

![Gate infidelity without robustness](a)

![Gate infidelity without robustness](b)

Figure 5.1: An SCP optimization algorithm is run without robustness for time points running
from 1 ns to 100 ns, at each time point 20 random initial guesses are made to start the
optimization from. The figure displays the maximum and average infidelities reached for each
time point out of the initial random starts. (a) Full display of infidelity versus time for \( T = 0 \)
to 100 ns. (b) Close up of Figure 5.1a showing where \( F > 0.99 \). (Reproduced from [251])
5.3. **MINIMAL TIME SEARCHES**

In Figure 5.1 it is seen that after 40 ns the average and maximum fidelities at all times are $F > 0.99$. Further, after 80 ns the maximum fidelity has $F > 0.9999$, while after 95 ns the average fidelity has $F > 0.9999$. The fidelity values of $F > 0.99$ after 40 ns are a factor 4 improvement in the duration of the gate for the same fidelity over the state-of-the-art implementation [74]. Additionally, in less than 100 ns, higher fidelity values are achievable; values that are important to fault-tolerant quantum computing [17, 77, 94, 252].

With the promising results laid out in the non-robust benchmarking search, the minimal time search is then applied using the robust optimal control methods. For these robust searches, a varying size of uncertainty in the $J$ coupling is considered, ranging from 1% to 10% error. The $J$ coupling is generally the dominant source of uncertainty in measured system parameters due to the way in which it is measured and estimated. The range of uncertainties considered is experimentally realistic and therefore of interest to the wider community.

![Gate infidelity (transmon no crosstalk)](image1)

(a)

![Gate infidelity (transmon no crosstalk)](image2)

(b)

**Figure 5.2:** The optimization is run with uncertainty in the $J$ coupling ranging from 1% uncertainty to 10% uncertainty. At each time point the average minimum infidelity from the random starts is displayed. The figure shows that within a time of 52 ns a robust pulse can be achieved with an average minimum fidelity $F_{\text{min}} > 0.99$ for uncertainty up to 10%. The graphs further show that the range of uncertainty becomes important for the achievable fidelity as the infidelities tend to some value for each level of uncertainty as time increases, with only uncertainties less than 10% achieving $F > 0.999$. (a) The average infidelity for varying uncertainty is plotted against the operation time of the gate from 1 ns to 100 ns. (b) A closer view of 5.2a showing the time taken to achieved fidelities $F > 0.99$ and higher. (Reproduced from [251])

Figure 5.2 shows that, with up to 10% error in the $J$ coupling, the optimiser has found pulses that can achieve a fidelity of $F > 0.99$ in approximately 52 ns. This is 12 ns slower than...
for the non-robust case, but is still a factor of 3 faster the state-of-the-art implementation. Additionally, it can be seen that for uncertainty levels up to 3%, fidelities of $F > 0.999$ can be achieved in times of less than approximately 77 ns. At these short times incoherent errors will be at a minimum, if not negligible, as most transmon qubits have coherence times in the 10’s of microseconds \[74\], while the state-of-the-art is around 0.1 ms \[235\].

The trend of the fidelities with time in Figure 5.2 shows that the fidelity tends to some value as time increases and it would appear to show that for uncertainties greater than 3% the fidelities tend to values less than $F = 0.999$, within the constraints of the system that has been simulated. This suggests that the optimal level of uncertainty for this system is 3% or less; if this level of measurement uncertainty for the $J$ coupling can be reached, then high fidelity short robust pulses can be achieved.

5.3.2 Two Three-level Qubits with Classical Control Cross-talk

The previous section looked at the idealised case of no classical crosstalk. However, in reality there is likely to be some amount of crosstalk. In this section we are interested in the inclusion of classical crosstalk, where we have $\lambda_j = 0.1$ for both drives, simulating 10% crosstalk from both. This is generally considered to be a realistic but high level and non-trivial amount of classical crosstalk due to the drives. As with the previous section, it is instructive to look at the situation in which there are no uncertainties in the system. Figure 5.3 shows the results of the search without uncertainty compared with the results shown in figure 5.1. Although it was considered that the level of crosstalk involved in the Hamiltonian is sub-optimal, Figure 5.3 shows that the crosstalk case very closely follows the results where there was no crosstalk.

Figure 5.4 displays the average infidelity against time for the multiple random starts, following the same search method as described above. The graph shows that within a time of approximately 55 ns, all the error ranges achieve an average worst-case fidelity of $F = 0.99$. This is only marginally slower than for the no crosstalk situation, which achieves the result in a time of approximately 52 ns. As with the no crosstalk case, Figure 5.4 further shows that the optimal level of uncertainty for fast gate operation times is less than 3% as fidelities of $F > 0.999$ can be achieved with this maximum level of uncertainty in times less than 80 ns.
5.3. MINIMAL TIME SEARCHES

Figure 5.3: A comparison of the average infidelities when there is classical crosstalk within the system versus the case when there are only direct drives with no crosstalk. In this case 10% of the pulse is affecting the other qubit. It is noted that this amount of crosstalk does not inhibit the optimizer from finding high fidelity solutions. (Reproduced from [251])

Figure 5.4: The level of infidelity of a robust optimal pulse where a level of 10% crosstalk is assumed. The figure shows that within a time of 55 ns a robust pulse can be achieved with an average worst-case fidelity \( F_{\text{min}} > 0.99 \), with uncertainty up to 10%. This is extremely close to the time for the no crosstalk situation. Additionally, the optimum level of uncertainty is less than 3% as fidelities \( F > 0.999 \) are achievable. (Reproduced from [251])

The above shows extremely promising results for a robust cross-resonance gate in transmon devices. In both cases, with and without crosstalk, robust pulses are achieved with average worst-case fidelities \( F > 0.99 \) in times of less than 60 ns. This is approximately a factor of 3 speed up on the state-of-the-art implementation of cross resonance gates. The inclusion of crosstalk makes the results more experimentally relevant, while further restricting the piecewise constant amplitudes to 2 ns resolution (the limit of current state-of-the-art AWGs) further adds weight to the promising results for future experiments.
5.3. MINIMAL TIME SEARCHES

5.3.3 Two-level Qubits

While multi-level qubits with weak anharmonic structures are currently widely used by many superconducting research groups, work is still being progressed in qubits with more isolated two-level structures where the non-computational levels are far enough away that there is no significant leakage out of the computational subspace [42-44, 253-256]. As all the dynamics during the gate operation are contained within the computational subspace, it would indicate that two-level systems would be the preferable choice for the cross-resonance gate and should achieve higher fidelity, shorter gate times due to the lack of leakage.

To simulate two-level qubits, eqn. 5.2 is adapted with reduced dimensions down to two levels for each transmon to effectively consider two two-level systems. With this alteration, the same initial search is performed as previously with no uncertainty in the system in order to give an indication of the minimal time for the two-level qubits. Figure 5.5 displays the results of this search and compares them with the three-level case, which displays a somewhat unexpected and interesting feature. For the two-level qubits, as expected, fidelities at the lower times are higher than for the three-level qubits. It is expected that the limiting factor is the leakage level where the potentially large amplitude pulses are driving the higher level interactions and limiting the fidelity. However, as the time is increased the fidelities increase more gradually for the two-level qubits than for the three-level qubits; eventually the fidelities of the three-level qubits become greater than the two-level qubits for the same time values. Figure 5.5 further shows that three-level qubits reach fidelity values of $F > 0.99$ in times of approximately $T \geq 40$ ns, whereas for two-level qubits this is achieved for $T \geq 58$ ns.

