Time Optimal Quantum State Control

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Contents:

Synopsis:

Optimisation is the efficient and effective use and allocation of resources. This project considers the processes of time-optimisation and control theory in a form suitable for application to the quantum state. Time-optimisation is directly relevant to the production of stable and useful quantum computational devices, as fast chips and processors translate directly into fast calculations when coupled with efficient programming. Using this theory it then becomes possible to derive external control fields from within the formalism which minimise the time taken for some desired transition to occur within the quantum system, whilst respecting the constraints on possible operations that may be conducted and using only finite energy. The explicit forms of these driving fields are evaluated using linear algebra and matrix differential techniques.

The time-optimal Hamiltonian controls are proven to be periodic for a number of constrained examples on SU(2), SU(3) and SU(4). Some more general cases are considered which exhibit a type of non-linearity; the degree of difficulty in solving the dynamical equations appears to be related to the relative amount of symmetry chosen in the initial control system.

Statement of Candidate:

This thesis is the personal work of P. G. Morrison BSc. and has not been submitted for a higher degree to any other university or institution. All sources have been acknowledged and appear as necessary in the references section of this document.

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"*To co-ordinate a definite cause to a definite effect has sense only when both can be observed without introducing a foreign element disturbing their interrelation.....there exist no infinitesmals by the aid of which an observation might be made without appreciable perturbation.*"

Werner Heisenberg, in *The Physical Principles of the Quantum Theory* [1].

Chapter 1: Introduction to Classical Control Theory

Physics is concerned primarily with the determination of physical law. Scientists claim they have developed a law of nature, and seek to verify whether the predictions generated by such a law agree with experience. Control theory generalises this by considering the modification of the dynamical operator which is assumed to govern the behaviour of the system. By asking whether the system is useful, controllable, optimal, observable and stable we are considering problems that will extend our domain of knowledge beyond physics and into engineering.

The joint criteria of utility, controllability, observability and stability are key ideas within classical control theory. Utility states that there exists some measure function against which we may rank the possible control strategies in terms of efficiency. Controllability gives us that for any proper input and output, then a system is completely controllable if it is possible to associate a unique control function which steers the input state to the desired output state. Optimality allows us to examine such issues as costing of strategies and their improvement with respect to figures of merit. Observability concerns the question as to whether all states of a system may be observed during a measurement, and the actual determination of the state itself. The consideration of stability presents us with the possibility that our control strategy itself may not be perfect; due to the presence of non-removable noise in our measurement, there may be some departure from the ideal control. As a consequence of this it is important to analyse mathematically what would happen to the outputs produced by the system if the control was to depart infinitesmally from its optimal functional value. These are all significant factors that must be taken into account in the devices we use in our daily lives, including the servos in aeroplane wing-flaps, the captain's wheel on a ship and even such ordinary objects as swings, hoops and electric circuits. Classical control theory is relevant on a macroscopic level everywhere there is an external driving force that interacts with the system in question.

In classical control there exists an implicit assumption that one is able to control the dynamics such that it is possible to reverse the uncertainties imparted to the system by the measurements of a noisy observer. This is achieved by the application of a counter-sequence of operations that wind back the errors [2]. As we are able to measure and predict the average dynamics of the noise, it is also possible to correct for the errors which occur in our control system by performing some slightly altered future interaction which contains the relevant corrective factor.

Classical control theory may then be understood in analogy with the actions of a captain who is sailing a ship in relatively calm seas. The ship, representing the state of the system, is pushed about by the waves of the ocean. A clever captain seeks to flow along the path of least time from the pick-up point to the destination. Current pushes the ship off course, bending the ideal straight line into a curve. This may be accounted for directly in the setting of the rudder. By fixing an appropriate angle as a function of time it is possible to take the effect of the external perturbation into account.

The mathematics of classical control theory is based on the addition of a control variable to the differential equation of state, given in [2] by

$$\frac{\mathrm{d}\vec{x}}{\mathrm{dt}} = f(\vec{x}\,,\vec{y}\,). \tag{1.00}$$

where the variable $\vec{x}$ represents the state of the system and $\vec{y}$ gives the functional dependence of the control variable. The function f is not necessarily linear; however for many of the cases we will consider it is given by a linear operator which can be explicitly written as a matrix. In classical control it is possible to explicitly analyse the effects of the external control within the equation of state for the system. This is done by using a particular form of f in the equation of state

$$\frac{d\vec{x}}{\mathrm{d}t} = \hat{A}\,(t)\vec{x} + \hat{B}\,(t)\,\vec{y}\,. \tag{1.01}$$

The operators $\hat{A}$ and $\hat{B}$ and variable $\vec{y}\,(t)$ define the time dependence of the state and control variables, and are linear operators (matrices). Without a control interacting with the system, the equation of state does not have any of the y-dependent terms. To analyse how the state changes with time we must solve the differential equation for $\vec{y}$ as a function of time and substitute into the first equation of state. This represents a generalisation from classical dynamics which deals exclusively with closed systems which do not interact with a control variable. We may assume a simple control related linearly to the state [2]:

$$\vec{y} = \hat{N}\vec{x} \tag{1.02}$$

where $\hat{N}$ is a time-independent linear operator. We then substitute into (1.01) to obtain

$$\frac{\mathrm{d}\vec{x}}{\mathrm{dt}} = (\hat{A} + \hat{B}\hat{N})\vec{x}.$$

(1.03)

The behaviour of the system is governed by the eigenvalues of the matrix $(\hat{A} + \hat{B}\hat{N})$, which may be calculated using linear algebra. Once this has been carried out, we may use the theory of dynamical systems to find the time dependence of the state variable and control. Let us examine a driven harmonic oscillator in one dimension as a case study of classical control. The control in this case is the external driving force, which we can vary in time as required to alter the state of the system. Our equation of motion from Newton's Law reads as

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + \frac{k}{m}x(t) = u(t)$$

(1.04)

where $u(t)$ is our control variable, $x(t)$ is the position of the particle and k/m is the stiffness constant of the oscillator. Our two system parameters are the position $x_1 = x(t)$ and velocity $x_2 = \dot{x}(t)$ and hence defining our control vector $\vec{x}(t) = (x_1, x_2)^T$, we obtain

$$\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \begin{pmatrix} x_2 \\ u - \frac{k}{m}x_1 \end{pmatrix} = \hat{A}\vec{x} + \vec{b}(t); \quad \vec{b}(t) = \begin{pmatrix} 0 \\ u(t) \end{pmatrix}.$$

(1.05)

The dynamical law is now in the standard form for application of the transition matrix. The transition matrix (or kernel) gives the time evolution of the system for a specific initial state.

Writing the dynamics for the free system

$$\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \hat{A}\vec{x}; \qquad \hat{A} = \begin{pmatrix} 0 & 1 \\ -k/m & 0 \end{pmatrix}$$

(1.06)

This is readily solved using the free kernel equations:

$$\hat{U}(t,0) = \exp(-\int_0^t \hat{A}(s)\mathrm{d}s); \qquad \hat{U}(t_0,t_0) = \hat{1}; \qquad \vec{x}(t) = \hat{U}(t,t_0)\vec{x}(t_0).$$

(1.07)

The kernel or transition matrix takes the initial state to some future state; it is particularly important that the matrix $\hat{A}$ is correctly exponentiated. Although the example we have considered does not contain time-dependent operators it is important to understand how to deal with these more complicated cases. Many important examples in this thesis have periodic $\hat{A}$ with particular symmetry; for these examples the relevant mathematics is contained within the Floquet theory [3]. Once we have computed the free evolution we may then consider the generalised problem with control, given by

$$\frac{d\vec{x}}{\mathrm{dt}} = \hat{A}(t)\vec{x} + \hat{B}\vec{u}\,. \tag{1.08}$$

This has an explicit solution which may be written in the form

$$\vec{x}\,(t) = \hat{U}\,(t,t_0)\vec{x}\,(t_0) + \int_{t_0}^{t} \hat{U}\,(t,s)\hat{B}\,(s)\vec{u}\,(s)\mathrm{ds} \tag{1.09}$$

where $\hat{U}\,(t,\,t_0)$ is the transition matrix for the free system (1.06). The steps in the calculation are to initially find the transition matrix of the free system and then use the above expression to find the time-dependence of the state. For our particular example, the control is only on the velocity component. Consequently, one may write down the matrices for the relevant operators which define the control system (1.08) for application in (1.07) and (1.09):

$$\hat{A} = \begin{pmatrix} 0 & 1 \\ -k/m & 0 \end{pmatrix}$$

$$\hat{B} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \vec{u}\,(t) = \begin{pmatrix} 0 \\ u_2(t) \end{pmatrix} \tag{1.10}$$

These matrices are sufficient to define the time-dependence of the state variables $\vec{x}\,(t)$, given the controls $\vec{u}\,(t)$. To find the time dependence of the control variables we must look elsewhere. This demonstrates the necessity of having a well-defined and physically-based method which specifies the functional time-dependence of the control variables, as without this information we are prevented from proceeding further.

In the field of classical control, this has resulted in the development of the science of optimisation. The optimal control is the strategy that maximises (or minimises) the associated physical action function such that its value is an extremum. This action functional specifies the necessary physics and dynamics of the controls; it also gives the constraints or limitations on our available operations. Any modification of the form of the optimal control parameter away from its extremal results in a value for the functional that is sub-optimal. We shall demonstrate how to derive the Euler-Lagrange equation for the action function. We start from Hamilton's action principle

$$S(q_1,...,q_n|\dot{q}_1,...,\dot{q}_n\,;t) = \int_0^T \mathfrak{L}(q_1,...,q_n|\dot{q}_1,...,\dot{q}_n\,;s)\,\mathrm{d}s. \tag{1.11}$$

The function appearing under the integral sign is referred to standardly as the Lagrangian. Our premise is that the observed physical behaviour of the system is that for which the action principle is an extremum. To find this special set of variables we note that the variation of the action gives us that

$$\frac{\partial S}{\partial \alpha} = 0$$

(1.12)

as it is an extremal value and hence we may differentiate (1.11) under the integral sign and integrate by parts to evaluate the equations of motion. The expressions obtained take the form:

$$\frac{\partial \mathfrak{L}}{\partial q_j} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathfrak{L}}{\partial \dot{q}_j}\right) = 0.$$

(1.13)

These equations (henceforth referred to as the Euler-Lagrange formulae) enable us, given a suitable costing, to write down differential equations that govern the time-dependence of the system. They are equivalent in all respects to Hamilton's equations

$$\mathfrak{H} = \sum_i p_i \dot{q}_i - \mathfrak{L} \qquad \frac{\partial \mathfrak{H}}{\partial p_i} = \dot{q}_i \qquad \frac{\partial \mathfrak{H}}{\partial q_i} = -\dot{p}_i$$

(1.14)

where $\mathfrak{H}$ is the Hamiltonian of the system and the p_i are the conjugate momenta associated with the co-ordinate q_i. In our case, the functional is the time of evolution for our system to evolve from one configuration to another. Classically this is similar to treating the equations which define the unique curve called the brachistochrone, solved originally by J. Bernoulli and set as a challenge to the scientists of the day. This curve has the property that a particle moving along such a curve and obeying Newton's Law of Gravitation as well as the friction-free condition will travel between any two points in least time. The action principle may be written in terms of the time minimisation for the curve

$$S = \int \mathrm{d}t = \int \frac{\mathrm{d}s}{v} \quad ; \quad v = \frac{\mathrm{d}s}{\mathrm{d}t} \; ; \qquad \mathrm{d}s = \sqrt{\mathrm{d}x^2 + \mathrm{d}y^2}$$

(1.15)

where x and y represent the horizontal and vertical components of the particle on the curve. The conservation law for the energy of the system is

$$\frac{m v^2}{2} = m g y$$

(1.16)

m gives the mass of the particle and g is the standard gravitational constant. Simple algebra implies that $v = \sqrt{2gy}$. Our action principle then reads

$$S = \int \mathrm{d}x \sqrt{\frac{1 + y'^2}{2gy}}.$$

(1.17)

Our Lagrangian is then

$$\mathfrak{L}(y(x), y'(x)|x) = \sqrt{\frac{1+y'^2}{2gy}};\ y' = \frac{\mathrm{d}y}{\mathrm{d}x}. \tag{1.18}$$

Applying the Euler-Lagrange equations we obtain

$$\frac{\partial \mathfrak{L}}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial \mathfrak{L}}{\partial y'} = 0 \implies \sqrt{\frac{1+y'^2}{2gy}} - \frac{(y')^2}{2gy}\sqrt{\frac{2gy}{1+y'^2}} = \text{const.} = A. \tag{1.19}$$

Rearranging yields the simple differential equation that defines the brachistochrone

$$(1+y'^2)\,y(x) = \frac{1}{2gA^2} = B. \tag{1.20}$$

Equation (1.20) is neatly solved by the parametric formulae

$$y(\theta) = B(1-\cos\theta)\ ; \qquad x(\theta) = B(\theta - \sin\theta). \tag{1.21}$$

This is a classic problem of time optimality; the principal mathematical apparatus used to address it has been the calculus of variations. We will use this technique several times in this document, and it is a useful trick that can be applied to many different situations.

We now move forward to consider controllability of dynamical systems. Controllability of a dynamical system is defined in mathematical terms as an existence and uniqueness theorem [4]. A system is completely controllable if and only if there exists a control that steers the system from every proper input state to every proper output state. The close relationship between this definition and the notion of reachability may be used to determine many useful properties of control systems. Reachability is defined in terms of the transition matrix or kernel which is given by the time evolution operator for the classical system. The reachable set
$\mathfrak{R}[t, \vec{u}\,(t)|\vec{x}_0]$ for a particular input $\vec{x}_0$ and control $\vec{u}\,(t)$ by time t is the set of points such that:

$$\mathfrak{R}[t, \vec{u}\,(t)|\vec{x}_0] := \{\vec{x}\,(\tau)|\ \ \vec{x}\,(\tau) = \hat{X}_{u}(\tau, 0)\cdot\vec{x}_0\ ;\ 0 \leqslant \tau \leqslant t < \infty\} \tag{1.22}$$

where $\hat{X}_u$ is the transition matrix. Now, if we were to have the particular situation whereby for *any* input state we were able to find a control strategy that maps the input to *every* conceivable output, we would then claim that the system is completely controllable. But this is just a statement on the reachable set, and merely states that the reachable set covers the entire state space. However, we must make a distinction here; we are always constrained in terms of time. Hence it is relevant to restrict the total time to be some finite arbitrary value for physical reasons. This is the meaning of the limits on t and τ in (1.22). For this thesis we concentrate completely on issues of time-optimal control, in that we are seeking to minimise the time taken to move between two basis states on the manifold.