The feature where the fidelities for the three-level qubits are greater than for the two-level qubits and tend towards higher fidelities more quickly suggests that the third level is actively used during the gate operation. Figure 5.6 shows plots of the value $1 - |\text{tr}(\prod_k U_k^\dagger \hat{O} \prod_k U_k \hat{O})|^2/d^2$ for each time point $k$ within the pulse length for gate operation times of $T = 10, 20, 40, 80$ ns; this is for the results from the three-level qubit simulations with no crosstalk that achieved the highest fidelity. This gives a representation of the leakage for each of the pulses, where it is assumed that leakage $= 1 - |\text{tr}(\prod_k U_k^\dagger \hat{O} \prod_k U_k \hat{O})|^2/d^2$. $\hat{O}$ is the projection operator into the four-level two-qubit subspace and $d = 2$ for the qubit case. $|\text{tr}(\prod_k U_k^\dagger \hat{O} \prod_k U_k \hat{O})|^2/d^2$
5.3. MINIMAL TIME SEARCHES

Figure 5.5: A comparison of the performance of two-level qubits, three-level qubits with no crosstalk, and three-level qubits with crosstalk, where the average infidelity for each time point is plotted. Initially the two-level qubit simulations produce higher fidelity pulses, however the improvement in fidelity for the two-level qubits is more gradual than for the three-level qubits, with the three-level qubits achieving higher fidelities in shorter time than the two-level qubits. This suggests that the third level is being used during the pulse time to gain higher fidelities. (Reproduced from [251])

would be unity if there was no leakage from the qubit subspace, and therefore the graphs display the level of leakage out of the two-qubit subspace. This figure shows that for each of the pulse length times there is a significant degree of leakage during the operation, suggesting that the third level is extremely important for these pulse shapes and eventually the higher fidelities that are able to be achieved in the three-level cases.

Figure 5.7 shows the fidelities with time for the robust pulses for the two-level qubits. Similar to the three-level system case the trend is the same as the no uncertainty case, with the fidelities decreasing for each increase in uncertainty. In this case, for the two-level qubits, Figure 5.7 shows that after a time of \( T = 70 \) ns average fidelities of \( \mathcal{F} > 0.99 \) are achieved for all ranges of uncertainty up to 10\%. This is again a speed up of gate time compared with current state-of-the-art implementation. For the two-level qubits, however, the trend of the fidelities shows that the optimal level uncertainty is less than 4\%, as opposed to the 3\% for the three-level qubits. In a time of approximately 95 ns, fidelities of \( \mathcal{F} > 0.999 \) are achievable with uncertainty up to 4\%. 

84
5.4. CONCLUSION

Figure 5.6: For each of the pulse length times chosen above, the value $\left| \text{tr}(\prod_k U_k^\dagger \prod_k U_k) \right|^2 / d^2$ is calculated at each time point, $k$, during the pulse. This then determines how unitary the evolution operator is at that time point, which indicates how much leakage there is at that time point. It is assumed leakage $= 1 - \left| \text{tr}(\prod_k U_k^\dagger \prod_k U_k) \right|^2 / d^2$, where $d = 4$ for a two qubit ideal system. (a) Representation of leakage for 10 ns pulse. (b) Representation of leakage for 20 ns pulse. (c) Representation of leakage for 40 ns pulse. (d) Representation of leakage for 80 ns pulse. (Reproduced from [251])

Figure 5.7: Average worst-case infidelity is given for the two-level qubit optimization. The figure shows that within a time of 70 ns a robust pulse can be achieved with an average worst-case fidelity $\bar{F_{\text{min}}} > 0.99$, with uncertainty up to 10%. This is longer than for the three-level qubits which suggests more third level interactions. (Reproduced from [251])

5.4 Conclusion

We have shown that the robust SCP algorithm can achieve robust pulses with fidelities $F > 0.99$ in a time of approximately 55 ns for three-level systems and approximately 70 ns for two-level qubit systems. This is a factor of three faster than the current state-of-the-art implementation for the three-level case and a factor of two faster for the two-level qubits [74]; this is while being robust to one of the most uncertain parameters in the system, the $J$ coupling. Fidelities of $F = 0.99$ are suitable for surface code quantum error correction [101, 103, 104]; this is ideal as there has been much work looking towards implementing surface codes in superconducting qubit devices [77, 257–260]. The robustness of the results
also ensures there is less variability in the performance in multi-qubit processors which is ideal for scaling up quantum computers. We have further shown that for short gate times there is an optimal level of uncertainty for each of the devices. For the multi-level qubits, uncertainty levels up to 3% can achieve fidelities $F > 0.999$ in gates times of 75 ns. For two-level qubits, uncertainty levels up to 4% can achieve fidelities $F > 0.999$ in gates times of 95 ns.

It has also been shown that in theory the coupled three-level qubits can outperform the coupled two-level qubit systems as the addition of a third level can allow for more complicated dynamics and give an extra dimension to be used during the operation. This has led to a faster convergence of higher fidelity results for the three-level qubits, achieving fidelities $F > 0.99$ in a time of 15 ns faster. However, care must be taken when considering this result as the simulation was limited to just the three level system and no other dynamics. In this case of two closed three-level systems, the excitations can return to the computational basis. In reality this may not be the case and the fidelities given may be lower due to permanent loss from the computational basis. Further work would look to include higher levels than the third. Nonetheless, these results show promise for transmons. Additionally, there are certain multi-level superconducting qutrits for which these results could be directly applicable [261, 262]. Nitrogen-vacancy centres could also benefit from these results as the level structure is more like a three-level system with the fourth level being far away [263], similar to the simulations in this paper.

There is also the possibility of other dynamics coming into play, particularly if the pulses have high amplitudes and rapidly fluctuate, causing high frequency components to be excited. As the simulations directly diagonalized the coupled transmon/qubit equations, this will have removed some assumptions in the cross-resonance equation. However, this is still based on a closed system and as such assumes no external interactions. Further work could look to incorporate an open system approach to account for these dynamics, particularly when looking toward implementing the robust pulses in experiments.

While the best achievable fidelities are limited by uncertainty (for the case of constant piecewise control lengths of 0.5 ns), the results nonetheless show that uncertainty can be dealt with if a certain duration of gate time is accepted. Given the current interest in noise
5.4. CONCLUSION

intermediate-scale quantum (NISQ) technologies [111], the results also show that shorter gate times on the order of $30\,\text{ns}$ can be implemented for the full range of uncertainty using our parameterization if lower fidelities can be accepted. This gate time would give fidelities of approximately $\mathcal{F} = 0.96$ for all cases, which is what NISQ technologies are targeting as a minimum gate fidelity for implementation.
Chapter 6

Towards Implementing a Robust Cross-Resonance Gate in a Two Coaxmon System

We have previously spoken about the need to scale qubit systems in order to build large scale quantum computers and perform all the necessary operations on the qubits, and how there are a variety of methods for achieving this. While scaling up the systems, in order for the quantum system to work at it’s best, it is desirable for the coherence time to be as long as possible, but also for the system to be controllable; this invariably introduces sources of decoherence into the system [57, 235, 264]. As an engineering challenge, as the systems are built larger and larger it becomes a problem of how to introduce the controls to all the qubits, particularly if the desire is to have individual control lines for all the qubits. Currently many implementations of the transmon device have the transmons, cavities, control lines, and readout lines fabricated on the same chips [56, 61, 65, 68, 69, 74, 77, 257, 265–270]. As the devices begin to be scaled up the issue of connectivity arises due the limited space available on the chip for the control and readout lines (the number of control and readout lines scales linearly with the number of qubits $N$, while the edges of a 2D array scale as $\sqrt{N}$) [271].

This chapter is based on work undertaken in collaboration with an experimental group
6.1. COAXMON DEVICE

at the University of Oxford [1]. The system developed there is a novel superconducting qubit device with out-of-plane control and read-out channels in order to help with the scaling of the quantum systems for large scale quantum computers [271]. We applied the robust optimization methods in order to find optimal pulses to perform the cross-resonance gate in their superconducting two-qubit system, while aiming to test the performance of the pulses produced after we had used the robust optimization methods in simulation. This work proved an interesting challenge as there are additional factors to take into account in actual experiment, including the translation of the simulation results into the actual system. There are also other error sources to account for such as filtering effects on the pulses.

The rest of the chapter is as follows: in Section 6.1 the Coaxmon device and its Hamiltonian for simulation is defined, in Section 6.2 the experimental limitations and the methodology used for the simulations in this chapter as well as other experimental considerations that affect the simulations are defined, in Section 6.3 the results of the simulations undertaken to find robust high fidelity pulses for the two-coaxmon device are presented, and Section 6.4 presents the conclusions of the work.

6.1 Coaxmon Device

The superconducting device of interest to this work is the novel implementation of a transmon designed and created by LeekLab, University of Oxford. Named the coaxmon, the device architecture is based on coaxial geometries, whereby the coaxially designed transmon is fabricated on one side of a sapphire chip while a coaxial LC resonator is fabricated on the other [271]. Due to the similar geometry of one another these two components can be strongly coupled across the dielectric of the sapphire chip, allowing for implementation of circuit QED experiments, for example dispersive readout of the qubit via the coupled cavity. The coaxial readout and control coupling ports are placed perpendicular to the plane of the chip, coming in from the top and bottom. This device has been shown to be a successful implementation of the transmon, displaying good coherence times and controllability with coherence times around 5 µs and single-qubit gate fidelities of $F = 0.995$.  

1LeekLab, University of Oxford, https://leeklab.physics.ox.ac.uk/
Due to the nature of the design the devices are promising for scaling to larger systems as the issue of on-chip connectivity has been removed. Naturally, since the qubits have exhibited good single-qubit fidelities and further research is examining how to improve these fidelities, examination of the two-qubit gates is the next step. Initial work has been performed implementing a cross-resonant gate in a two coaxmon system using the direct microwave drive capabilities, with best fidelity of $F = 0.94$ in a time of 215 ns [272]. This is not at the coherence limit for the coaxmon, which at this gate time would be $F = 0.957$, and therefore there is scope for improvement of the fidelity. Additionally, it would be ideal if the gate time can be reduced to improve the coherence limited fidelity. In particular, this device presents an interesting place to explore optimal control to improve the gate fidelity and test some of the outputs from robust quantum optimal control simulations.

In order to use optimal control for this system we must first determine the Hamiltonian of the system. Due to the device being a transmon we can make the approximation of simulating the device as a Duffing oscillator [145, 155]. The method for coupling the coaxmons is direct capacitive coupling, which is well understood in superconducting systems [58]. The cavities can effectively be ignored due to being off-resonance with the qubit transition frequencies and the fact that the control lines are on the other side of the chip to the cavities [25, 26]. One interesting factor to consider is the control lines - due to the design, whereby the control lines are not directly coupled to the transmons but are brought close to them for control, there will inevitably be some classical cross-talk of the control lines. In this case, some of the drive on one qubit will also drive the other qubit. Considering all these factors, we can use the below Hamiltonian to describe this superconducting device:

\[
H = \omega_1 b_1^+ b_1 + \frac{\delta_1}{2} b_1^+ b_1 (b_1^+ b_1 - 1) + \omega_2 b_2^+ b_2 + \frac{\delta_2}{2} b_2^+ b_2 (b_2^+ b_2 - 1) + J (b_1^+ b_2 + b_1 b_2^+) \\
+ c_{1,X}(t) \left[ b_1^+ b_1 + m_{12} (b_2^+ b_2) \right] + ic_{1,Y}(t) \left[ b_1^+ b_1 + m_{12} (b_2 - b_2^+) \right] \\
+ c_{2,X}(t) \left[ b_2^+ b_2 + m_{21} (b_1^+ b_1) \right] + ic_{2,Y}(t) \left[ b_2^+ b_2 + m_{21} (b_1 - b_1^+) \right].
\] (6.1)
The first line describes the energy levels of the two coaxmons, approximated as Duffing oscillators, where $\omega_j$ is the frequency of coaxmon $j$ and $\delta_j$ is the anharmonicity of coaxmon $j$. The second line describes the direct capacitive coupling of the two coaxmons in the rotating wave approximation, where $J$ is the coupling strength of the coaxmons. Lines 3 and 4 of the equation give the drive terms for coaxmon 1 and 2 respectively. In these lines, $c_{j,A}(t)$ gives the time-dependent amplitude of the drive term for coaxmon $j$ in quadrature $A$ and $\alpha_j$ gives the classical crosstalk of the drive $j$ on the other coaxmon. In these drive terms we have assumed amplitude and phase control of the microwave drives, thus allowing two quadrature control of both coaxmons. This is the same Hamiltonian as was used for the previous chapters simulations, with the $m_{ij}$ terms being equivalent to the $\lambda_i$ terms of Chapter 5. The same methodology as was used in the previous chapters will be used for these simulations, where the first two lines of eqn. 6.1 are diagonalised and the control terms are transformed in to this basis.

6.2 Experimental Considerations and Methodology

As this is now the application of optimal control theory to experiments, there are some considerations that must first be taken into account.

Control Resolution

As previously stated in chapter 5 experimental realization of pulses is limited by the the finite bandwidth of the AWGs used to shape the pulse. In this case the bandwidth is 5 GHz, allowing for 0.5 ns resolution of the pulses. Therefore, when implementing the piecewise constant approximation of the pulse for optimal control we can allow for the control dimension to be twice the number of pulse amplitudes as the length of time in nanoseconds for each control channel.
6.2. EXPERIMENTAL CONSIDERATIONS AND METHODOLOGY

Filtering

While the resolution may be 0.5 ns, as mentioned in chapter 3 the pulse that will actually reach the qubits will be filtered by attenuation through the dilution fridge plus the finite bandwidth of the AWGs [208]. Therefore it is desirable to be able to accurately simulate the filtered situation in optimal control to produce the correct pulse [190, 241]. In this case the filter would be included in the simulation via the transfer function

\[ s_{k,l} = \sum_{j=0}^{N-1} T_{k,l,j} u_{k,j}, \]  

(6.2)

where \( T_{k,l,j} \) is the transfer function, \( u_{k,j} \) is the piecewise constant amplitude for time slot \( j \) and control channel \( k \), while \( s_{k,l} \) is the new piecewise constant amplitude for new time slot \( l \) [208]. In the initial case we can assume that the filter is a Gaussian filter effect, as in chapter 4 however this may not accurately represent the effect on the pulse of the attenuation it goes through passing down into the fridge. Ideally the filter function for the specific device could be determined. This was attempted by the research group at LeekLab whilst undertaking these experiments but unfortunately we were unable to find the transfer function and implement it in time.