The definition of controllability may be extended in several ways, as it may be possible to map certain set of inputs to any output, but some other input states possess reachable sets which do not cover the entire state space. In this case we could say that the system is "conditionally controllable" in that some inputs may be controlled and some may not. This type of system must

be handled very carefully to avoid difficulties in analysis and definition. Higher dimensional problems with non-linear systems are also difficult, as it may not be possible to find a unique control operator which minimises the time globally.

The question as to whether a system is optimal and completely controllable may then be answered in terms of existence and uniqueness of control functions, and the determination of the reachable set for all possible input states. If it is in fact possible to find a control function such that we can steer any input to any output, then we would claim that the system is completely controllable. If, in addition to this, we can prove that the time taken for transfer between any two states on the manifold is a minimum for our control operator then the control strategy is time optimal. This definition can be broadened in order to take more general costings and constraints into account; it is also important to note that this is in general a multi-dimensional problem and very difficult to solve analytically.

There are several different types of control functions that have been studied widely by control theorists. These are known as open loop and closed loop control. Open loop controls are time-dependent functions that do not depend explicitly on the state of the system other than at the initial and final times; closed loop controls have an updating process whereby the results from past measurements are fed-forward into the future state of the control.

A stable control system is not sensitive to small perturbations away from the optimal control. By this we mean that, given our optimal control function, if we were to depart from this idealised functional value by some infinitesimal amount, then the amount by which the output departs from the original value vanishes as the perturbation from the control is taken to zero. A system where the departure is disproportionately large given only a small change in the control is then defined as unstable. In mathematics this may be written as:

$$\text{For optimal } u(t) \text{ we have } \lim_{\Delta u \longrightarrow 0} [[\hat{U}_{u+\Delta u}(t,t_0) - \hat{U}_u(t,t_0)] \cdot \vec{x}(t_0)] = \begin{cases} = 0 \text{ stable} \\ \neq 0 \text{ unstable} \end{cases} \tag{1.23}$$

Control theory is primarily concerned with the dynamical law which operates on the state (1.07)-(1.09). By considering those states which have special behaviour under the dynamical law it is possible to gain a great deal of information about the nature of the dynamical system itself.

A system is defined to be observable if, given the outputs of a particular process, we can figure out the internal state of the system in finite time [2,4]. In classical control theory this would correspond to knowledge of what is coming out of a factory production line at some point in time being sufficient to calculate the current state of affairs within the factory by algorithmic means. For example, we might examine the boxes of products that are coming out of the factory; since we have a description of all possible processes that occur to manufacture the products and the cycle within the factory it is possible to find out (after investing some time) the exact stage of the production process that the factory *was* in. However, time didn't stand still while we did our calculation, so we must account for this by adding this time into our calculation as well. Next we give our prediction on the state of affairs next time the trucks leave the factory, check the boxes and re-do our calculations again, remembering that time has moved on even for the mathematician. This enables us from measuring the outputs and knowledge of the internal machinery to draw out a history of the processes that are occurring in the factory. This is what we mean by observability.

"*We have assumed that the processes of production and detection are well separated and that one can talk of an amplitude that characterizes the object. This hypothesis has always been made (particularly in field theory) no matter how small the distance between the apparatus and the detector. It may turn out that this is not valid if these are too close together.*"

Richard P. Feynman, in *The Theory of Fundamental Processes* [8].

Chapter 2: Introduction to Quantum Control

As the size of the structures we are investigating shrinks ever smaller, quantum mechanical effects will become increasingly important in the operation of devices within technology. Most apparent is the change in the physical dynamics from continuous and predictable to discrete, quantised and probabilistic in nature. Examining quantum control of quantum systems is a useful avenue of investigation, in that this investigation of this area of science may lead to significant new methodologies which are of use in the engineering of real computational devices. At present much effort is being invested in examining the use of quantum effects within computer systems, as they offer a variety of interesting and novel features which may be directly applicable to the next generation of information technology development.

As a result of the difference in dynamics between quantum and classical systems, standard control theory becomes inapplicable, as the methods used to control objects in the classical domain contain assumptions which are no longer valid in the quantum regime. Many of the mathematical tricks and techniques of the classical theory do tend to show up in interesting ways. This is to be expected as the equations of state are related, if not identical. The key assumption in classical control theory that must be examined from a quantum perspective is the hypothesis that it is possible to observe the state of the system without disturbance. The quantum mechanics of closed systems is concerned with the free evolution of the system *between* observations. The key goal of quantum state control is to arrange for the probability of some useful configuration to be high at some particular time, and to be able to calculate this time from theory and confirm its applicability by experiment.

In time optimal open-loop quantum control this entire methodology is no longer applicable as the system is non-observable in a *physical* sense. We cannot specify the trajectory of the system deterministically; it exists in a superposition state in the time between when the clock starts and the measurement is executed. The idea of a chronologically arranged order of internal processes and procedures no longer makes any sense as in quantum mechanics *all* states which are possible have some amplitude. As a result of this it is not possible to associate particular outputs with particular inputs via some deterministic cycle which occurs internally; in fact we must deal with a much more difficult problem. We must find the quantum-mechanical distribution that describes the correlation of the input states with the outputs via the device.

Our quantum mechanical control system will be an open-loop system in that we are not measuring the state at a particular time and making decisions on how to control it in the future with respect to some fixed rules; rather we are attempting to control it by variation of some external time dependent parameters which influence the evolution of the system directly and avoiding measurement as far as possible. One simple physical example of an open-loop control system would be the application of time-dependent magnetic fields on an atom to cause it to move from one base state to another. Some useful descriptions of these types of quantum controls are found in the papers of Khaneja et. al [5,6] and Boscain [7].

The configuration of the closed quantum system is specified by a complex vector in a multi-dimensional Hilbert space. It is natural to ask whether it is possible to find an operator on the space of possible inputs and outputs which is derived from some physical action principle. There has been some experimental and theoretical research carried out in this direction, most prominently including the work of Khaneja and Glaser et al. [5,9] who analyse the problem of time optimal control in terms of Lie algebras on sub-Riemannian geometries. The work of Khaneja et. al directly assumes a matrix expansion of the Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \sum_j u_j(t)\hat{H}_j \tag{2.00}$$

where the "drift" Hamiltonian $\hat{H}_0$ is a constant operator, the $\hat{H}_j$'s and $\hat{H}_0$ are Hermitean matrices, and the second part of the Hamiltonian is a time-dependent function that is specified by the control variables $u_j(t)$. The schemata of [10] which we use throughout this thesis does not require this assumption of the constancy of the drift operator. It also differs in that we do not require any assumption of neglible time taken for 1-qubit gates.

Nielsen, Dowling and Gu cover the analysis of quantum circuits using Riemannian geometry in [11]. This system of analysis is different from that used in [5,9] and the method of [10] in that it seeks to minimise the computational complexity of operations that occur in a particular implementation. The optimisation process in this case recovers an efficient circuit design which is useful from a computer science perspective. Our system of time optimality does not necessarily minimise this computational complexity. As physicists and engineers we are simply trying to find devices which use least physical time given finite energy and constraints. This is crucial to the operation of any functional computer system.

It is important to note that the literature already available on quantum control is vast and it is unfeasible to categorise the entire spectrum. Many different types of control of quantum systems are in use, including feedback-based methods and unitary control. Feedback quantum control [12] assumes that one may allow closed control loops that transfer conditional information about the state from the past to the future, such that we can alter our controls in real time. Open-loop unitary control [13] is concerned with arranging the time-evolution operator to be in a particular configuration in the future, given some controls available on the Hamiltonian, and a known initial condition.

These approaches are to be distinguished from the method in this thesis, as it contains no assumption of time-dependent adaptive measurement or feedback control as in [12] and we impose our boundary conditions upon the quantum state, given by the projection operator. Time optimal open loop state control theory asserts the existence of Hamiltonian operators that drive from one state to another in least physical time, whilst respecting the constraints imposed on the system and using only finite energy. To find these optimal Hamiltonian operators we are required to specify an initial state, a final state and a constraint law.

There are other differences in the technique that diverge from the standard methodology that must be approached with care. For a chosen initial state, it may be that not every final state is reachable given the physical constraints on the system. We claim time-optimal state control in the restricted sense such that for any two states that are linkable by an arbitary time-dependent Hamiltonian, our method will specify the time-dependence of the Hamiltonian that uses the least physical time to complete the evolution, if it exists.

There are complexities associated with this as it is not necessarily guaranteed that the equations which define the Hamiltonian variables for given boundary conditions will have an analytical solution, as they are non-linear. For a small number of finite dimensional and highly-symmetric examples it has proved possible to surpass these difficulties and evaluate the solutions without resorting to numerical methods. These are new and novel calculations which have been carried out using the formulae derived initially in [10]. Due to this fundamental non-linearity there is no reason to expect a decrease in the difficulty for time-optimally controlling larger quantum systems, even with an increase in our capacity for control of small systems, as the equations which define the control variables generally become coupled in a very complicated fashion as the dimension of the space increases. There is hope as the use of symmetry, linear algebra and group theoretical techniques has already been of significant utility so far in conducting research in this field.

Quantum control as it relates to computation involves the development of strategies that optimise time and resource costs for our algorithmic implementation. The research of Law et. al [14] focuses on the design of implementations (sequences of Hamiltonian operators) that drive the input to a desired output state. Their approach is not time-optimal; they are concerned only with finding a way of driving from one state to any other. Our approach finds the *fastest* way, but it may not be possible to link two arbitary states, whereas Law and Eberly [14] are able to move from one configuration to another but not necessarily time optimally. In either case the boundary conditions, both past and future, must be carefully applied.

Law and Eberly in their paper of 1996 [14] outline a methodology for control of an atom in a cavity which interacts with continuous and quantised fields. We shall consider a simplified version of their model in order to compare the results with that produced by the time-optimal theory. Their paper is important to the development of open-loop quantum state control as it details the basic mathematical apparatus which we will expand upon and extend to more complicated systems. The key ideas are those of time evolution and control fields. The state of the atom, given an initial condition, moves forward in time under the influence of the time evolution operator, which is a functional of the control variables. If we can engineer the final state to be in a particularly useful configuration after applying a sequence of control operations, our task in the laboratory is greatly simplified. It is relevant to examine this work as it describes a method for evolving states from the ground state to some higher energy level by using a sequence of interactions with an external control field, which is an important case study and milestone.

Although this document focuses exclusively on quantum state control we shall repeatedly resort to using the time-evolution operator representation of quantum physics, invented by Werner Heisenberg [1]. This matrix will be given the symbol $\hat{U}(t,t_0)$ throughout this document, and its utility is unique among functionals. Its mathematical definition is the direct quantum parallel of the transition matrix used in classical control theory (1.07), with one exception: its evolution is governed by the Schrödinger equation

$$i\frac{\mathrm{d}\hat{U}(t,t_0)}{\mathrm{d}t} = \hat{H}(t)\hat{U}(t,t_0) \tag{2.01}$$

instead of (1.07) provided that the system is not subject to external disturbance. As we are working only with closed quantum systems this will be the case considered throughout this document. The time evolution operator representation is very useful in that given the initial state $|\psi(t_0)>$ we may find the final state

$$|\psi(t)> = \hat{U}(t, t_0)|\psi(t_0)> .$$

(2.02)

This means we are not restricted to a particular set of states or initial condition; we may solve (2.01) for the evolution operator and then substitute into (2.02) for a given set of basis states and boundary conditions and examine the output. This enables us to find the probability that for chosen initial and final states that a particular process happens by time t. However, we are not placing the boundary conditions upon the time-evolution operator, but upon the state. This is what is meant by quantum state control.

The techniques of [14] are relevant as they use a similar mathematical apparatus on an equivalent problem to [10]. This will enable us to make a comparison at the end of the calculation about the relative applicability and strengths of both methods. Law and Eberly [14] (also Khaneja [5]) postulate that given a Hamiltonian operator described by

$$\hat{H}(\tau) = \hat{H}_0 + \sum_j u_j(\tau)\hat{H}_j$$

(2.03)

as explained in (2.00) then there exists an optimal sequence of controls ($u_j(\tau)$'s) that drives the system from a known input to a target state while satisfying certain constraints or limitations. Let us follow a simplified version of the calculation of [14]. The physical system in question is a spin-1/2 particle in a time dependent magnetic field. The control functions in this example are given by the magnetic fields in the x- and y- directions and the drift term is a constant magnetic field along the z-axis. The Hamiltonian operator is given by

$$\hat{H} = \frac{1}{2}\omega_0\hat{\sigma}_z + v_x(t)\hat{\sigma}_x + v_y(t)\hat{\sigma}_y = \hat{H}_0 + \hat{V}(t).$$

(2.04)

If we have a Hamiltonian operator of this form, it is possible to remove the drift term by moving to the interaction picture. Some useful relationships enable us to eliminate the drift term ($\hat{H}_0$) as follows:

$$\text{Let } \hat{U} = \hat{Q}\hat{P} \quad \text{where} \quad i\frac{d\hat{Q}}{\mathrm{dt}} = (\sum_j u_j \hat{H}_j)\hat{Q} \quad \text{and} \quad i\frac{d\hat{P}}{\mathrm{dt}} = (\hat{Q}^{-1}\hat{H}_0\hat{Q})\hat{P} \tag{2.05}$$

so that:

$$i\frac{d\hat{U}}{\mathrm{dt}} = i\frac{d\hat{Q}}{\mathrm{dt}}\hat{P} + i\hat{Q}\frac{d\hat{P}}{\mathrm{dt}} = (\sum_j u_j \hat{H}_j)\hat{Q}\hat{P} + \hat{Q}(\hat{Q}^{-1}\hat{H}_0\hat{Q})\hat{P} = (\hat{H}_0 + \sum_j u_j \hat{H}_j)\hat{U} \tag{2.06}$$

So in order to solve the problem, we need only consider the expressions for $\hat{Q}$ and $\hat{P}$ in (2.05) to find the evolution operator. In this reference frame, the equations of motion (2.05) reduce to:

$$\hat{U}_I = \exp(-i\hat{H}_0 t)\hat{U}; \quad \hat{H}_{\mathrm{int}}(t) = \exp(-i\hat{H}_0 t)\hat{V}(t)\exp(+i\hat{H}_0 t)\ ; \quad i\frac{\mathrm{d}\hat{U}_I}{dt} = \hat{H}_{\mathrm{int}}(t)\hat{U}_I \tag{2.07}$$

It is impossible to proceed further without assumptions or constraints on the form of the control fields. The simplest example for the control fields which is analytically solvable is

$$u_{\pm}(t) = \sum_j \begin{cases} |r_j|\exp(\mp i(\omega_0 t + \theta_j)) & t_{j-1} < t < t_j \\ 0 \quad \text{otherwise} \end{cases} \qquad \text{where } r_j = |r_j|e^{i\theta_j} \tag{2.08}$$

Then the Hamiltonian operator in the interaction picture (2.07) may be written as:

$$\hat{H}_{\mathrm{int}}(t) = \sum_j \begin{pmatrix} 0 & r_j \\ r_j^* & 0 \end{pmatrix} \tag{2.09}$$

The evolution of the system has been broken up into discrete time steps; at each interval a constant magnitude control field is applied. The control fields in this case are independent (as they only apply to a single time step) and the evolution may therefore be evaluated as the net result of the individual time steps. For the interval $t_{j-1} < t < t_j$ the time evolution can be solved quite neatly using:

$$\hat{H}_j = \begin{pmatrix} 0 & r_j \\ r_j^* & 0 \end{pmatrix} \ , \ \hat{H}_j^2 = r_j^* r_j \mathbf{1}$$

$$\Rightarrow \hat{U}^j(t,T) = \exp(-i(t-T)\hat{H}_j)$$

$$= \begin{pmatrix} \cos(|r_j|(t-T)) & -i\cdot\sin(|r_j|(t-T))\exp(i\theta_j) \\ -i\cdot\sin(|r_j|(t-T))\exp(-i\theta_j) & \cos(|r_j|(t-T)) \end{pmatrix} \tag{2.10}$$

Finally the total time evolution operator reads as:

$$\hat{U}(t,0) = \prod_{k=0}^{n-1} \hat{U}^{k}(t_{k+1}, t_k)$$

(2.11)

If the limit is taken such that the time step distance ϵ tends to zero, whilst allowing the number of increments n to proceed to infinity, and maintaining the condition that $n\epsilon = t_f - t_0$ it is possible to derive an expression for the time evolution matrix as a function of the control field. A more general example of Law and Eberly [14] uses the Hamiltonian operator

$$\hat{H} = (r(t) + g(t)\hat{a})\hat{\sigma}_+ + (r^*(t) + g^*(t)\hat{a}^+)\hat{\sigma}_-$$

(2.12)

where the $\hat{a}$ ($\hat{a}^+$) refer to the creation (annihilation) operators of the electromagnetic field. Using the standard matrix definitions of these operators, and breaking the system evolution into $2m$ discrete time steps during which either the classical ($r(t)$) or quantum ($g(t)$) control fields are active, we arrive at the following expression for the time evolution operator

$$\hat{U}(t,0) = \hat{U}_Q(2m, 2m-1)\hat{U}_C(2m-1, 2m-2).....\hat{U}_Q(2,1)\hat{U}_C(1,0).$$

(2.13)

The individual time evolutions under classical and quantised interactions, labelled by C and Q respectively, are given by

$$\hat{U}_Q(j, j-1) = \exp(-i\tau(g_j\hat{a}\hat{\sigma}_+ + g_j^*\hat{a}^+\hat{\sigma}_-))$$

$$\hat{U}_C(j, j-1) = \exp(-i\tau(r_j\hat{\sigma}_+ + r_j^*\hat{\sigma}_-)).$$

(2.14)

Difficulty remains with this formulation of control theory in that we have the evolution operator but must take a tedious limit on the control fields to apply it to any real time dependent example outside the simple situation we set up. The other key concern is that we must also evaluate the transition probability that a chosen process occurs and then find a particular time at which its value is unity in order to be able to claim a degree of control over the system. There is no specific guarantee from the theory of Law and Eberly [14] that this derived time is a minimum. This is the topic that we will specifically address in the next chapter.

"*...suppose we have succeeded in measuring in some way one physical property of an atomic system. Now we go on to make a measurement of the second physical property. That measurement necessarily will involve an interaction, the strength of which is not arbitrarily weak and the effect of which is not controllable, in such a way that it will, in general, produce changes in the physical circumstances that specify the conditions of the first measurement.*"

Julian Schwinger, in *Quantum Mechanics: Symbolism of Atomic Measurements* [15].

Chapter 3: Time Optimal Quantum Control

The branch of time-optimal quantum control that we will now explore uses a particular form of Hamilton's principle of least action. This action principle and mathematical technique is similar to the variational calculus historically developed and initiated by the researches of J. Bernoulli and P. Fermat, aimed at finding solutions of time optimality. This formalism may be applied to find the particular solutions for the motion of a particle travelling under the influence of the gravitational force and the path that a ray of light takes when travelling through a medium of variable refractive index. There is a long history throughout physics of use of action principles with many famous names including Maupertius, Euler, Lagrange, Fermat, Bernoulli, Hamilton, Feynman, Schrödinger and Schwinger using it to solve problems that were relevant to their times.

Time optimal open-loop quantum control does not simply come from nowhere; its working parts contain useful information that comes from physical reasoning about the nature of the control system we are able to apply. Aharanov and Anandan [16] derived an equation relating the metric of the projective state space to the energy variance $\Delta E^2 = <\psi|(\tilde{H} - <\tilde{H}>\mathbf{1})^2|\psi>$:

$$\frac{\mathrm{d}s}{\mathrm{d}t} = \Delta E \tag{3.00}$$

where $\mathrm{d}s$ is the Fubini-Study metric of the complex projective space $\mathbb{CP}^N$ and $\mathrm{d}t$ is the increment of physical time. This is the quantum control equivalent of (1.15), used in the classical brachistochrone problem. The Fubini-Study metric is discussed by Braunstein and Caves in [17] and Wootters [18]. It may be derived by extending the notion of a statistical distinguishability metric for probability distributions to quantum pure states, by considering a state expanded in an orthonormal basis

$$|\psi> = \sum_j \sqrt{p_j} e^{i\varphi_j} |j> \tag{3.01}$$

where the p_j's are a set of probabilities, φ_j representing the quantum phases.

We then construct a metric using an infinitesmal translation on the state

$$\frac{1}{4}\mathrm{d}s^2 = 1 - |<\psi + \mathrm{d}\psi|\psi>|^2 = <\mathrm{d}\psi|(1-\hat{P})|d\psi> \tag{3.02}$$

where $\hat{P} = |\psi><\psi|$. For our quantum mechanical control problem the action principle needs to be recast in such a way that we can apply it to find optimal transfers between two states of the quantum system. We are seeking a time-dependent Hamiltonian that takes us time optimally from one state to another. We do not rule out the existence of systems where there are a number of extremal trajectories; however, we are searching for a global extremum where the time is a minimum regardless of the given initial and final states. Our mathematical apparatus departs from that of Khaneja et. al [5] in that we do not use the Cartan decomposition of the algebra of generators of the unitary operators. We also do not make the assumption that 1-qubit gates take arbitary time. The techniques of [5,9] are relevant in their own right as the matrices which define our operational spaces have structure which may be examined rigorously using group theory, as in [19].

The expression that justifies the hard work ahead is the quantum brachistochrone equation. It is algebraically equivalent to the Heisenberg equation of motion for operators, and its specific use is to derive the time dependence of the external controls (voltages, laser frequencies etc.) that we must execute in order to arrive at the correct configuration in least time, given some specified initial condition. The derivation of the quantum brachistochrone equation (QBE) consists of several steps. Firstly, we postulate on physical grounds the existence of an action functional whose extremal values give the time-dependence of the optimal Hamiltonian. This action functional contains the information regarding experimental constraints and the physical dynamics of the wave-function. This functional is then varied and the Euler-Lagrange equations are derived. In this case the resulting expressions are the Schrödinger equation for the wave-function and an operator equation for the Hamiltonian describing the boundary value problem with a set of constraint laws. Once we have these expressions we use algebraic manipulation to obtain quantum control laws for our system. These laws take the form of time-dependent operator equations, and generalise the Heisenberg equations of motion for quantum systems.

Writing out the expression for the time-optimal quantum control action from [10] we have

$$S = \int_{t_0}^{t_f} (\mathfrak{L}_T + \mathfrak{L}_S + \mathfrak{L}_C)\,\mathrm{d}t \tag{3.03}$$

where the constituent Lagrangian functions in (3.03) have the explicit forms

$$\mathfrak{L}_T = \frac{1}{\Delta E}\frac{\mathrm{d}s}{\mathrm{d}t} \;\; ; \;\; \begin{cases} \frac{\mathrm{d}s}{\mathrm{d}t} = \sqrt{<\dot{\psi}|(1-\hat{P})|\dot{\psi}>} \\ \Delta E^2 = <\psi|(\tilde{H} - <\tilde{H}>\mathbf{1})^2|\psi> \end{cases}$$

$$\mathfrak{L}_S = +i(<\phi|\dot{\psi}> - <\dot{\psi}|\phi>) - (<\phi|\tilde{H}|\psi> + <\psi|\tilde{H}|\phi>);$$

$$\mathfrak{L}_C = \sum_j \lambda_j\, f_j(\tilde{H}) \tag{3.04}$$

We are working with the traceless part of the Hamiltonian

$$\tilde{H} = \hat{H} - \frac{\mathbf{1}_N}{N}\mathrm{Tr}(\hat{H}).$$

(3.05)

In doing so, we are making a specific choice of the gauge, being the traceless reference frame. The constituent parts of the total Lagrangian ensure minimisation of total time ($\mathfrak{L}_T$), the wave functions obey the Schrodinger equation ($\mathfrak{L}_S$) and experimental constraints ($\mathfrak{L}_C$) are obeyed throughout the quantum evolution. The variations that must be carried out are with respect to the set $(|\phi>, |\psi>, \tilde{H}, \lambda_j)$. $\hat{P}$ is the projection operator, $|\psi>$ is the wavefunction, $\tilde{H}$ is the traceless part of the Hamiltonian operator, $|\phi>$ is a Lagrange multiplier, λ_j are arbitary time-dependent functions to be specified by the calculation and the $f_j(\tilde{H})$ are functionals of the Hamiltonian itself. The first term is unity using the Aharanov-Anandan relationship

$$\mathfrak{L}_T = \frac{\Delta E}{\Delta E} = 1$$

(3.06)

and therefore contributes a term $\int \mathrm{d}t$ to the action, justifying our claim of time optimality. The second term in the Lagrangian ($\mathfrak{L}_S$) ensures that the correct Schrödinger dynamics of the system is maintained throughout the evolution. The third term ($\mathfrak{L}_C$) gives the necessary constraints on our Hamiltonian. These constraints take the form of functionals of the Hamiltonian, and enable us to eliminate experimentally unfeasible terms from our analysis. Writing the Euler-Lagrange equations that result from the variation of (3.03)

$$\delta|\phi> \quad : \qquad i|\dot{\psi}> = \tilde{H}|\psi>; \qquad (A)$$

$$\delta|\psi> \quad : \qquad -\frac{i}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\tilde{H} - <\tilde{H}>\mathbf{1}}{\Delta E^2}\right)|\psi> = i|\dot{\phi}> - \tilde{H}|\phi>; \qquad (B)$$

$$\delta\tilde{H} \quad : \qquad \frac{(\{\tilde{H}, \hat{P}\} - 2<\tilde{H}>\hat{P})}{2\Delta E^2} + (|\phi><\psi| + |\psi><\phi|) = \sum_j \lambda_j \frac{\partial f_j}{\partial \tilde{H}}; \qquad (C)$$

$$\delta\lambda_j \quad : \qquad f_j(\tilde{H}) = 0 \quad \forall j \qquad (D)$$

(3.07)

We now define the F-operator as

$$\hat{F} = \sum_j \lambda_j \frac{\partial f_j}{\partial \tilde{H}} = (|\phi><\psi| + |\psi><\phi|) + \frac{(\{\tilde{H}\,,\hat{P}\} - 2<\tilde{H}>\hat{P})}{2\Delta E^2}.$$

(3.08)

The trace of the second term on the right of (3.08) may be easily computed

$$\mathrm{Tr}(\{\tilde{H}\,,\hat{P}\} - 2<\tilde{H}>\hat{P}) = 2<\tilde{H}> - 2<\tilde{H}> = 0.$$

(3.09)

Taking expectation values of the same term yields the result

$$<\{\tilde{H}\,,\hat{P}\} - 2<\tilde{H}>\hat{P}> = 0.$$

(3.10)

Using this we evaluate the trace and expectation value (w.r.t. $|\psi>$) of the F-operator as

$$<\hat{F}> = \mathrm{Tr}(\hat{F}) = <\psi|\phi> + <\phi|\psi>.$$

(3.11)

Computing the anticommutator of the F-operator and the projector we finally obtain

$$\{\hat{F}\,,\hat{P}\} = \hat{F}\hat{P} + \hat{P}\hat{F}$$

$$= (|\phi><\psi| + |\psi><\phi|) + \frac{(\{\tilde{H}\,,\hat{P}\} - 2<\tilde{H}>\hat{P})}{2\Delta E^2} + (<\psi|\phi> + <\phi|\psi>)\hat{P}\ .$$

(3.12)

This results in the F-operator boundary condition

$$\{\hat{F}\,,\hat{P}\} = \hat{F} + <\hat{F}>\hat{P}.$$

(3.13)

Defining the G-operator we arrive at the boundary condition equations (BCEs):

$$\hat{G} = \hat{F} - <\hat{F}>\hat{P};$$

(3.14)

$$\{\hat{G}(t),\hat{P}(t)\}=\hat{G}(t)\,;\ \text{ with }\ \mathrm{Tr}(\hat{G})=2<\hat{G}>=0$$

(3.15)

This is an important relationship that we will use repeatedly throughout this thesis. It enables us to specify the exact form of the time-optimal Hamiltonian using the boundary conditions on the quantum state.