Frequency Constraint

Additional to the filtering effect above, it is also wise and potentially necessary to include some kind of constraint on the frequency components of the pulse [157, 173, 273]. In general, if left unconstrained, the simulation results may produce pulses that have extreme changes in amplitude; this is due to the simplified model used to simulate the system in order to keep the computational complexity down. Pulses with these fast changes in infinitesimally small times will have potentially detrimental high frequency content that may drive unwanted transitions or simply introduce processes of decoherence. Additionally, the AWGs do not have the ability to change the amplitude of the pulses as quickly as may be produced by the simulation. Although some kind of smoothing of the pulses will occur in the simulation when the filter
6.2. EXPERIMENTAL CONSIDERATIONS AND METHODOLOGY

effect is included, this will not necessarily remove the high frequency contributions. This is when it becomes wise to include a frequency constraint.

To include this constraint a penalty is added to the cost function to penalise high frequency contributions from the pulse. This extra part to the cost function must be included as a search parameter, so that at every iteration the new cost is calculated and compared with the previous one. Additionally, the gradient of this new cost function with respect to time step must be calculated at every step and included for the search. The standard way to include new cost functions [32, 33, 120, 157], $\phi_i$, in the total, final cost function, $\Phi$ is to sum them all and give the extra cost functions some weighting $\alpha_i$

$$\Phi = \mathcal{F} + \sum_i \alpha_i \phi_i.$$  \hspace{1cm} (6.3)

The gradient is straightforward to calculate if the approximate gradient formulation is used, as is used in this work. In this case the gradient for each time slot is given by

$$\nabla \Phi_{k,j} = \frac{\Delta \Phi}{\Delta u_{k,j}} = \frac{\Phi(u_{k,j} + \epsilon) - \Phi(u_{k,j})}{\epsilon},$$  \hspace{1cm} (6.4)

where $\epsilon$ is some small predefined perturbation to the control. This can then be straightforwardly included in the simulations.

For the frequency constraint, the cost function implemented is to take a Fourier transform of the control pulse at each iteration and take a sum of the frequency components. This penalises the higher frequency terms as the cost function increases with the addition of more of the higher frequency terms [157]. The weighting factor used here is $\alpha = 0.001$

Quantum Process Tomography and Fidelity

In simulations it is straightforward to determine whether the output of the algorithm was successful. Generally there is some desired outcome, in the case of this thesis this will be some desired unitary operator that performs a gate. The inputs into the algorithm are some
known Hamiltonian and an initial pulse. When the algorithm ends it outputs an ideal pulse, constructs the time evolution operators for the system using the output pulse and compares this to the desired outcome via the fidelity function. In experiment it is not so straightforward as the system dynamics will not be unitary. In this case a procedure known as Quantum Process Tomography (QPT) is used to determine the quantum dynamical process of the applied pulse sequence which is then compared with the desired operator [17, 274, 275]. A full description of Quantum Process Tomography is beyond the scope of this thesis, but a brief summary is given below.

Quantum Process Tomography is concerned with determining the map

\[
\xi(\rho_i) \mapsto \rho_f
\]  

(6.5)

which maps the full quantum state of the two qubit system prior to the quantum process, \( \rho_i \) to the full quantum state afterwards, \( \rho_f \) [17, 274]. In order to do this we must be able to determine the density matrix of the two-qubit system, which is done by quantum state tomography. The density matrix of a two-qubit system can be written as the sum of the 16 two qubit Pauli matrices:

\[
\rho = \frac{1}{4} \sum_{i,j=0}^{3} \langle \sigma^i \otimes \sigma^j \rangle \sigma^i \otimes \sigma^j
\]  

(6.6)

where \( \sigma^0 \) is the identity matrix, \( \sigma^1 = \sigma_x \), \( \sigma^2 = \sigma_y \), \( \sigma^3 = \sigma_z \) [17]. The expectation values can be measured by performing 9 different experiments (averaged over many times). To measure qubits in the \( X \) or \( Y \) basis we must first perform a \( \pi/2 \) pulse around the \( Y \) or \( X \) axis respectively. This rotates the state of the qubit around the centre of the Bloch sphere, mapping the \( X \) or \( Y \) axis on the \( Z \) axis where it can be directly measured. Using this procedure, known as Quantum State Tomography, the state matrix of the system can be constructed.

The map \( \xi(\rho) \) can be described by using the transfer matrix \( \lambda \) in the simple form:
6.2. EXPERIMENTAL CONSIDERATIONS AND METHODOLOGY

\[ \xi(\rho)_i = \sum_j \lambda_{ij} \rho_j, \quad (6.7) \]

where \( \rho_j \) is the input matrix flattened into vector form (for convenience in calculation and description), \( \xi(\rho)_i \) is the final state matrix after the operations now in vector form, and \( \lambda_{ij} \) is the 16x16 (in the two-qubit case) transfer matrix. Preparing 16 linearly independent state matrices, \( \sigma^n, n = 1 \ldots 16 \), applying the process to each of these states now yields the resultant density matrices in vector form:

\[ \rho^n_i = \sum_j \lambda_{ij} \sigma^n_j. \quad (6.8) \]

As \( \rho^n_i \) can be measured using quantum state tomography, and \( \sigma^n_j \) is known (since it is simply the initial prepared states), the \( \sigma^n_j \) can be inverted to re-arrange the equation and determine \( \lambda_{ij} \).

With knowledge of the transfer matrix a fidelity function can be defined for experimental outputs compared with ideal unitary operations. The average gate fidelity is defined as the average fidelity between the actual output state and the ideal output state over all possible input states [165]. It is defined as

\[ F(\xi, U) = \frac{\sum_j \left( U A_j^\dagger U^\dagger \xi(A_j) \right) + d^2}{d^2(d + 1)}, \quad (6.9) \]

where we can use the transfer matrix above to define the map \( \xi, U \) is the ideal gate operation, \( A_j \) are chosen to be the set of 16 two-qubit Pauli matrices and \( d \) is the dimension of the Hilbert space.

Recapping the above, in order to find the fidelity of the actual implemented gate compared with the desired operation the following procedure is followed:

- Create a set of 16 linearly independent input states (for the two-qubit case);
6.3 Simulations for Implementation

Given the above experimental considerations it was desired to perform quantum gates, both single and two-qubit, with high fidelity and ideally in shorter times than had previously been performed with the two-coaxmon system. Additionally, testing of the robustness of the pulses was desired and a method for translating the results of the Matlab simulations into actual test pulses for the two-coaxmon system was sought. This section details the simulation side of the experiments including developing robust single-qubit gates for performing QPT when including filtering effects and cross-talk, and two-qubit gates for the same cases.