We now move through some simple algebraic manipulations. Firstly ketting the Schrödinger equation (3.07A) with $<\phi|$ and the conjugate of (3.07B) with $|\psi>$ we obtain:

$$i<\phi|\dot{\psi}>=<\phi|\tilde{H}\,|\psi>\,; \qquad (A)$$

$$i<\dot{\phi}\,|\psi>=-<\phi|\tilde{H}\,|\psi>-\frac{i}{2}<\psi|\frac{\mathrm{d}}{\mathrm{d}t}(\frac{\tilde{H}-<\tilde{H}>\mathbf{1}}{\Delta E^2})|\psi>;\ \ (B)$$

(3.16)

Evaluating the time-derivative of the expectation value of the Hamiltonian and using (3.07A) we find

$$\frac{\mathrm{d}}{\mathrm{d}t}<\tilde{H}>=<\dot{\psi}\,|\tilde{H}\,|\psi>+<\psi|\tilde{H}\,|\dot{\psi}>+<\frac{\mathrm{d}\tilde{H}}{\mathrm{d}t}>\,;$$

$$\Rightarrow\ \frac{\mathrm{d}}{\mathrm{d}t}<\tilde{H}>=<\frac{\mathrm{d}\tilde{H}}{\mathrm{d}t}>\,.$$

(3.17)

This means we may effectively differentiate under the expectation sign. Calculating the time-derivative of the inner product using (3.16)

$$\frac{\mathrm{d}}{\mathrm{d}t}<\phi|\psi>=-\frac{1}{2}<\frac{\mathrm{d}}{\mathrm{d}t}(\frac{\tilde{H}-<\tilde{H}>\mathbf{1}}{\Delta E^2})>=0.$$

(3.18)

Hence we obtain a constant of the motion given by

$$<\phi|\psi>=\mathrm{const}=-<\psi|\phi>+<\hat{F}>\,.$$

(3.19)

Taking the Euler-Lagrange equation that comes from the variation $\delta\tilde{H}$ (3.07C) and right-multiplying by $|\psi>$ we arrive at the result

$$|\phi>=(<\psi|\phi>-\frac{(\tilde{H}-<\tilde{H}>\mathbf{1})}{2\Delta E^2}+\hat{G})|\psi>\,.$$

(3.20)

After differentiating both sides of (3.20) with respect to time and substituting the constant of the motion into the equation the derived expression is given by

$$(i\frac{\mathrm{d}\hat{G}}{\mathrm{d}t}+[\hat{G}\,,\tilde{H}\,])|\psi>=0.$$

(3.21)

Some trivial algebra using hermitian conjugates and right-multiplication proves that the G-operator and projection operator follow the Heisenberg equation of motion

$$i\frac{\mathrm{d}\hat{G}}{\mathrm{d}t} = [\tilde{H}, \hat{G}] \qquad (A)$$

$$i\frac{\mathrm{d}\hat{P}}{\mathrm{d}t} = [\tilde{H}, \hat{P}] \qquad (B).$$

(3.22)

We then use these expressions to evaluate the time-derivative of the F-operator by direct differentiation of (3.14) and (3.15) to yield

$$i\frac{\mathrm{d}\hat{F}}{\mathrm{d}t} = [\tilde{H}, \hat{F}] + i\hat{P}\frac{\mathrm{d}}{\mathrm{d}t} < \hat{F} > = [\tilde{H}, \hat{F}] \quad \text{since} \quad \frac{\mathrm{d}}{\mathrm{d}t} < \hat{F} > = 0.$$

(3.23)

and hence

$$i\frac{\mathrm{d}\hat{F}}{\mathrm{d}t} = \tilde{H}\hat{F} - \hat{F}\tilde{H}$$

(3.24)

So it is proved that the G-operator, F-operator and projection operator all obey the Heisenberg equation of motion. We shall refer to this important relationship as the Quantum Brachistochrone Equation (QBE) throughout this text. Equations (3.24) and (3.15) form the foundations of applied time optimal quantum control theory, and we will refer to them repeatedly.

It is important to point out that we will consider an energetic constraint as part of our quantum control methodology in practice. Restrictions or constraints take the mathematical form of Lagrange multipliers in the action functional. The energetic restriction restricts the total energy used in the process to be finite, and is given by

$$f_0(\tilde{H}) = \mathrm{Tr}(\frac{\tilde{H}^2}{2}) - k = 0.$$

(3.25)

The other constraints which restrict the degrees of freedom for the Hamiltonian of the system will often be linear in $\tilde{H}$

$$f_j(\tilde{H}) = \mathrm{Tr}(\tilde{H}\hat{g}_j).$$

(3.26)

The $\hat{g}_j'$ s are Hermitean operators over a space of the same dimension as the Hamiltonian. In this case the Hamiltonian and F-operator will obey the equation

$$\hat{F} = \lambda_0\tilde{H} + \hat{F}';$$

$$\mathrm{Tr}(\tilde{H}\hat{F}') = 0; \qquad \hat{F}' = \sum_j \lambda_j\hat{g}_j.$$

(3.27)

as well as the quantum brachistochrone equation (QBE) (3.24) which may be rewritten in a form suitable for direct application

$$i\frac{\mathrm{d}}{\mathrm{d}t}(\tilde{H}+\hat{F}')=[\tilde{H}\,,\hat{F}'] \quad \text{as} \quad [\tilde{H}\,,\tilde{H}]=0. \tag{3.28}$$

We will apply this expression to many different mathematical and physical examples within this thesis. The basic methodology is to separate the group into Hamiltonian and constraint generators; we then may write down the open-loop quantum control equations by matrix addition, differentiation and multiplication.

Chapter 4: Optimal Qubit Control

Qubit is information science terminology for a two-level quantum system, as the two basis states may be conveniently mapped into the logical values **0** and **1**. The physical degree of freedom we are interested is the spin state of the electron. An electron may be spin up or down. Our first real time optimal state control problem is then to arrange the electron to be in some final configuration given the initial condition and a certain set of constraints on the physical Hamiltonian.

The subject of control of qubits is extensive as is to be expected, and it is impossible to name all the papers relevant to two-level quantum state control. Boscain et. al [7] examine a trajectory-based approach with a quantum Pontraygin principle to find time-minimal paths for two-state systems. The method we use, developed by the author and originating in [10] differs from [9] in that the equations of motion which define the Hamiltonian and state are found without complicated algebra other than basic matrix multiplication. The main objective is to evaluate the differential equations arising from direct application of (3.28) to a two-level system with a simple toy constraint.

One of the simplest quantum systems to analyse is that of an isolated electron spin, which we can control using magnetic fields. In our case, we wish to consider a situation where a two level system has a Hamiltonian which cannot generate rotations around the z-axis in the Bloch sphere, as well as the standard finite energy restriction. The following calculation (up to scaling) is equivalent to that contained in [10]. It is included as a demonstration of the basic mathematical techniques we will use throughout the document when solving time optimal quantum control problems. In particular we assume the constraints on the Hamiltonian may be written

$$
\begin{aligned}
f_0(\tilde{H}) &= \mathrm{Tr}(\frac{\tilde{H}^2}{2}) - k = 0 \qquad (A) \\
f_1(\tilde{H}) &= \mathrm{Tr}(\tilde{H}\hat{\sigma}_z) = 0 \qquad (B) \\
\mathrm{Tr}(\tilde{H}) &= 0 \qquad (C)
\end{aligned}
\tag{4.00}
$$

From (3.08) we have the expression for the F-operator

$$\hat{F} = \lambda_0(\tilde{H}(t) + \Omega\hat{\sigma}_z) \quad \text{where } \Omega = \lambda_1/\lambda_0.$$

(4.01)

The results derived in this section are not new work, but the matrix analysis methods we use to reach the same answer as [10] are novel and developed solely by the author. Assume that the Hamiltonian is some arbitary matrix on SU(2), given by a linear combination of Pauli matrices

$$\tilde{H} = \begin{pmatrix} \alpha & \varepsilon \\ \varepsilon^* & -\alpha \end{pmatrix} \quad \text{where} \quad \varepsilon = u - iv.$$

(4.02)

Computing (4.00B) directly we find that $\alpha = 0$ which implies that $\tilde{H} = u\hat{\sigma}_x + v\hat{\sigma}_y$. Writing the quantum brachistochrone equation (3.28) and evaluating the right hand side by ordinary matrix multiplication:

$$i\frac{\mathrm{d}\hat{F}}{\mathrm{d}t} = [\tilde{H}, \hat{F}] = \tilde{H}\hat{F} - \hat{F}\tilde{H};$$

$$i\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \Omega & \varepsilon \\ \varepsilon^* & -\Omega \end{pmatrix} = 2\Omega\begin{pmatrix} 0 & -\varepsilon \\ \varepsilon^* & 0 \end{pmatrix}$$

(4.03)

By inspection, $\Omega = \text{const}$. We may write the differential equations for the complex control fields in the form

$$i\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \varepsilon(t) \\ \varepsilon^*(t) \end{pmatrix} = 2\Omega\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \varepsilon(t) \\ \varepsilon^*(t) \end{pmatrix}$$

(4.04)

and hence our solution for the Hamiltonian is

$$\tilde{H}_{\mathrm{opt}}(t) = \begin{pmatrix} 0 & \varepsilon(0)e^{2i\Omega t} \\ \varepsilon^*(0)e^{-2i\Omega t} & 0 \end{pmatrix}.$$

(4.05)

We must now apply the boundary conditions of the initial and final state (3.15) to completely specify the Hamiltonian. Using an initial state of $|\Psi(0)> = \frac{1}{\sqrt{2}}[1,\ 1]^T$ in (3.15) we find that $\varepsilon(0) = -\varepsilon^*(0)$ and therefore

$$\tilde{H}_{\mathrm{opt}}(t) = v_0(\sin 2\Omega t\,\hat{\sigma}_x + \cos 2\Omega t\,\hat{\sigma}_y)$$

(4.06)

The isotropic condition (4.00A) gives us that $v_0^2 = k$. Using the final state $|\Psi(T)> = \frac{1}{\sqrt{2}}[1,-1]^T$ in (3.15) gives us another boundary condition on the Hamiltonian, yielding $\varepsilon(T) = -\varepsilon^*(T)$.

We may rewrite this as

$$\sin(2\Omega T) = 0$$

(4.07)

and this gives us the quantisation condition

$$\Omega T = \frac{n\pi}{2} \quad n \in \mathbb{N}.$$

(4.08)

We now move to consideration of the unitary operator which drives the state. The F-operator evolves unitarily as per (3.24), and therefore we may write a solution as

$$\hat{F}(t) = \hat{U}(t,0)\hat{F}(0)\hat{U}^+(t,0).$$

(4.09)

Rearranging and substituting (4.01) on both sides:

$$(\tilde{H}(t) + \Omega\hat{\sigma}_z)\hat{U} = \hat{U}(\tilde{H}(0) + \Omega\hat{\sigma}_z)$$

(4.10)

and after using the Schrödinger equation, we find the dynamical equation for the unitary, given by

$$i\frac{\mathrm{d}\hat{U}}{\mathrm{d}t} = \hat{U}(\tilde{H}(0) + \Omega\hat{\sigma}_z) - \Omega\hat{\sigma}_z\hat{U}$$

(4.11)

which has an explicit solution

$$\hat{U}(t,0) = \exp(i\,t\,\Omega\hat{\sigma}_z)\exp(-i\,t(\tilde{H}(0) + \Omega\hat{\sigma}_z)).$$

(4.12)

After some algebra we find the unitary operator has matrix representation

$$\hat{U}(t,0) = [\cos(\Omega t)\cos(\Omega' t) + \frac{\Omega}{\Omega'}\sin(\Omega t)\sin(\Omega' t)]\mathbf{1}$$

$$- i\frac{v_0}{\Omega'}\sin(\Omega' t)[\hat{\sigma}_x \sin(\Omega t) + \hat{\sigma}_y \cos(\Omega t)]$$

$$+ i\hat{\sigma}_z[\cos(\Omega' t)\sin(\Omega t) - \frac{\Omega}{\Omega'}\cos(\Omega t)\sin(\Omega' t)] \tag{4.13}$$

where $\Omega' = \sqrt{k + \Omega^2}$. We require a unitary that satisfies boundary conditions of the form

$$\hat{U}(T,0)\hat{\sigma}_x \hat{U}^+(T,0) = -\hat{\sigma}_x. \tag{4.14}$$

and after some work we derive a second quantisation condition, given by $\Omega' T = m\pi/2$, $m \in \mathbb{N}$. After some simple manipulation of the two quantisation conditions we finally find the minimum time of transfer

$$\Omega'^2 = k + \Omega^2 \;\Rightarrow (\Omega' T)^2 = kT^2 + (\Omega T)^2$$

$$\text{where} \quad \Omega T = \frac{n\pi}{2} \quad \text{and} \quad \Omega' T = m\pi/2 \qquad n, m \in \mathbb{N}$$

hence

$$T^2 = \frac{\pi^2}{4k}(n^2 - m^2) \tag{4.15}$$

The left-hand side of (4.15) is the square of a real number, and is therefore positive. We then derive the inequality $n > m$, assuming both non-negative integers and $T > 0$. Our minimum time of operation is then given by

$$T_{\min} = \frac{\pi}{2\sqrt{k}} = \frac{\pi}{2v_0} \tag{4.16}$$

as being inversely proportional to the strength of the control Hamiltonian (4.06).

This section has merely reproduced the results of [10], using the machinery of matrix mechanics. It is this technique, utilised originally by Werner Heisenberg [1], that we will focus on within this document. The matrix mechanics method of time-optimal quantum control is particularly useful and concise, as it enables us to calculate all the useful properties of the quantum control system without getting tied up in tedious algebra.

Chapter 5: Optimal Qutrit Control

Let us consider a more general example, to which we can apply the open-loop quantum control. Until now we have concentrated only on control of two-level systems. As we have a binary computation system at present, qubit control is naturally interesting and useful. In general it is difficult to find analytical solutions on higher-level systems. This is due to the relative complexity in calculating time evolution operators for time-dependent Hamiltonians on SU(N) for $N \geq 3$. To avoid this complication, we use a mathematical technique developed by Laufer in [20].

The control problem we are going to analyse in this chapter is that of a qutrit, being a three level quantum system which may be pumped by external control fields. One physical representation of this would be a group of three quantum dots in a line; the state is represented by the presence of a single electron in this system. For the time being we neglect completely the effects associated with the spin degree of freedom of the electron, and assume that we can perform our operations without influencing the spin. This is simply for mathematical simplicity, and its physical meaning is clear: we are measuring the charge present in the dots and not the spin. The quantum behaviour of the charged spinning electron in the three dot system *is* different, and if we were to perform a joint control of the spin and charge we would find a quite different (and more complex) result as our answer. For now, we are going to leave this as a problem for the future and consider the simplest case possible.

By applying voltages in the correct fashion, it is possible to cause the charge to hop from one location to another. We may set up the experimental situation such that the energies required to move the charge between the pairs of dots (1,2), (1,3) and (2,3) are all well separated. There are then three distinct energy levels and a basis of three states designated $|1>$, $|2>$ and $|3>$ which indicates the presence of the charge in dot 1, 2 or 3. By then choosing various experimental regimes we may examine the different control Hamiltonians which affect the quantum system's behaviour. This whole section and the remainder of the document is new work developed solely by the author. The Lie Algebra relevant to the qutrit system is SU(3). We shall use the Gell-Mann basis for SU(3); its properties and concrete representation are contained in Appendix 5.

SU(3) is already significantly more complicated in structure than SU(2), and this makes it harder to find analytical solutions for the wavefunction and unitaries. The fundamental reason for this is the difficulty in solving the polynomial equations which describe the eigenvalues and energy levels of the system. This does not negate the use of effective and clever factorisations to solve these problems, and it turns out that these are relationships of great utility. Useful algebraic properties of the relevant matrix groups are contained within [21] and [22]. Boscain [23] also looks at a three-state quantum control system as a generalisation of his SU(2) techniques. Again, his method is very different to ours, as we do not have to perform anything other than matrix multiplication and solve coupled differential equations.