Table 6.1 gives the parameters for each of the coaxmon devices. The parameters $f_{01}$, $f_{12}$ are measured with little uncertainty, however the parameter $J$ is determined with the greatest error of approximately 10%. Ultimately the $J$ parameter is the one which we will desire the pulses to be robust to the uncertainty in. For the simulations, the Hamiltonian in eqn. 6.1 is truncated to include only the first three levels; the first two as the computational basis and the third as a leakage level.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Coaxmon 1</th>
<th>Coaxmon 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f_{01}$</td>
<td>5.9037 GHz</td>
<td>6.6434 GHz</td>
</tr>
<tr>
<td>$f_{12}$</td>
<td>5.56 GHz</td>
<td>6.34 GHz</td>
</tr>
<tr>
<td>$T_1$</td>
<td>7.1 $\mu$s</td>
<td>6.4 $\mu$s</td>
</tr>
<tr>
<td>$T_2$</td>
<td>7.4 $\mu$s</td>
<td>7.6 $\mu$s</td>
</tr>
<tr>
<td>$\Delta$</td>
<td>7.397 MHz</td>
<td></td>
</tr>
<tr>
<td>$J$</td>
<td>11.4 MHz</td>
<td></td>
</tr>
</tbody>
</table>

Table 6.1: Coaxmon parameters
6.3. SIMULATIONS FOR IMPLEMENTATION

6.3.1 No Robustness

The initial start point for the simulations was without including robustness and testing the non-robust pulses to determine how well they performed on the device. The computation is faster without including robustness which ensured there were some immediate results to test with. Additionally, determining how to implement the output from the simulations in the experiment was needed so immediate results were desired. While this configuration process was going on, the robust pulses could then be simulated.

Single Qubit Gates Simulations

Initially sixteen single-qubit gates were optimised for the two-coaxmon device in the presence of crosstalk. It had previously been determined that the amplitude of classical crosstalk for each coaxmon was $m_{12} = 0.0599$ and $m_{21} = 0.149$ due to the proximity of the coaxial control lines with the chip [272]. In this case both qubits will be driven by each of the control drives to varying degrees. Additionally, due to the coupling of the qubits, the cross-resonance interaction is always on in this case which needs to be optimised for in the simulations. The sixteen single-qubit gates for QPT that were optimised are defined in Table 6.4 below, where each single-qubit target unitary gate includes both qubits. The table also gives the fidelity for each of the gates in the different cases that were optimised, namely without any constraints, with only the Gaussian filter, with only the bandwidth constraint, and with both Gaussian filter and bandwidth constraint. This is for the initial case of no robustness.

For each of the simulation runs, the initial starting pulse for the optimizer was based on a Gaussian shape as this is the typical pulse shape used for single qubit gates [58, 72, 73, 271]. Figure 6.1 shows the initial pulse shape. For each gate the amplitude is chosen as $A = \theta / T_{\text{fin}}$ where $\theta$ is the angle of the gate to be optimized and $T_{\text{fin}}$ is the gate time. This initial guess is entered into the relevant quadrature for the desired gate. The resolution of the AWGs was 0.5 ns, as such this has been chosen as the length of each piecewise constant part of the pulse for the simulations. The total gate time for each case was 50 ns. This is not the fastest time for single-qubit gates in the coaxmon device, but is approximately the same time as they are currently running at with a fidelity of $\mathcal{F} = 0.995$ [271]. It is worth noting that the
6.3. SIMULATIONS FOR IMPLEMENTATION

Figure 6.1: Initial pulse shape for the single-qubit gate optimization. The amplitude is chosen as $A = \theta / T_{\text{fin}}$ where $\theta$ is the angle of the single-qubit gate to be optimized and $T_{\text{fin}}$ is the final time of the gate. This pulse is set in the control quadrature determined by which gate is being optimized.

<table>
<thead>
<tr>
<th>Single-qubit gate</th>
<th>No Con-</th>
<th>Gaussian Filter Only</th>
<th>Frequency Constraint only</th>
<th>Both Gaussian filter and Frequency Constraint</th>
</tr>
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<tr>
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</tr>
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</tr>
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</tr>
</tbody>
</table>

Table 6.2: Fidelity for each single-qubit gate without robustness for the different constraint cases simulated.

The reported level of fidelity in [271] is for a single-qubit device only, whereas these results are for a two-qubit device with an always on interaction between them due to the coupling.

From the table 6.4 we see improvements on the reported fidelity in the cases of no constraints and also with the Gaussian filter applied. In the cases where only the frequency constraint is applied and both Gaussian filter and frequency constraint are applied, it is found...
to be much more difficult to overcome the constraints and find high fidelity results (for this specific set of searches). This is likely due to the location of the initial pulse within the control landscape, as it may be stuck in an area with sub-optimal local maxima [159, 173, 174, 222]. Due to the limited nature of the search the pulse has likely become stuck in one of these local maxima, particularly due to the inclusion of the constraints [173, 222].

Comparing the pulse shapes, it is noted that the addition of the bandwidth constraint does ensure that there are fewer large changes in amplitudes between each piece-wise constant section of the pulse. However, it appears to have substantially limited the ability of the optimizer to search the area as the optimized pulse shapes have only slight differences compared with the original pulse. Interestingly, the largest amplitude shifts come from the Gaussian filtered pulse. However, it is to be noted that when the Gaussian filter is included this would not be the pulse shape as applied to the device. Figure 6.3 shows the pulse shapes with the Gaussian filter included. This shows that the amplitude shifts are less severe and the pulses are more smoothed out, as is to be expected with the Gaussian filter function.

Further to the above, when looking at the frequency components of the pulses as shown in Figure 6.4, it can be seen that the bandwidth constraint is effective at limiting the high frequency components but at the expense of high fidelity. The unfiltered, no constraint case does have a high frequency component. In the case of the Gaussian filter only, there is also significant contribution to the high frequency components. When the bandwidth constraint is included it is seen that the high frequency components are limited, showing the successful implementation of the constraint. Nonetheless, given the weighting of the bandwidth cost function, it has highly constrained the pulses and limited the optimizer in finding high fidelity optimized pulses.

**Two Qubit Gate Simulations**

Following on from the single qubit gate simulations and experimental tests, which were implemented with mixed success, it was desired to move on to the two-qubit gate cases for testing and tweaking. The best experimental cross-resonance pulse achieved for this device at the time achieved a fidelity of $F = 0.94$ with a gate time of $T = 215$ ns [272]. This was achieved
6.3. SIMULATIONS FOR IMPLEMENTATION

Figure 6.2: Pulse shapes for the four different constraint cases for the $X_{\pi/2}I$ gate. The blue line gives the pulse shape for $c_{1,X}(t)$, the orange line is $c_{1,Y}(t)$, the yellow line is $c_{2,X}(t)$, and the purple line is $c_{2,Y}(t)$. (a) Pulse shape for no frequency constraint or Gaussian filter. (b) Pulse shape with only Gaussian filter during search. (c) Pulse shape with frequency constraint only. (d) Pulse shape with both frequency constraint and Gaussian filter.
6.3. SIMULATIONS FOR IMPLEMENTATION

Figure 6.3: Actual pulse shapes after Gaussian filter is applied. These pulse shapes show the smoothing that the pulses undergo and how the amplitude fluctuation is shown in the Figure 6.2 is not as extreme due to the filtering. The blue line gives the pulse shape for $c_{1,X}(t)$, the orange line is $c_{1,Y}(t)$, the yellow line is $c_{2,X}(t)$, and the purple line is $c_{2,Y}(t)$. (a) Smoothed pulse shape for the single-qubit gate with only Gaussian filter applied. (b) Smoothed pulse shape for both bandwidth constraint and Gaussian filter included in search.

by using a similar scheme to that described in ref [74]. At this gate time, incoherent errors become a factor, particularly with the lifetime of the coaxmon device; the coherence limit on the fidelity at a gate time of $T = 215$ ns is $F = 0.957$. The simulations for the two-qubit gate were run with the intention of improving the fidelity while also bringing the gate time down to a comparable time with the state-of-the-art implementation and to allow the higher coherence limited fidelity values. To this end, initially the simulations were performed with a fixed gate time of $T = 150$ ns for the four constraint cases as above. The results of these runs are given in Table 6.3 where it can be seen that in all cases the gate fidelity is better than the current best fidelity with the coaxmon device. This is promising for the future implementation of the gate with the device.