5I. Lambda System

We consider a lambda type system first, with an intermediate level |2> which links states |1> and |3>. The transition from |1> to |3> can only occur via some intermediate process through |2>. We may write this as a simple chemical reaction chart

$$|1> \rightleftharpoons |2> \rightleftharpoons |3> .$$

It is quite straightforward to write down the form of the Hamiltonian, by requiring that the matrix is Hermitean and using the generators of SU(3) in Appendix 5. The matrix is given by

$$\tilde{H} = u_1(t)\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + v_1(t)\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + u_2(t)\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} + v_2(t)\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}; \; u_1, u_2, v_1, v_2 \in \mathbb{R}. \tag{5.00}$$

The explicit time-dependence of the control functions is to be determined from the quantum brachistochrone equation (3.28). Let us consider first the isotropic constraint; this restricts the total energy available to the system during the evolution to be less than some finite constant

$$\mathrm{Tr}(\tilde{H}^2/2) = u_1^2 + u_2^2 + v_1^2 + v_2^2 = k < \infty. \tag{5.01}$$

The linear constraints may be written in the form

$$\mathrm{Tr}(\tilde{H}\hat{F}') = 0$$
$$\hat{F}' = \sum_{j \in S} \lambda_j(t)\hat{\eta}_j \; ; \quad \lambda_j \in f\colon \mathbb{R} \to \mathbb{R}. \tag{5.02}$$

where the set S is SU(3) without the generators which appear in the Hamiltonian operator (5.00). We use the standard Gell-Mann basis of SU(3) (see [24] and Appendix 5) to conduct our calculations. It is straightforward to determine the matrix of the constraints as

$$\hat{F}' = \begin{pmatrix} \lambda_8/\sqrt{3} + \lambda_3 & 0 & \lambda_4 - i\lambda_5 \\ 0 & \lambda_8/\sqrt{3} - \lambda_3 & 0 \\ \lambda_4 + i\lambda_5 & 0 & -2\lambda_8/\sqrt{3} \end{pmatrix}. \tag{5.03}$$

Evaluating the quantum brachistochrone equation is then a matter of commuting the Hamiltonian matrix with the constraint operator $\hat{F}'$, and setting it equal to the time derivative of their sum (3.28). The principal result is that the control variables $(\lambda_3, \lambda_4, \lambda_5, \lambda_8)$ which appear in the constraint are in fact constant functions, and the control fields associated with the Hamiltonian satisfy the matrix equation

$$\frac{d}{d\tau}\begin{pmatrix} u_1(t) \\ v_1(t) \\ u_2(t) \\ v_2(t) \end{pmatrix} = \begin{pmatrix} 0 & 2\lambda_3 & \lambda_5 & -\lambda_4 \\ -2\lambda_3 & 0 & -\lambda_4 & -\lambda_5 \\ -\lambda_5 & \lambda_4 & 0 & -\lambda_3+\sqrt{3}\lambda_8 \\ \lambda_4 & \lambda_5 & \lambda_3-\sqrt{3}\lambda_8 & 0 \end{pmatrix}\begin{pmatrix} u_1(t) \\ v_1(t) \\ u_2(t) \\ v_2(t) \end{pmatrix} \tag{5.04}$$

where we have rescaled the time using $t = \lambda_0 \tau$. This is written in terms of *real* functions of time; in this particular case the solvable form of the equations is reached by examining the *complex* functions of time. Both sets are isomorphic to each other. Interestingly, the matrix equation for the real control functions (5.04) can be written in the form

$$i\frac{d\vec{x}}{\mathrm{dt}} = \hat{A}\vec{x}. \tag{5.05}$$

where the matrix $\hat{A}$ is Hermitean, a constant and tracefree. This is relevant as it means that the control fields themselves satisfy a Schrödinger-type equation. This is not always true, and seems to hold only for special cases. The equations which define the control variables may be non-linear for even slightly more complicated cases, and we demonstrate why in Appendix 4. The process of solving for the control fields often involves embedding the problem inside a larger space and at the end removing the extra degrees of freedom. In this general sense it is similar to the approach of Bellman [25] in classical control theory. The reason for the constraint in this case being a constant matrix is such: the generators in $\hat{F}'$ spanning the subgroup $G_{\hat{F}'}$ have the property that when they are operated on by the commutator with any generator which appears in $G_{\tilde{H}}$ then the result always lies in $G_{\tilde{H}}$. In mathematics this property can be written as

$$\forall\ \hat{\eta}_j \in G_{\tilde{H}} \quad \text{and} \quad \hat{\eta}_k \in G_{\hat{F}'} \quad \text{then} \, [\hat{\eta}_j, \hat{\eta}_k] \in G_{\tilde{H}} \ \forall\, j,k \longleftrightarrow \hat{F}' = \text{const.} \tag{5.06}$$

Appendix 4 shows *why* the structure of the algebra is to be directly associated with the form of the control system. For this particular situation, the Hamiltonian and associated constraint can be compactly rewritten in matrix form as

$$\tilde{H}(t) = \begin{pmatrix} 0 & \varepsilon_1(t) & 0 \\ \varepsilon_1^*(t) & 0 & \varepsilon_2(t) \\ 0 & \varepsilon_2^*(t) & 0 \end{pmatrix} \qquad \text{and} \qquad \hat{F}' = \begin{pmatrix} \omega_1 & 0 & \kappa \\ 0 & \omega_2 & 0 \\ \kappa^* & 0 & -(\omega_1+\omega_2) \end{pmatrix} \tag{5.07}$$

We have introduced the control variables

$$\varepsilon_1 = u_1 - i\,v_1\ ;\ \ \varepsilon_2 = u_2 - i\,v_2\ ;\ \ \kappa = \lambda_4 - i\,\lambda_5$$

$$\omega_1 = \lambda_3 + \lambda_8/\sqrt{3}\ ; \qquad \omega_2 = -\,\lambda_3 + \lambda_8/\sqrt{3}.$$

(5.08)

Using (3.28) again we find

$$i\frac{d}{\mathrm{dt}}\begin{pmatrix} \omega_1 & \varepsilon_1 & \kappa \\ \varepsilon_1^* & \omega_2 & \varepsilon_2 \\ \kappa^* & \varepsilon_2^* & -(\omega_1+\omega_2) \end{pmatrix} = \begin{pmatrix} 0 & -(\omega_1-\omega_2)\varepsilon_1 - \kappa\varepsilon_2^* & 0 \\ (\omega_1-\omega_2)\varepsilon_1^* + \kappa^*\varepsilon_2 & 0 & \kappa\varepsilon_1^* - (\omega_1+2\omega_2)\varepsilon_2 \\ 0 & -\kappa^*\varepsilon_1 + (\omega_1+2\omega_2)\varepsilon_2^* & 0 \end{pmatrix}$$

(5.09)

from which we immediately observe that ω_1, ω_2 and κ are constants. Now assume that the wave-vector is initially in state $|1>$ at $t=0$ and ends in state $|3>$ at $t=T$. We then have boundary conditions on the projector given by

$$\hat{P}(0) = |1><1| = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \hat{P}(T) = |3><3| = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

(5.10)

Since we have the initial and final conditions, we may use the quantum control equation (3.15) to write

$$\begin{cases} \hat{G}(0) = \{\hat{G}(0), \hat{P}(0)\} \\ \hat{G}(T) = \{\hat{G}(T), \hat{P}(T)\} \end{cases} \qquad \hat{G} = \hat{F} - <\hat{F}>\hat{P} \qquad \hat{F} = \lambda_0\tilde{H} + \hat{F}'.$$

(5.11)

The boundary conditions on the state translate into boundary conditions on the control fields (epsilons). These are derived by substitution of (5.10) into (5.11) and using elementary linear algebra. We find that the boundary conditions are equivalent to the expressions

$$\omega_1 = \omega_2 = 0$$

$$\varepsilon_2(0) = \varepsilon_2^*(0) = 0$$

$$\varepsilon_1^*(T) = \varepsilon_1(T) = 0.$$

(5.12)

As the diagonal elements of $\hat{F}'$ in (5.07) are constant in time, and by eq. (5.12) are originally zero, then they are zero always.

We then have the interaction picture equation of motion

$$\hat{F}(t) = \hat{U}(t,0)\hat{F}(0)\hat{U}^{+}(t,0)$$

(5.13)

and may rewrite the time evolution operator in the form

$$\hat{U}(t,0) = \exp(i\hat{F}'t)\cdot\exp(-i(\tilde{H}(0)+\hat{F}'(0))t) = \hat{U}_1\hat{U}_2$$

(5.14)

where we have absorbed the constant λ_0 into the Hamiltonian as a scaling factor. We will evaluate this in parts; firstly, let us examine $\hat{U}_2$. In this case we are required to calculate

$$\hat{U}_2 = \exp(-i[\tilde{H}(0)+\hat{F}'(0)]t) = \exp(-i\begin{pmatrix} 0 & \varepsilon_1(0) & \kappa(0) \\ \varepsilon_1^*(0) & 0 & 0 \\ \kappa^*(0) & 0 & 0 \end{pmatrix}t) = \exp(-i\hat{B}t)$$

(5.15)

as $\omega_1,\ \omega_2,\ \varepsilon_2(0),\ \varepsilon_2^*(0) = 0$. We now refer the reader to the paper of Laufer [20] which outlines the exponentiation of general matrices over SU(n) in terms of the eigenvalues. We wish to apply his formalism to SU(3); firstly we evaluate the eigenvalue equation

$$0 = \det(\hat{B}-\alpha\hat{\mathbf{1}}) = -\alpha^3 + \alpha(|\varepsilon_1(0)|^2 + |\kappa(0)|^2)$$

(5.16)

which has solutions

$$\alpha_1 = 0, \quad \alpha_2 = +\sqrt{|\varepsilon_1(0)|^2+|\kappa(0)|^2} = +\Delta, \qquad \alpha_3 = -\Delta.$$

(5.17)

Laufer's formulae [20] allow us to write the exponential of a general matrix in SU(3) as

$$\hat{U}_2 = \exp(-i\hat{B}t) = f_1(t)\hat{\mathbf{1}} + f_2(t)\hat{B} + f_3(t)\hat{B}^2$$

$$f_1(t) = \frac{1}{m}(\alpha_2\alpha_3(\alpha_2-\alpha_3)e^{-i\alpha_1 t} + \alpha_1\alpha_3(\alpha_3-\alpha_1)e^{-i\alpha_2 t} + \alpha_1\alpha_2(\alpha_1-\alpha_2)e^{-i\alpha_3 t})$$

$$f_2(t) = \frac{1}{m}(\alpha_1(\alpha_2-\alpha_3)e^{-i\alpha_1 t} + \alpha_2(\alpha_3-\alpha_1)e^{-i\alpha_2 t} + \alpha_3(\alpha_1-\alpha_2)e^{-i\alpha_3 t})$$

$$f_3(t) = \frac{1}{m}((\alpha_2-\alpha_3)e^{-i\alpha_1 t} + (\alpha_3-\alpha_1)e^{-i\alpha_2 t} + (\alpha_1-\alpha_2)e^{-i\alpha_3 t})$$

$$m \stackrel{\circ}{=} (\alpha_1-\alpha_2)(\alpha_1-\alpha_3)(\alpha_2-\alpha_3)$$

(5.18)

and hence using (5.17) in (5.18) we obtain the formula

$$\Delta = \sqrt{|\varepsilon_1(0)|^2+|\kappa|^2}$$

$$\hat{U}_2 = \begin{pmatrix} \cos(t\Delta) & \frac{-i}{\Delta}\varepsilon_1(0)\sin(t\Delta) & \frac{-i}{\Delta}\kappa\sin(t\Delta) \\ \frac{-i}{\Delta}\varepsilon_1^*(0)\sin(t\Delta) & \frac{1}{\Delta^2}(|\kappa|^2+|\varepsilon_1(0)|^2\cos(t\Delta)) & \frac{1}{\Delta^2}(\varepsilon_1^*(0)\kappa)(\cos(t\Delta)-1) \\ \frac{-i}{\Delta}\kappa^*\sin(t\Delta) & \frac{1}{\Delta^2}(\varepsilon_1(0)\kappa^*)(\cos(t\Delta)-1) & \frac{1}{\Delta^2}(|\varepsilon_1(0)|^2+|\kappa|^2\cos(t\Delta)) \end{pmatrix}.$$

(5.19)

We find the other time evolution operator $\hat{U}_1$ from this by making the substitutions $\varepsilon_1(0) = 0$ and $t \longmapsto -t$. The result is

$$\hat{U}_1 = \begin{pmatrix} \cos(|\kappa|t) & 0 & \frac{i\kappa}{|\kappa|}\sin(|\kappa|t) \\ 0 & 1 & 0 \\ \frac{i\kappa^*}{|\kappa|}\sin(|\kappa|t) & 0 & \cos(|\kappa|t) \end{pmatrix}. \tag{5.20}$$

Now our state vector at some future time is given by

$$|\psi(t)> = \hat{U}_1\hat{U}_2|\psi(0)>. \tag{5.21}$$

For our particular experimental situation we require that initially the system is in $|1>$ and finally at $|3>$ after time T. Hence we may write the state after some matrix multiplication as

$$|\psi(t)> = \begin{pmatrix} \cos(t\Delta)\cos(|\kappa|t) + \frac{|\kappa|}{\Delta}\sin(|\kappa|t)\sin(t\Delta) \\ \frac{-i\varepsilon_1^*(0)}{\Delta}\sin(t\Delta) \\ i\kappa^*[\frac{1}{|\kappa|}\sin(|\kappa|t)\cos(t\Delta) - \frac{1}{\Delta}\sin(t\Delta)\cos(|\kappa|t)] \end{pmatrix}. \tag{5.22}$$

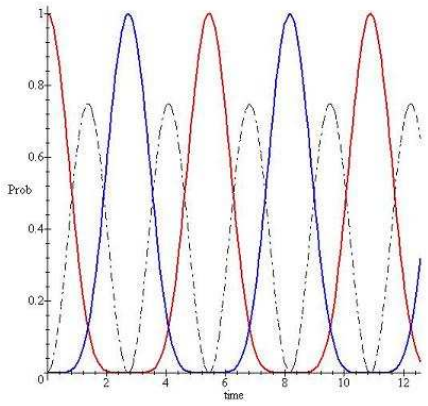

Figure 1. Probability and time curves for the optimally-controlled V-system

In the above figure, the solid line starting at **1** on the y-axis represents the probability that the state is in $|1>$; the dashed line is the probability that the state is in $|2>$ and the solid line starting at **0** is the corresponding curve for $|3>$. As can be seen, initially all the probability is at $|1>$; after some time, amplitude is transferred to state $|2>$ and begins feeding into the final state $|3>$. The whole system is periodic and cyclical, the minimum time of transfer being given by the time taken for the probability to anneal into the state $|3>$. We have chosen a scaling $|\varepsilon| = \sqrt{|\varepsilon_1|^2 + |\varepsilon_2|^2} = 1$ to plot the curves.