<table>
<thead>
<tr>
<th>Single-qubit gate</th>
<th>No Constraints</th>
<th>Gaussian Filter Only</th>
<th>Bandwidth Constraint only</th>
<th>Both Gaussian filter and Bandwidth Constraint</th>
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</thead>
<tbody>
<tr>
<td>$ZX^{1/4}$</td>
<td>0.9985</td>
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<td>0.9919</td>
<td>0.9574</td>
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</tbody>
</table>

Table 6.3: Fidelity for the cross-resonance gate for each constraint case

Given the relative success of these runs, it was desired to see how much the gate time
6.3. SIMULATIONS FOR IMPLEMENTATION

Figure 6.4: Frequency components of the pulse shapes for the four different constraint cases for the $X_{\pi/2}I$ gate. Here, $c'_1(f)$ is the Fourier transform of $c_{1,X}(t)$, $c'_2(f)$ is for $c_{1,Y}(t)$, $c'_3(f)$ is for $c_{2,X}(t)$, and $c'_4(f)$ is for $c_{2,Y}(t)$. (a) Frequency components for no bandwidth constraint or Gaussian filter. (b) Frequency Components for only Gaussian filter during search. (c) Frequency components for bandwidth constraint only. (d) Frequency components for both bandwidth constraint and Gaussian filter.
could be decreased and still keep high fidelity. To this end the simulations were run with increasing time after each successful run, starting at 50 ns and increasing up to 200 ns. This would then suggest a minimum time for the cross-resonance gate in the coaxmon device. Figure 6.5 shows the results of this run for each of the four cases. As expected, the case of no filters achieves very high fidelities in short time. After a time of approximately 120 ns almost all solutions have fidelities $\mathcal{F} > 0.99$ and it can be seen that there are solutions with fidelities $\mathcal{F} > 0.9999$ which is closer to the ideal situation for fault-tolerant quantum computation. As the filters are included the expected drop in fidelity is seen, however there are still solutions for all cases which are improvements on the current best fidelity in times much shorter than 215 ns. Indeed, the maximum fidelity for the Gaussian filter only case is $\mathcal{F} = 0.9999$ for $T = 198$ ns. However, for the case of only bandwidth constraint the maximum fidelity found in this time range is $\mathcal{F} = 0.7841$ for $T = 125$ ns, while for both filters we also have $\mathcal{F} = 0.7841$ for $T = 125$ ns.

6.3.2 Robust Pulses

Following the runs of the optimizer while not including robustness, the main goal was to find robust pulses for the four different constraint cases and test these out for the coaxmon device. This was performed for both the single-qubit tomography gates and the cross-resonance gate. Although the previous results were mixed, with particularly negative results for the bandwidth constraint cases, it was still desired to use the same weighting for the constraint with the same initial start point. The uncertainty to be optimised for was $\pm 10\%$ in the $J$ coupling, which was considered to be the largest source of uncertainty in the coaxmon device.

Single Qubit Gates

As with the non-robust case, all sixteen gates were simulated with each of the four different constraint cases for a fixed gate time. Table 6.4 below shows the results of these runs, displaying the worst-case fidelities. In the robustness protocol, it was the worst-case fidelity that was being optimized at every iteration.

Most surprisingly, with the addition of the robust condition, the minimum fidelities all
Figure 6.5: Logarithmic plot of pulse infidelity against time in the cases where there is no uncertainty in the system.
### 6.3. SIMULATIONS FOR IMPLEMENTATION

<table>
<thead>
<tr>
<th>Single-qubit gate</th>
<th>No Constraints</th>
<th>Gaussian Filter Only</th>
<th>Bandwidth Constraint only</th>
<th>Both Gaussian filter and Bandwidth Constraint</th>
</tr>
</thead>
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<td>$X_{\pi/2}I$</td>
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<tr>
<td>$IY_{-\pi/2}$</td>
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<td>$IY_{-\pi}$</td>
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<td>0.9992</td>
<td>0.9948</td>
<td>0.9946</td>
</tr>
</tbody>
</table>

Table 6.4: Minimum fidelity for each single-qubit gate. All fidelity values in the error range have the same fidelity as the minimum range, having full robustness to ±10% uncertainty in $J$.

Improved compared with the fidelities for the non-robust case. This was unexpected as it is believed that adding a range of parameters to optimize for should inevitably lead to lower minimum fidelity in the range compared with the fidelity for the non-robust case. One possible reason for this improvement in fidelity is that including robustness effectively adds another control dimension during the search. During the the algorithm the optimizer must find the optimum increment $\tilde{\varepsilon}$ that satisfies the linear constraint of Eqn. 3.16 and ensures this is greater than $F(\varepsilon, \delta_i)$ for all points in the uncertain range $\delta_i \in \Delta$. As there are multiple points in the error range this effectively creates multiple control landscapes to optimize over and therefore the search path is vastly different than the non-robust case. This result shows promise for the two-qubit gate for this device also.

### Two Qubit Gates

Further to the single qubit gates case and the promising results obtained, robustness was included for the two-qubit gate case, again with the desire to find the minimal time for which
6.3. SIMULATIONS FOR IMPLEMENTATION

The pulse was robust but also had high fidelity. Figure 6.6 shows the results of this search, where the minimum fidelity of the robust range is plotted against the time for which the gate was run. For the case where no filters are included the maximum worst-case fidelity reached for the cross-resonance gate was $F = 0.9973$ for a time of $T = 133$ ns. This is a promising result for the coaxmon device as this is a much improved fidelity for the gate with much faster gate time than the initial one of 215 ns. However, in the case where the filters begin to be included the fidelities are again extremely limited. For the Gaussian filter case the maximum worst-case fidelity reached was $F = 0.9893$ in a time of $T = 187$ ns. While this result is not ideal from a quantum computing standpoint this is still a promising result for the coaxmon device with an improved fidelity in a faster gate time.

Figure 6.6: Logarithmic plot of pulse minimum infidelity against time in the cases where there is uncertainty in the system.
6.4. **CONCLUSION**

However, as the bandpass filter was included, the problem became too constrained again and the achieved fidelities in times less than 200 ns were further reduced. For the case of both Gaussian filter and bandpass constraint, the maximum fidelity achieved in less than 200 ns was $\mathcal{F} = 0.4948$ in a time of 142 ns. Further to these results, it would be ideal to run the simulations with longer gate times to find the optimal time for high fidelity gates for this specific device with the bandpass filter included.