We are interested in the form of the projection operator, given by the outer product of the state with itself. By setting the initial and final boundary conditions as outlined above, we may derive the minimum time of evolution as follows. Firstly, calculating the projection operator

$$\hat{P}(t) = |\psi(t)><\psi(t)| = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} (c_1^*, c_2^*, c_3^*) = \begin{pmatrix} |c_1|^2 & c_1 c_2^* & c_1 c_3^* \\ c_1^* c_2 & |c_2|^2 & c_2 c_3^* \\ c_1^* c_3 & c_2^* c_3 & |c_3|^2 \end{pmatrix}. \tag{5.23}$$

The next step is to realise that after the optimal time of operation given by $t = T$, which is the minimum time required for the transition from $|1>$ to $|3>$ to occur, the matrix elements of the projection operator satisfy

$$\begin{gathered} |c_3(T)|^2 = 1 \\ |c_2(T)|^2 = |c_1(T)|^2 = c_1(T)c_2^*(T) = c_1(T)c_3^*(T) = c_2(T)c_3^*(T) = 0. \end{gathered} \tag{5.24}$$

Hence we may write the above set of boundary conditions as

$$\begin{gathered} |c_2(T)|^2 = \frac{1}{\Delta^2}|\varepsilon_1(0)|^2 \sin^2(T\Delta) = 0 \\ \Rightarrow \quad \sin(T\Delta) = 0 \\ \Rightarrow \quad T = \frac{n\pi}{\sqrt{|\kappa|^2 + |\varepsilon_1(0)|^2}} \quad n \in \mathbb{N}. \end{gathered} \tag{5.25}$$

Considering the boundary conditions on the parameter $|c_1(T)|^2 = 0$ we obtain $\cos(|\kappa|T) = 0$. This implies

$$T = (2n' + 1)\frac{\pi}{2|\kappa|} \quad n' \in \mathbb{N}. \tag{5.26}$$

Now for these to both be the minimum time, we must have them equal. From this we find the important relationship

$$|\kappa|^2[1 - (\frac{n' + 1/2}{n})^2] = (\frac{n' + 1/2}{n})^2 |\varepsilon_1(0)|^2. \tag{5.27}$$

The quantity on the right hand side is the square of a real number, and hence is positive. This means that the function multiplying $|\kappa|^2$ on the left hand side must be positive, and hence

$$\begin{gathered} 1 - [\frac{n' + 1/2}{n}] \geqslant 0 \\ \Rightarrow n \geqslant n' + 1/2. \end{gathered} \tag{5.28}$$

This means that the minimum time is obtained for $n=1, n'=0$ and reads

$$T_{\min} = \frac{\pi}{2|\kappa|} = \frac{\sqrt{3}\pi}{2|\varepsilon_1(0)|} \tag{5.29}$$

where we have used from (5.27) that $|\kappa| = |\varepsilon_1(0)|/\sqrt{3}$. Remembering that the diagonal terms in $\hat{F}'$ are zero from boundary conditions we may write the control matrix equation (5.09) as

$$i\frac{d}{\mathrm{dt}}\begin{pmatrix} \varepsilon_1 \\ \varepsilon_1^* \\ \varepsilon_2 \\ \varepsilon_2^* \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -\kappa \\ 0 & 0 & \kappa^* & 0 \\ 0 & \kappa & 0 & 0 \\ -\kappa^* & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_1^* \\ \varepsilon_2 \\ \varepsilon_2^* \end{pmatrix}. \tag{5.30}$$

After some further algebra we obtain

$$\tilde{H}_{\mathrm{opt}}(t) = \begin{pmatrix} 0 & |\varepsilon_1(0)|\cos(|\kappa|t) & 0 \\ |\varepsilon_1(0)|\cos(|\kappa|t) & 0 & \varepsilon_2(T)\sin(|\kappa|t) \\ 0 & \varepsilon_2^*(T)\sin(|\kappa|t) & 0 \end{pmatrix}. \tag{5.31}$$

This may be written in an equivalent form as

$$\tilde{H}_{\mathrm{opt}}(t) = |\varepsilon_1(0)| \begin{pmatrix} 0 & \cos(|\kappa|t) & 0 \\ \cos(|\kappa|t) & 0 & e^{-i\theta}\sin(|\kappa|t) \\ 0 & e^{+i\theta}\sin(|\kappa|t) & 0 \end{pmatrix} \tag{5.32}$$

where $\varepsilon_2(T) = |\varepsilon_2(0)|e^{-i\theta}$ and we have used the normalisation condition $|\varepsilon_1(0)| = |\varepsilon_2(T)|$. Note that as the constraint $\hat{F}'$ was a constant matrix, even though the Hamiltonian is of a fairly complex form we were able to evaluate the evolution operator without having to use the full time-dependent Hamiltonian. All that was required was the time dependence of the constraint $\hat{F}'$ (in this case a constant), the initial condition of the Hamiltonian operator and the boundary conditions on the state. This is a useful trick and readily extended to many different circumstances. This is the first solution for open-loop time optimal state control on qutrits.

5II. Lambda System with Self-Interaction

Our next control problem on SU(3) is one in which the Hamiltonian has only the (13) and (31) terms forbidden. Using the standard Gell-Mann basis for SU(3) contained in Appendix 5 we may write

$$\tilde{H} = \begin{pmatrix} u_7 + u_8/\sqrt{3} & u_1 - i\cdot u_2 & 0 \\ u_1 + i\cdot u_2 & -u_7 + u_8/\sqrt{3} & u_3 - i\cdot u_4 \\ 0 & u_3 + i\cdot u_4 & -2u_8/\sqrt{3} \end{pmatrix}; \quad u_1, u_2, u_3, u_4, u_7, u_8 \in \mathbb{R} \tag{5.33}$$

for which the operator $\hat{F}'$ is given by the matrix

$$\hat{F}' = \lambda_4(t)\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} + \lambda_5(t)\begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & \kappa \\ 0 & 0 & 0 \\ \kappa^* & 0 & 0 \end{pmatrix}; \quad \kappa = \lambda_4 - i\lambda_5. \tag{5.34}$$

Evaluating the quantum brachistochrone equation (3.28) by direct differentiation and matrix multiplication, we obtain the set of differential equations given by the matrix identity (setting $\lambda_0 = 1$)

$$i\frac{d}{\mathrm{dt}}\begin{pmatrix} u_7 + u_8/\sqrt{3} & u_1 - i\cdot u_2 & \kappa \\ u_1 + i\cdot u_2 & -u_7 + u_8/\sqrt{3} & u_3 - i\cdot u_4 \\ \kappa^* & u_3 + i\cdot u_4 & -2u_8/\sqrt{3} \end{pmatrix}$$

$$= \begin{pmatrix} 0 & -\kappa(u_3 + i\cdot u_4) & \kappa(u_7 + \sqrt{3}u_8) \\ \kappa^*(u_3 - i\cdot u_4) & 0 & \kappa(u_1 + i\cdot u_2) \\ -\kappa^*(u_7 + \sqrt{3}u_8) & -\kappa^*(u_1 - i\cdot u_2) & 0 \end{pmatrix}. \tag{5.35}$$

This may be written in control-matrix form as

$$i\frac{d}{\mathrm{dt}}\begin{pmatrix} \varepsilon_1 \\ \varepsilon_1^* \\ \varepsilon_2 \\ \varepsilon_2^* \\ \kappa \\ \kappa^* \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -\kappa & 0 & 0 \\ 0 & 0 & \kappa^* & 0 & 0 & 0 \\ 0 & \kappa & 0 & 0 & 0 & 0 \\ -\kappa^* & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \omega & 0 \\ 0 & 0 & 0 & 0 & 0 & -\omega \end{pmatrix}\begin{pmatrix} \varepsilon_1 \\ \varepsilon_1^* \\ \varepsilon_2 \\ \varepsilon_2^* \\ \kappa \\ \kappa^* \end{pmatrix}. \tag{5.36}$$

where control variables have been defined as

$$\varepsilon_1 = u_1 - i\cdot u_2$$

$$\varepsilon_2 = u_3 - i\cdot u_4$$

$$\omega = u_7 + \sqrt{3}u_8 = \text{const.} \tag{5.37}$$

The control fields u_7 and u_8 are constants, as can be seen from examining the diagonal elements from equation (5.35). The equations for κ, κ^* inside the matrix in (5.36) decouple from the rest of the system; we may therefore analyse them separately

$$i\frac{d}{\mathrm{dt}}\begin{pmatrix} \kappa \\ \kappa^* \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \kappa \\ \kappa^* \end{pmatrix} \tag{5.38}$$

with a solution $\kappa(t) = \kappa(0)e^{-i\omega t}$. Explicit substitution of this formula into the upper block of the matrix in (5.36) yields the matrix equation

$$i\frac{d\vec{x}}{\mathrm{dt}} = \hat{\mathcal{A}}\vec{x}$$

$$\vec{x}\,(t) = \begin{pmatrix} \varepsilon_1 \\ \varepsilon_1^* \\ \varepsilon_2 \\ \varepsilon_2^* \end{pmatrix}$$

$$\hat{\mathcal{A}} = \hat{\mathcal{A}}\,(t) = \begin{pmatrix} 0 & 0 & 0 & -\kappa_0 e^{-i\omega t} \\ 0 & 0 & \kappa_0^* e^{+i\omega t} & 0 \\ 0 & \kappa_0 e^{-i\omega t} & 0 & 0 \\ -\kappa_0^* e^{+i\omega t} & 0 & 0 & 0 \end{pmatrix}. \tag{5.39}$$

We may write the control-matrix equations for the complex control fields in the form

$$i\frac{d}{\mathrm{dt}}\begin{pmatrix} \varepsilon_1 \\ \varepsilon_1^* \\ \varepsilon_2 \\ \varepsilon_2^* \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -\kappa_0 e^{-i\omega t} \\ 0 & 0 & \kappa_0^* e^{i\omega t} & 0 \\ 0 & \kappa_0 e^{-i\omega t} & 0 & 0 \\ -\kappa_0^* e^{i\omega t} & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \varepsilon_1 \\ \varepsilon_1^* \\ \varepsilon_2 \\ \varepsilon_2^* \end{pmatrix}. \tag{5.40}$$

By inspection, it is apparent that there is cross-coupling between the $\varepsilon_1 - \varepsilon_2^*$ and $\varepsilon_1^* - \varepsilon_2$ subsystems. The differential equations are just

$$\begin{aligned} i\frac{d\varepsilon_1}{\mathrm{dt}} &= -\kappa_0 e^{-i\omega t}\varepsilon_2^* \qquad (A) \\ i\frac{d\varepsilon_2^*}{\mathrm{dt}} &= -\kappa_0^* e^{i\omega t}\varepsilon_1 \qquad (B) \end{aligned} \tag{5.41}$$

and their complex conjugates. Direct differentiation of (5.41A) gives

$$i\left(\frac{d^2}{\mathrm{dt}^2} + |\kappa_0|^2\right)\varepsilon_1 = i\omega\kappa_0 e^{-i\omega t}\varepsilon_2^*. \tag{5.42}$$

Back-substitution of (5.41A) into (5.42) yields the second-order differential equation

$$\frac{d^2\varepsilon_1}{\mathrm{dt}^2} + i\omega\frac{d\varepsilon_1}{\mathrm{dt}} + |\kappa_0|^2\varepsilon_1 = 0. \tag{5.43}$$

It is quite straightforward to evaluate the rest of the equations of motion in a similar fashion. The resulting differential equation is

$$\frac{d^2\varepsilon_{1,2}}{\mathrm{dt}^2} + i\omega\frac{d\varepsilon_{1,2}}{\mathrm{dt}} + |\kappa_0|^2\varepsilon_{1,2} = 0.$$

(5.44)

Using a trial exponential solution, we obtain the form of the control fields

$$\varepsilon_{1,2}(t) = e^{-i\omega t/2}(R_+^{1,2}\exp(i\chi\omega t/2) + R_-^{1,2}\exp(-i\chi\omega t/2))$$

$$\text{with} \quad \chi = \sqrt{1 + \frac{4|\kappa_0|^2}{\omega^2}}$$

(5.45)

where the $R_\pm^{1,2}$'s and $W_\pm^{1,2}$'s are constants.

Let us now analyse the transformation laws which apply between the various qutrit sub-problems; this is an important calculation as it can save a large amount of work and tedious algebra. Firstly, let us transform the (31)-(13) system such that it turns into the (23)-(32) system. This may be achieved by application of the permutation from $\mathcal{S}^3$ with matrix representation

$$\hat{W}_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \tilde{H}_1 = \begin{pmatrix} 0 & 0 & \varepsilon \\ 0 & 0 & 0 \\ \varepsilon^* & 0 & 0 \end{pmatrix}$$

$$\tilde{H}_3 = \hat{W}_3\tilde{H}_1\hat{W}_3^+ = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon^* & 0 \end{pmatrix}.$$

(5.46)

In fact, we may transform the constraint and Hamiltonian for a more general case where two complex control fields are applied to the state. This transformation causes the Hamiltonian to change form to

$$\tilde{H} = \begin{pmatrix} 0 & \varepsilon_1 & 0 \\ \varepsilon_1^* & 0 & \varepsilon_2 \\ 0 & \varepsilon_2^* & 0 \end{pmatrix} \quad \longrightarrow \quad \tilde{H}_{W_3} = \hat{W}_3\tilde{H}\hat{W}_3^+ = \begin{pmatrix} 0 & \varepsilon_1^* & \varepsilon_2 \\ \varepsilon_1 & 0 & 0 \\ \varepsilon_2^* & 0 & 0 \end{pmatrix}$$

(5.47)

whereas the constraint operator changes in the following fashion

$$\hat{F}' = \begin{pmatrix} a+b & 0 & \kappa \\ 0 & -a+b & 0 \\ \kappa^* & 0 & -2b \end{pmatrix} \longrightarrow \hat{F}'_{W_3} = \hat{W}_3 \hat{F}' \hat{W}_3^+ = \begin{pmatrix} -a+b & 0 & 0 \\ 0 & a+b & \kappa \\ 0 & \kappa^* & -2b \end{pmatrix}. \tag{5.48}$$

Evaluating the QBE (3.28) we obtain the equivalent control problem

$$i\frac{\mathrm{d}\vec{X}_G}{\mathrm{dt}} = \hat{\mathcal{A}}_G \vec{X}_G \qquad a, b, \kappa \ \text{ constants.} \tag{5.49}$$

where the relevant vectors and matrices have the structure

$$\hat{\mathcal{A}}_G = \hat{G}\hat{\mathcal{A}}\hat{G}^{-1}; \quad \hat{G}^{-1} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; \quad \hat{\mathcal{A}} = \begin{pmatrix} 2a & \kappa^* & 0 & 0 \\ \kappa & a-3b & 0 & 0 \\ 0 & 0 & -2a & -\kappa \\ 0 & 0 & -\kappa^* & -a+3b \end{pmatrix}; \quad \vec{X}_G = \begin{pmatrix} \varepsilon_1^* \\ \varepsilon_2 \\ \varepsilon_1 \\ \varepsilon_2^* \end{pmatrix}. \tag{5.50}$$

Thus it is demonstrated that the permutation group plays a useful role in the simplifying calculations in open loop quantum control. The physical meaning is clear; the control fields may be relabelled, but the dynamical law possesses various symmetries which must be preserved under such a transformation. It is for this reason that we keep encountering the same equations for a number of different constrained systems.