### 6.3.3 Comments on experiment

With the promising results shown in all the simulations it was hoped that these could be implemented and replicated in the actual device. Unfortunately, due to time constraints, this was not possible. Initial tests with the single-qubit gates showed promise, but also revealed some errors in the implementation. Work was being done to calibrate the input so that the AWGs could fully produce the desired result. Additionally, it was desired to determine the actual filter function for the device in order to simulate it in the algorithm to produce pulses that the device would actually see. Future work would look to determine this so that it could be included in simulation to produce much more realistic pulse shapes for the specific device. While all the full desired outcomes were not achieved, this work was a very useful preparatory process that highlighted areas that were successful and others that required more calibration and thought. This process will be taken up in the next phase of the UK Quantum Hubs and the work undertaken in support of this chapter will inform this next next phase.

### 6.4 Conclusion

For this work the intention was to test pulses optimized using the SCP algorithm in a two-coaxmon device. To this end the optimizer was run for single-qubit gates to develop the gates for quantum process tomography. Additionally the optimizer was run to find pulses that performed the cross-resonance gate in the coaxmon device with high fidelity and in a shorter time than the best case fidelity for the device. It was further desired to test the robust pulses in a device to determine the actual fidelity and the effectiveness of robust simulations. In
particular, it was desired to find and test pulses that had improved fidelity on the current best performing non-optimal gates for the device while they are also robust. It was also key to ensure that the pulses that were developed by the algorithm were experimentally valid; if the pulses are left unconstrained in an optimal control search, they can often be returned with unphysical results that are impractical to implement. To this end, various filters and constraints were included in the simulations in an attempt to find experimentally valid pulses. Additionally, the control dimension was chosen such that the pulses could be implemented.

The simulations have shown that for the single-qubit case there are pulses that have improved fidelity over the best fidelity pulses for the coaxmon device, while also being robust to the $J$ measurement uncertainty. This is for all the filter cases and shows promise for the device. In the case of the cross-resonance gate, it was shown that when robustness is not included there are solutions that show improved fidelity compared with the best case gate for the device, in a time much more comparable to state-of-the-art gates in other devices. When the robust condition was added the algorithm was able to find a solution for improved fidelity in short time for the case of no filters and the case of Gaussian filter, however when the frequency constraint was added this severely restricted the search and the optimizer was unable to find high fidelity solutions. Nonetheless, with the high fidelity solutions found for the no filter and Gaussian filter cases, this set the results up in a good place to be tested in the device. Most surprisingly, in the single-qubit gate implementations, it appears that adding robustness as a condition allowed the optimiser to find higher fidelity solutions than for those without robustness. This should be explored further as it shows adding the robust feature can aide in finding high fidelity solutions.

As previously mentioned, this work is to be picked up in the next phase of the UK Quantum Hub investments and, therefore, the work undertaken in support of this chapter should greatly inform the next round of simulations and experimental implementation. Areas of success have been highlighted as well as areas that will require further work and thought to implement the simulation results in the device. At present, much work is looking into improving the results of the optimiser; this, in conjunction with improvements in the experimental application of the results, will yield a very exciting set of experiments and results.
Chapter 7

Conclusions

The focus of this thesis was the cross-resonance gate in superconducting quantum devices. This gate has been used successfully in the IBM quantum computer currently available to access via the cloud and is a fairly straightforward gate to implement on a new device, albeit not necessarily with high fidelity. This thesis sought to use optimal control techniques to find pulse shapes that performed high fidelity cross-resonance gates in a variety of superconducting qubit architectures. In particular, the focus was on the robust optimal control technique to find pulses that produced a high fidelity gate while also being robust to some inevitable uncertainty in a measured system parameter. Additionally, in each chapter it was desired to find experimentally feasible pulses to ensure that the designed controls would be directly applicable to experimental application. This conclusion will review each chapter and end with some discussion on future directions from this work.

In Chapter 4 the system under investigation was two superconducting qubits within a 3D cavity. In order to control the qubits in this setup and take advantage of the long lifetime offered by the 3D cavity, the microwave drive was coupled with the resonator so that there was a single global drive on both qubits. This was to ensure fewer control avenues, thus decreasing the likelihood of decoherence, while also keeping the overall number of control lines down to aid in scaling up to larger scale quantum computing. The simulations performed for this setup were initially for a true two-level system, which is applicable to a variety of superconducting qubits. Following from this the simulations were performed for an anharmonic multi-level
system applicable to the transmon qubit. It was found that with uncertainty in one qubit frequency parameter, robust pulses could be found with high fidelity. However, in both cases, when finding pulses robust to uncertainty in both qubit frequencies, high fidelity pulses were more difficult to achieve. This could be due to the parameterisation of the controls and the specific device parameters chosen to be simulated. Future work could perhaps extend this so that certain device parameters were also optimisable, as in ref [233]. This technique could then be used to find the best device parameters that could also achieve high fidelity pulses robust to multiple uncertainties.

In Chapter 5, a more traditional setup of the cross-resonance gate was investigated in which each qubit has a direct control line. Three situations were looked at: three-level device with direct control lines that exhibited no classical crosstalk, three-level device with a realistic level of classical crosstalk, and two-level qubits with no classical crosstalk. In this chapter it was desired to find the minimal operation time for the cross-resonance gate with controls that still exhibited high fidelity and robustness to some realistic uncertainty in one of the device parameters. It was found that for all cases it was possible to improve the gate time by at least a factor 2 while still finding high fidelity robust pulses. This is extremely valuable as improving the gate time improves the possible fidelity of the gate as the operation will no longer be coherence limited. Additionally, all three cases are experimentally relevant, particularly the crosstalk case where many devices will exhibit some amount of crosstalk. Further, the two-level qubit case is unique as there has been interest in implementing the cross-resonance in a flux qubit device which has a level structure more similar to a two-level system; the work in this chapter proves a good starting point for this implementation.

Chapter 6 recounted the simulations undertaken during the collaboration with LeekLab in Oxford in which it was desired to perform high fidelity, robust single-qubit and two-qubit gates in their novel quantum qubit device. It was particularly desired to find pulses to perform the cross-resonance gate in a time faster than their current best implementation and, ideally, faster than the current best cross-resonance gate from IBM. The work built on that carried out in Chapters 4 and 5 and wanted to further ensure that the pulses were experimentally feasible by applying more constraints in order to get around some features of pulses produced
in simulation such as potential high frequency components in the pulses due to the truncation of the simulation space. It was also desired to test optimal control pulses in a real device and test the robustness of the pulses to determine the effectiveness of the methodology. Without constraints the optimizer was able to find high fidelity robust pulses for all cases of gates, both single-qubit and two-qubit. However, as the number of constraints increased, particularly with the inclusion of the frequency, the high fidelity pulses were harder to achieve in the short gate times desired. This work has proven to be a very useful preparatory process that will be continued in the next phase of the UK Quantum Hubs. Therefore, future work will look to use these results and progress with implementing the pulses on the device and improve the gate fidelities in the coaxmon device.

Naturally, during the research and now at the end, many further questions have arisen producing many ideas for future work following on from this thesis. This next section will summarise some key ideas that arose during the research.

The first big step is to follow on the work from Chapter 6 and complete the implementation of robust optimal pulses in the coaxmon device. This will require further calibration of their device and further simulation of the device to find high fidelity pulses for all cases of constraint to find experimentally feasible pulses.