Chapter 6: Dual Qubit Optimal Control

Quantum control on a four-level system then seems to be the logical extension of the techniques considered thus far in this thesis. One major axiom that is currently in use in coupled-qubit computation is that of arbitrarily fast transformations on single qubits [26, 27, 28]. We will not assume this postulate, but rather work directly with the algebra and compute the optimal Hamiltonian for a simple two-qubit (4-level) system to begin with.

6I. Heisenberg Model

Assume that we may perform control operations on each qubit without individual addressing. This means that the Hamiltonian must be of the form

$$\tilde{H} = \lambda_0 \, \hat{\sigma}_z \otimes \hat{\sigma}_z + \lambda_x \, \hat{\sigma}_x \otimes \hat{\sigma}_x + \lambda_y \, \hat{\sigma}_y \otimes \hat{\sigma}_y \tag{6.00}$$

This has explicit matrix representation:

$$\tilde{H} = \begin{pmatrix} \lambda_0 & 0 & 0 & \lambda_- \\ 0 & -\lambda_0 & \lambda_+ & 0 \\ 0 & \lambda_+ & -\lambda_0 & 0 \\ \lambda_- & 0 & 0 & \lambda_0 \end{pmatrix}; \quad \lambda_\pm = \lambda_x \pm \lambda_y \tag{6.01}$$

Our constraint may be expanded in the Hermitean basis:

$$\hat{F}' = [\vec{m}(t) \cdot \vec{\sigma}] \otimes \mathbf{1} + \mathbf{1} \otimes [\vec{n}(t) \cdot \vec{\sigma}] + \sum_{\substack{j,k \in \{x,y,z\} \\ j \neq k}} \chi_{j,k}(t) \, [\hat{\sigma}_j \otimes \hat{\sigma}_k] \quad \text{where } \vec{m}, \vec{n} \in \mathbb{R}^3 \tag{6.02}$$

Evaluating (3.28) for this particular example we obtain the differential equations for the controls:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\lambda_0\\ \lambda_x\\ \lambda_y\end{pmatrix}=\mathbf{0} \tag{6.03}$$

and hence we may write the equation for the state vector at time t in the form:

$$|\psi(t)>=\exp(-it\tilde{H})|\psi(0)> \tag{6.04}$$

We choose an initial condition given by $|\psi(0)>=|00>$. Using (3.15) we find that $\lambda_x=-\lambda_y$. Evaluating (6.04) gives the time dependence of the wave-vector:

$$|\psi(t)>=\begin{pmatrix}\cos(2\lambda_x t)\\ 0\\ 0\\ -i\sin(2\lambda_x t)\end{pmatrix} \tag{6.05}$$

Hence after a time $T=\pi/8\lambda_x$ we find that the state has evolved to $\frac{1}{\sqrt{2}}(|00>-i|11>)$. Evaluating the boundary conditions using this state and (3.15), we find that $\lambda_0=0$. The isotropic condition $\mathrm{Tr}(\tilde{H}^2/2)=k$ yields the result that $\lambda_x=\sqrt{k}/2$ and therefore our optimal Hamiltonian is

$$\tilde{H}_{\mathrm{opt.}}=\sqrt{k}/2(\hat{\sigma}_x\otimes\hat{\sigma}_x-\hat{\sigma}_y\otimes\hat{\sigma}_y) \tag{6.06}$$

Discussions and Conclusions

D0. Principal Results

The results contained out in sections 5I, 5II and 6 are new and developed solely by the author. The main conclusion is that when the optimal quantum control system exists, the minimum time of evolution follows an empirical law of the form

$$(\text{Strength of control field}) \times (\text{Minimum time}) = \text{constant}. \tag{D0.00}$$

as observed in equations (4.16), (5.29) and under (6.05). This is qualitatively similar to the Heisenberg Uncertainty Principle for energy and time, $\Delta E \Delta t = \text{const}$. Physically this requires that to lower the time of evolution we must impart more energy to the system. By obeying the Heisenberg lower bound on energy-time, we have indeed found optimal systems.

The time-optimal Hamiltonian operators we were able to find, including (4.06) and the new results of (5.32), (5.37) and (6.03) were either constant matrices or composed of periodic functions. The constant matrices are geodesics, but it is the structure of the resonant operators that contains useful information about the physics of optimal quantum control.

Our methodology is able to be precisely summarised: find the experimental constraints, given a class of Hamiltonian operators (3.27); then apply the quantum brachistochrone equation (3.28) with an appropriate set of boundary conditions on the quantum state as outlined in (3.15).

Symmetry has been a necessary and useful tool in this investigation, both for error correction and throughout the calculation and for translation between different matrix groups. Time optimal quantum control is an area in which many matrix groups are related to each other in a fashion that is apparent to the observer. For example, the differential equations produced from the quantum brachistochrone can often appear as a Hamiltonian problem on higher dimensions, and as such it is possible to relate SU(2) with SU(4) via equation (4.11). In doing so, we are moving between the matrix and vector representations, going from an $n \times n$ matrix to a vector with n^2 entries. The object which operates on this new vector is an $n^2 \times n^2$ matrix. We may then define a new optimal control problem using this matrix, as in Chapter 5.II, create a vector and move up the dimensional chain.

The phenomena contained within the spectrum of time-optimal quantum state control is quite vast and complex. The results of this thesis would seem to indicate that analytical solutions are plentiful and evaluation of optimal control problems straightforward and formulaic. In reality this is not the case and there exist many problems, particularly of a non-linear type, that are resistant to simple analysis and remain unsolved.

DI. Methodology of Open Loop Quantum Control

For our standard quantum control we have the F-operator as being given by:

$$\hat{F} = \lambda_0 \tilde{H} + \hat{F}'$$

(DI.00)

where the first part represents the isotropic constraint, and the second is related to restrictions on $\tilde{H}$. For the time being, we restrict our discussion to the special case where the constraint is a constant matrix. In this particular example, the quantum brachistochrone (3.28) would read as:

$$i\frac{d\tilde{H}}{\mathrm{dt}} = [\tilde{H}\,, \hat{F}'\,]$$

(DI.01)

which is solved by the Heisenberg ansatz:

$$\tilde{H}(t) = \exp(i\hat{F}'t)\tilde{H}(0)\exp(-i\hat{F}'t)$$

(DI.02)

This is revealing of the subtleties of time optimal quantum control as discussed in [10]; even in the simplest example of a constant constraint we are not solving for the time-evolution operator given the time dependence of the Hamiltonian but for the optimal Hamiltonian operator itself. For a particular choice of initial and target states, the process of open-loop quantum control seeks to determine the functional time dependence of the Hamiltonian operator which steers from one state to another whilst minimising the time taken during the evolution [10], as well as respecting constraints on the total energy imparted to the system and on the degrees of freedom which are accessible to the experimentalist. What this achieves is a restriction within the group of all physical Hamiltonians to a subclass of time optimal operators; these remaining operators satisfy various physical properties in their functional form and time dependence.

The isotropic condition ensures that the amount of energy imparted to the system in reaching the target is bounded from above. This is essential as without it there is a possibility that operators may arise from within the control formalism that would require an infinite amount of energy to be imparted to the system in order to reach the target from our input state, which is not physically reasonable.

Other constraints on the accessible degrees of freedom available may be necessary to eliminate the experimentally difficult or unfeasible terms from our control operators. In a certain implementation of quantum computation it may be that some types of operations are straightforward whereas other operations are experimentally complicated. Therefore it is natural to attempt to find Hamiltonian operators which excite only feasible transitions and examine the time dependence of a chosen process occurring.

The quantum brachistochrone equations are similarity invariant, as are the constraint equations themselves due to the cyclic invariance of the trace. This is a very useful result, as it allows the application of symmetry, group theory and matrix analysis.

It is interesting to note that for the examples we have calculated explicitly, the control vector obeys a Schrödinger-type equation. This is not the case in general, and more difficult examples are highly non-linear. Because of this complication the variables which define the optimal Hamiltonian control variables may no longer be well-behaved in a mathematical sense, and the optimal control regimen which influences the system is no longer defined. The difficulties that arise may be sidestepped through a clever use of symmetry on the group in question. As we move to higher dimensional spaces, the symmetries become more complex and making a good choice of control and constraint groups is critical to finding a well-defined open-loop optimal control for the quantum system.

The control functions in any standard quantum mechanical system are normally defined by the actions of the experimentalist. The process of optimisation could therefore be viewed as a variational calculus over all possible experimental constructions to find the time-minimal arrangement between chosen initial and final states.

In this sense we are moving beyond quantum mechanics proper, and into quantum engineering as a discipline in its own right. Science seeks to observe systems for how they are, and from these observations make predictions which are confirmed at later times by experiment. Engineering takes this in another direction, in making a particular demand for an outcome to occur at some chosen time, and then asking if it is possible to steer the system such that it meets this criterion.

This result is useful to the field of quantum computation, as the computational device requires the delivery of predictable, regular and controllable outcomes for its practical operation.

DII. Physics of Quantum Control

In classical control and engineering the basic operational axioms are that:

1. The system under observation may be measured without disturbance, or any disturbance may be corrected for perfectly [2]

2. Errors within the system do not operate in superposition, but only independently [31]

3. The controls on individual components may be scaled to fit the numbers of components on the whole device

The first axiom implies that one may "find" the error, being the external disturbance beyond the necessary that the experiment has imparted to the system, and correct for it by including a complementary term during the next interaction such that it is compensated for.

The second statement makes clear the assumption on the physical nature of the errors which occur within the physical system itself. If we had a suitable physical system for computation, intuitively you would hope that the probability of a single error might be the greatest, two errors would be much less probable, three errors even less probable, etc. Within the computational system it would be definitely to the benefit of the engineer if there were no collective or exhange effects with the errors themselves, as this might have some strange effects on the data itself which might be difficult to reverse or correct for.

The third statement implies that it is possible to make a control mechanism for a device that is made of a number of different component parts, if we can make control mechanisms for the individual parts themselves and find a geometrical arrangement such that the components are adjacent to their associated controllers. It is a physical axiom, and necessary for the construction of a realistic architecture of a control system that is functional.

In quantum mechanics it is possible that these operational axioms of classical control are no longer useful, as the axioms upon which they depend become invalid as we move to the nanoscopic realm. However, many of the old mathematical techniques (with care taken to handle i!) translate into a useful quantum context. Let us consider the nature of these classical axioms with respect to quantum control theory, and see where the classical error correction and control theory may be extended. For simplicity of discussion, we consider an atom, located within a closed system upon which we may shine light of a known frequency.

Firstly, it is *not* possible to measure a quantum system without imparting some arbitrary, non-reversible disturbance to it. Our only way to observe the quantum state is to absorb some light which is scattered out of the system. Now, given that the system was initially in the ground state, this implies that we must shine light onto it in order to observe light being scattered out at some later time. However, we cannot predict with certainty *the time of absorption/emission*, *the position we detect at*, *what final momentum* and *how much energy* the photon will have. The best we can do is predict the possible distributions of these characteristics, and say that each variable has an associated Heisenberg conjugate. This means that during the intermediate step between when our input photon is absorbed by the atomic system and when it is observed to be emitted, we cannot assign a direct trajectory to the internal state of the system. The best we can do is say that the internal state has travelled over all indistinguishable intermediate states which lie between the initial and final states which were observed.

Even more interesting than this is that we never actually know what the internal state of the system *is*, only what it *was*. When we observe a photon being absorbed/emitted, we know for a fact that the atom has been excited/relaxed. However we only know with certainty what *happened*, not what is going to *happen*. The best we can do for predicting the future is give the distributions calculated from quantum mechanics; also, if there were indistiguishable alternatives which both could contribute to the observed result, we are not able to specify which one of these actually occurred. In order to be consistent we are required to allow all these indistinguishable pathways to operate in superposition.

To expand upon the second statement, let us imagine a physical system which consists of a one dimensional chain of spin-1/2 particles. Initially the spin of the atomic sites is identically down on all sites throughout the crystal. We might think of the "data" in this system as being represented by a spin-flip on a particular atomic site, which we achieve by lasing a certain atom in the chain with the correct frequency and polarisation of radiation.

An error in this situation would consist of either an incorrect labelling of the atomic sites (in which case we excite the wrong atom) or an incorrect timing of the shutter on our laser which causes us to excite more than what we were intending to. In either case, we may understand that the error particle is itself another spin-wave which also resides within the crystal. Much of the probability is concentrated around the "correct" site; however, it is possible that there is some small (but non-zero) component of the wavefunction which is distributed around the intended site of the excitation. In this sense we are required to analyse a system of interacting particles in the spin chain.

It is possible for these particles to scatter off each other. During this process, the error and the data may form a complex which possesses exchange characteristics which cannot be assigned to the composite parts. So it is not consistent in a quantum mechanical sense to think of the error and the data as being physical quantities that are independent of one another; in fact the *interaction* and *exchange* processes between the initial data and the intrinsic error creates the observed data output from the computational system. It would be interesting to investigate whether the system may be arranged in such a way that the error is negligible at appropriate instances of time, such that we may sample the data to receive the correct output with high probability.

The third statement of classical control states that if we have a technique for controlling one component (call it A) and another component (B), then if we would like to develop a device that contains both components then our only problem is to find a geometrical arrangement such that the controllers do not overlap. In a classical system this is completely acceptable, as there is negligible interaction and cross-talk between the external controllers. We could assume the errors arriving from each controller were independent and uncorrelated. The quantum system will behave quite differently, in that it is possible that control pulses targeted for a specific subspace may not arrive in the correct place or correct time, and may be correlated. The errors from the controllers and the errors from the environment may interact and cause change within the system.

In this general circumstance it is then necessary to move to a fully quantum control regime. Such a system would control the device by ensuring that targeted outcomes were reached by as many of the available data streams of intermediate states as possible. By maximising the numbers of routes to the target (and refusing to distinguish between them), the device is highly likely to be in the target state at the chosen time.

Imagine the microscopic flow of information along two wires in a computer chip. At the classical level, the data which flows in one wire is completely independent of the other. As we shrink the wires to the quantum level and bring them closer and closer together, we find that there comes a point where what is happening in one wire is affecting the operation of the other, regardless of the height of the potential barrier between them. The information in one wire represents the data; the information in the other wire is the associated error with respect to the chosen data source and vice versa.

We cannot even analyse one nanowire independent of the rest of the device. Consequently there is a direct requirement to model the whole mechanism in order to achieve open-loop optimal control.