Currently it appears that adding constraints can hinder the search for the optimal, high fidelity solution, even when the weighting attached to that particular constraint is kept very small. Further investigative work should look into why it is so limiting and to find ways to circumvent this. Additionally, new constraints could be investigated for the algorithm such as adding a cost function to penalise time which would include optimizing for time as part of the search. Further, in multi-level simulations a useful constraint may be to keep all the excitations within the computational subspace. Although in Chapter 5 it was apparent that the third level was being used to find time optimal solutions, this can prove problematic in practice as the non-computational levels may have a shorter lifetime and thus lead to more irreversible leakage. Further to this, simulations could be undertaken with more than three levels included to determine whether the excitations would just be contained to the three levels for the time optimal solutions or whether more levels might lead to further leakage. If
this is the case then adding the constraint of keeping within the computational subspace is a must as these levels will certainly lead to high levels of irreversible leakage.

In order to make the simulations more realistic it should be ideal to simulate the system as an open system since the devices do exhibit stochastic irreversible processes. Initially it could be viewed simply as an inevitability and results achieved without treating it as an open system should be compared with the result when treating it as an open quantum system to determine the potential true fidelity of the control. Currently there is much work being investigated in open system quantum optimal control, this could be used to inform the work from here on and the SCP algorithm could look to incorporate these techniques to find robust pulses in the presence of leakage as well as uncertainty. Some work had begun to look at this avenue, but was unable to be fully incorporated.

During the simulations for all of the Chapters it was found that the current implementation of the SCP algorithm could be optimized itself. There are many contributing factors in helping with the convergence of the algorithm, such as how much to increase and decrease the trust-region by and how many iterations the optimizer should run for. These can be altered for different problems and work could look to include these as adjustable parameters during the optimization so that perhaps they wouldn’t be constant but would adjust as necessary. In certain situations, if the optimizer found itself in a plateau, the convergence on a good solution would be slow. If the trust-region size change were modified to speed up the convergence this would lead to a more powerful, quicker algorithm. It was generally found during throughout this work that the computational time for the optimisation was relatively long, sometimes taking weeks to complete simulations; optimising these parameters could aide in this process and speed up the computation time.

As the SCP algorithm was a local search algorithm it, any solution produced by the algorithm inevitably leads to the question of whether it is the global optimum. The ultimate goal for optimization is to find the global optimum. Although some work has shown that in certain situations the local optimum is also the global optimum, in our experience the solutions found in these cases are not the global solutions. Future work could potentially look to incorporate some form of global optimiser in conjunction with the local search optimiser.
for faster converging global optimizer. The gradient search algorithms are still powerful as they are fast converging, whereas many global optimisers such as simulated annealing can take a long time to converge. If these two were combined, for example in a way where, if the local search optimiser becomes stuck in plateau, the simulated annealing feature could be initiated to determine whether there is another region of the control landscape with higher fidelity and higher gradient to lead to a further increase in fidelity, then this would lead to a faster converging potentially global optimal solution. This had begun to be explored during this work but was unable to be taken far enough for testing.

Finally, robustness is a very interesting area to explore as there will always be some uncertainty in the experimental implementations. Simulations should generally always account for this otherwise the results can be misleading and the implementations can fail due to the system parameters not being exactly as simulated or drifting. Currently there is work looking into the robust technique and determining what makes a robust pulse and what is the mechanism for robustness. This will lead to many interesting results and should improve the minimum fidelities found in this thesis. Additionally, as Chapter 6 showed, including robustness can sometimes lead to improved fidelities over the non-robust case. Future work will ideally determine the mechanism for this and use it to further improve simulation results.
Appendix A

Schrieffer-Wolff Transformation

A Schrieffer-Wolff transformation is a method for deriving effective Hamiltonians where the high-energy and low-energy subspaces are decoupled that is a method of quasi-degenerate perturbation theory [276].

Start with a Hamiltonian composed of two parts, an unperturbed part $H^0$ with known eigenvalues and eigenfunctions and a small perturbation $H' = \epsilon V$:

$$H = H^0 + H' = H^0 + \epsilon V. \quad (A.1)$$

It is then assumed that the eigenfunctions of $H^0$ can be divided into two weakly interacting subset $A$ and $B$, which are separated by a spectral gap $\Delta$ that is never closed. The Schrieffer-Wolff transformation is defined as

$$\tilde{H} = e^{-S}H e^S, \quad (A.2)$$

where $S$ is chosen so that the block off-diagonal elements in $H_{eff}$ are removed up to the desired order.

The perturbation term $H'$ can be written as a sum of a purely block diagonal term $H^1$ and a purely block off-diagonal term $H^2$.
\[ H' = H^1 + H^2. \]  
(A.3)

\( S \) must then be constructed so that the Schrieffer-Wolff transformation converts \( H^2 \) into a block diagonal term, while keeping the block diagonal form of \( H^0 + H^1 \). Expanding \( e^S \) in series form

\[ e^S = 1 + S + \frac{1}{2!}S^2 + \frac{1}{3!}S^3 + \ldots \]  
(A.4)

and substituting this into eqn A.2 noting that \( S \) must be anti-Hermitian, gives

\[ \tilde{H} = \sum_{j=0}^{\infty} \frac{1}{j!}[H, S]^{(j)} = \sum_{j=0}^{\infty} [H^0 + H^1, S] + \sum_{j=0}^{\infty} [H^2, S]^{(j)}, \]  
(A.5)

where \([H, S]^{(j)} = [[H, S]^{(j-1)}, S]\) and \([H, S^{(0)}] = H\). As \( S \) must be block off-diagonal, the block diagonal term \( \tilde{H}_d \) of \( \tilde{H} \) contains the term \([H^0 + H^1, S]^{(j)}\) with even \( j \) and \([H^2, S]^{(j)}\) with odd \( j \)

\[ \tilde{H}_d = \sum_{j=0}^{\infty} \frac{1}{(2j)!}[H^0 + H^1, S]^{(2j)} + \sum_{j=0}^{\infty} \frac{1}{(2j + 1)!}[H^2, S]^{(2j+1)}. \]  
(A.6)

The block off-diagonal part \( \tilde{H}_n \) of \( \tilde{H} \) is then

\[ \tilde{H}_n = \sum_{j=0}^{\infty} \frac{1}{(2j + 1)!}[H^0 + H^1, S]^{(2j+1)} + \sum_{j=0}^{\infty} \frac{1}{(2j)!}[H^2, S]^{(2j)}, \]  
(A.7)

which must have the condition \( \tilde{H}_n = 0 \) as the transformation must remove these terms.

Writing \( S \) as a Taylor series of successive approximations to \( S \)

\[ S = \sum_{j=1}^{\infty} S^{(j)} \]  
(A.8)
and substituting it into eqn A.7 with the condition of $\tilde{H}_n = 0$ we can derive the following equations to define $S^{(j)}$

\[
[H^0, S^{(1)}] = - H^2 \tag{A.9}
\]
\[
[H^0, S^{(2)}] = - [H^1, S(1)] \tag{A.10}
\]
\[
[H^0, S^{(3)}] = - [H^1, S^{(2)}] - \frac{1}{3!}[[H^2, S^{(1)}], S^{(1)}]. \tag{A.11}
\]

Up to second order in $\epsilon$ the effective Hamiltonian gives

\[
\tilde{H} = H^0 + H^1 + [H^2, S^{(1)}] + \frac{1}{2}[[H^0, S^{(1)}], S^{(1)}] = H^0 + H^1 + \frac{1}{2}[H^2, S^{(1)}]. \tag{A.12}
\]

This is now a Hamiltonian with the block off-diagonal terms removed.
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