DIII. Future Extensions of Quantum Control

Quantum state control is the *targeted steering of transitions within quantum systems*. By tuning some external control fields it is possible to engineer the quantum state to be in some particular configuration at some future time, given that we knew the state at some point in the past. Quantum mechanics is different in that the knowledge of the initial state is not sufficient to determine the experimental outcomes at all times with certainty; we must actually examine the probability that for a given input state, we receive a particular outcome after some time. More generalised disciplines of quantum control are equally as powerful, and it is relevant to consider their future development. Let us start with chemistry, and chemical engineering.

For a chemical reaction process we have a known initial condition, being the amount (and state) of substance that we start with. Many chemical reactions proceed through a series of intermediate steps, with the key concern of the chemist being to maximise the experimental yield of the desired product from the reaction vessel. Each of these steps represents a energetic transition, whether it be an exothermic or endothermic process. Consequently, given the knowledge of the chemist in the reaction sequence and of the physicist in the energy released/absorbed during each step, we may use quantum control methods to help the reaction proceed efficiently.

This may be achieved by using external laser pulses tuned to the energetic transitions which are occuring within the reaction vessel. By a clever use of pulse timing sequences we can ensure that we obtain a high yield of product, given a known input mixture [32]. This might minimise the loss due to wastage during the transitional reactions. It would be interesting to consider a chemical reaction industry that is based on coloured light. As light also has a polarisation, by engineering the internal state of the system to have a particular spin, one may further selectively target the transitions desired.

The use of quantum control techniques and systems which have tunable external parameters which may be toggled in real time brings us to a new forefront of quantum mechanics. By considering Hamiltonians which are explicitly time dependent, a large new area of mathematics and physics is also opened up for exploration by a new generation of scientists. This area has traditionally been considered a difficult area of study. Now that some new mathematical framework has been laid down it will prove possible and productive to reconsider the formulations of quantum mechanics from a control-theoretical perspective.

In the future, it is likely we will see many more applications of quantum control theory in devices which are used in the solid-state, optics, photonics, nuclear magnetic resonance and ion traps. These applications may include new techniques for engineering these systems such that they are stable, predictable and can be used as components in larger computational devices. The time-optimal theory is also directly applicable for industry, as nobody in business is ever keen on wasting time for nothing.

A1. Mathematical Methods

The use of optimal quantum control theory may be given a systematic basis for its application in real-world problems. In this appendix we will outline the methodology by which one may carry out any linear calculation in finite dimensions and derive the quantum control equations, as well as the state vector and time-evolution operator as functions of time.

To start the calculation we are required to specify a unitary matrix algebra $\mathcal{A}(\mathcal{G})$, with group $\mathcal{G}$ containing hermitean generators given by the set $\{\hat{g}_1, \hat{g}_2, ..., \hat{g}_N\} = \mathcal{S}$. We then partition the generators in $\mathcal{S}$ into two subsets $\mathcal{H}$ and $\mathcal{F}$ such that the Hamiltonian operator contains time-dependent linear combinations of generators from $\mathcal{H}$ and the motional constraint contains only members of $\mathcal{F}$.

$$\tilde{H} = \sum_{j \in \mathcal{H}} \lambda_j(t)\, \hat{g}_j$$

$$\hat{F}' = \sum_{k \in \mathcal{F}} \beta_k(t)\, \hat{g}_k$$

(A1.00)

Given the quantum control action principle, and assuming some constraints as Lagrange multipliers, the first step is to write the isotropic condition and the motional restrictions out in full:

$$\mathrm{Tr}(\frac{1}{2}\tilde{H}^2) - k = 0 \qquad \text{[i]}$$

$$\mathrm{Tr}(\tilde{H}\hat{F}') = 0 \qquad \text{[ii]}$$

(A1.01)

Equation (A1.01) [ii] is automatically satisfied as we have partitioned a trace-normalised inner product algebra, and [i] gives us a restriction on the functional nature of the Lagrange multipliers. We then take the matrix representations of the Hamiltonian and motional constraint and substitute these operators into the Quantum Brachistochrone equation:

$$i\frac{\mathrm{d}}{\mathrm{dt}}(\tilde{H} + \hat{F}') = \tilde{H}\hat{F}' - \hat{F}'\tilde{H}$$

(A1.02)

and evaluate the right-hand side by ordinary matrix multiplication. We obtain the differential equations which specify the time dependence of the functions which multiply the generators. This is done by simply reading off the entries of the matrices on the left and right hand sides and setting them equal. If there are enough constants of the motion available, we may move forward using the formulae below, otherwise the full non-linearity examined in Appendix 4 is applicable. If they exist the form of the matrix differential equation is of type:

$$i\frac{\mathrm{d}}{\mathrm{dt}}\begin{pmatrix}\lambda_1\\ \vdots\\ \lambda_j\\ \beta_1\\ \vdots\\ \beta_k\end{pmatrix}=\begin{pmatrix}A_{1,1} & \cdots & & \cdots & A_{1,N}\\ \vdots & \ddots & & & \vdots\\ & & \ddots & & \\ \vdots & & & \ddots & \vdots\\ & & & & \\ A_{N,1} & \cdots & & \cdots & A_{N,N}\end{pmatrix}\begin{pmatrix}\lambda_1\\ \vdots\\ \lambda_j\\ \beta_1\\ \vdots\\ \beta_k\end{pmatrix}\qquad j+k=N \tag{A1.03}$$

In general, this is a difficult problem to solve, but there are a number of techniques which may be applied at this point. Firstly, if we are able to move the linear operator $\hat{A}$ into a representation where it is block-diagonal, we are a lot closer to being able to evaluate the solution. Secondly, it may be possible to evaluate the solutions of the differential equations by a process of back-substitution and elimination. Thirdly, if both of the first two techniques fail we are still in a position where the numerical solutions may be evaluated without too much difficulty on a computer.

Now that the time-dependence of the control fields and Lagrange multipliers (λ_j's and β_k's) has been determined, it is necessary to solve the Schrödinger equation for the time evolution operator. This is achieved by writing the time-evolution operator in the form:

$$\hat{U}(t,0)=\hat{U}_1\hat{U}_2=T[\exp(+i\int_0^t \hat{F}'(s)\mathrm{ds})]\exp(-i(\tilde{H}(0)+\hat{F}'(0))t) \tag{A1.04}$$

where the T indicates a time-ordered product in the exponential. For a constant motional constraint the solution may be reached quite efficiently by using Laufer's formulae [16]. If the motional constraint is not constant, one is required to use other methods. For a periodic time-dependence, use of Floquet matrix techniques will enable the exponential to be evaluated.

Once the time-evolution operator has been evaluated we then place boundary conditions on the state-vector. These translate into relations on the projection operator, which is then substituted into the boundary condition equations (BCE's). This is given by:

$$\hat{P}(0)=|\psi(0)><\psi(0)|;\quad \hat{P}(T)=|\psi(T)><\psi(t)|;$$

$$\{\hat{G}(0),\hat{P}(0)\}=\hat{G}(0);\qquad \text{(i)}$$

$$\{\hat{G}(T),\hat{P}(T)\}=\hat{G}(T);\qquad \text{(ii)}$$

$$\hat{F}=\tilde{H}+\hat{F}';$$

$$\hat{G}=\hat{F}-<\hat{F}>_\psi\hat{P} \tag{A1.05}$$

This will give extra information on the form of the control fields, which eliminates all un-necessary constants from the final expressions. Now that the time-dependent Hamiltonian operator, the time-evolution operator and the boundary conditions on the state vector have been written out, the explicit functional form of the state may be written out as:

$$|\psi(t)> = \hat{U}(t,0)|\psi(0)> \tag{A1.06}$$

and the problem is solved. There are several key points that must be noted:

- The sequence in which these calculations are carried out is fixed in that one must evaluate the time dependence of the Hamiltonian before the time evolution operator can be written down. However, the boundary conditions can sometimes simplify the form of the control fields so it is useful to evaluate it early to save extra work.

- If we can calculate the time-dependence of the Hamiltonian, using the equation $\mathrm{id}\hat{U}/\mathrm{dt} = \tilde{H}(t)\hat{U}$ we can write out explicit formulae for the differential equations of state. If the Hamiltonian is periodic then this leads itself naturally to the application of Floquet theory.

- In higher dimensional systems than n=2, it is possible to encounter non-linear control systems which do not obey the above formulae (see Appendix 4). It has not been immediately apparent to the author how to attack this fundamental difficulty, and consequently, to find stable time-optimal control Hamiltonians for closed quantum systems it has been necessary to seek out special examples which may be evaluated using standard group theoretical and linear algebraic techniques.

A2. Useful Operators and Transformations

Various interesting and useful mathematical formulae on coupled qubits may be derived by considering the relationship between the permutation group $\mathcal{S}_4$ and the group $\mathcal{SU}(4)$. Some matrices are members of both groups, some are members of one and not the other, and the multiplication and similarity transforms of members of one group by the other has some very interesting symmetry.

We include this discussion so as to demonstrate the wide variety of unique operators which exist in this interesting matrix analytical space. These operators are useful in a mathematical sense for conducting calculations as they have a number of properties which simplify computational procedures; they also have a number of symmetries which are relevant to physical systems.

Let us begin with the matrix which maps the data encoded on the standard computational basis to the Bell states, given by:

$$\hat{B} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}} (\hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_z \otimes \mathbf{1}) = \hat{B}^{-1}$$

(A2.00)

The Hamiltonian operator used in NMR quantum computation takes the following form:

$$\hat{H} = g(\hat{\sigma_1} \cdot \hat{\sigma_2} - 3(\vec{n} \cdot \hat{\sigma_1})(\vec{n} \cdot \hat{\sigma_2})) - \mu_B((\vec{B}_1 \cdot \hat{\sigma_1}) \otimes \mathbf{1}_2 + \mathbf{1}_1 \otimes (\vec{B}_2 \cdot \hat{\sigma_2}))$$

$$= \hat{H}_{\text{int}} + \hat{H}_{r.o.} + \hat{H}_1 + \hat{H}_2 \text{ where } \vec{n}, \vec{B}_1 \text{ and } \vec{B}_2 \in \mathbb{R}^3$$

(A2.01)

and when transformed under this matrix it is mapped to the new Hamiltonian:

$$\tilde{H}' = \hat{B}\tilde{H}\hat{B}^{-1} = \begin{pmatrix} -2g & 0 & 0 & m_1 \\ 0 & -2g & m_2 & 0 \\ 0 & m_2 & 0 & 0 \\ m_1 & 0 & 0 & 4g \end{pmatrix}$$

(A2.02)

This has placed the matrix differential equation $i\frac{\mathrm{d}|\psi>}{\mathrm{d}t} = \tilde{H}|\psi>$ where $|\psi> = (C_1, C_2, C_3, C_4)^T$ into an interesting and useful form. By direct differentiation and back-substitution it is possible to write the first component of the matrix differential equation in the form:

$$\frac{d^2C_1}{\mathrm{dt}^2} + i(6g)\frac{\mathrm{dC_1}}{\mathrm{dt}} + (m_1^2 - 8g^2)C_1 = 0$$

(A2.03)

What we can observe from this is that the component in the transformed reference frame behaves as if it was a complex damped exponential. The superposition of the two oscillatory solutions produces the observed total wavefunction. This equation is easily solved by the method of exponential solution for constant g and magnetic fields.

Let us now consider some more computational operators to observe how they transform under the Bell transformation (A2.00). We choose particular matrices that have a high degree of symmetry; the point of this is to examine whether the symmetry is preserved under the operation. Our first choice of operator is given by:

$$\begin{aligned}\tilde{H}_1 &= \varepsilon(t)\hat{N} + \varepsilon^*(t)\hat{N}^T \\ &= \begin{pmatrix} 0 & 0 & \varepsilon^* & \varepsilon \\ 0 & 0 & \varepsilon & \varepsilon^* \\ \varepsilon & \varepsilon^* & 0 & 0 \\ \varepsilon^* & \varepsilon & 0 & 0 \end{pmatrix}\end{aligned} \tag{A2.04}$$

where $\hat{N} = \frac{1}{2}(\hat{\sigma}_x \otimes (1 + \hat{\sigma}_x) - i\hat{\sigma}_y \otimes (1 - \hat{\sigma}_x))$. Making the standard ansatz for the control fields ($\varepsilon = u - \imath v$) we obtain the formula:

$$\tilde{H}_1 = (u\hat{\sigma}_x + v\hat{\sigma}_y) \otimes \mathbf{1} + (u\hat{\sigma}_x - v\hat{\sigma}_y) \otimes \hat{\sigma}_x \tag{A2.05}$$

Under the isometric mapping with the Bell transform this operator gets taken to the new Hamiltonian operator:

$$\tilde{H}_1^B = \hat{B}\tilde{H}_1\hat{B}^{-1} = (u\hat{\sigma}_z - v\hat{\sigma}_y) \otimes \mathbf{1} + (u\hat{\sigma}_z + v\hat{\sigma}_y) \otimes \hat{\sigma}_x \tag{A2.06}$$

where is apparent that the mapping *does* preserve the symmetry of the operator. Let us consider a second example to demonstrate the utility of this matrix transformation. Our second Hamiltonian operator is the matrix:

$$\begin{aligned}\tilde{H}_2 &= \varepsilon(t)\hat{Q} + \varepsilon^*(t)\hat{Q}^T \\ &= \begin{pmatrix} 0 & \varepsilon & \varepsilon^* & 0 \\ \varepsilon^* & 0 & 0 & \varepsilon \\ \varepsilon & 0 & 0 & \varepsilon^* \\ 0 & \varepsilon^* & \varepsilon & 0 \end{pmatrix}\end{aligned} \tag{A2.07}$$

where $\hat{Q} = \frac{1}{2}(1 \otimes \hat{\sigma}_x + \hat{\sigma}_x \otimes 1 - i(\hat{\sigma}_y \otimes \hat{\sigma}_z - \hat{\sigma}_z \otimes \hat{\sigma}_y))$. After some elementary algebra and using the standard ansatz for the control fields, one finds the formula for the Hamiltonian in terms of generators of SU(4):

$$\tilde{H}_2 = u(t)(\mathbf{1} \otimes \hat{\sigma}_x + \hat{\sigma}_x \otimes \mathbf{1}) + v(t)(\hat{\sigma}_y \otimes \hat{\sigma}_z - \hat{\sigma}_z \otimes \hat{\sigma}_y) \tag{A2.08}$$

Mapping this via the Bell transformation we obtain:

$$\tilde{H}_2' = \mathbf{1} \otimes (u\hat{\sigma}_x + v\hat{\sigma}_y) + \hat{\sigma}_z \otimes (u\hat{\sigma}_x - v\hat{\sigma}_y) \tag{A2.09}$$

A3. Time Evolution Operators

Sometimes it can be difficult to directly solve the Schrödinger equation for the time evolution operator; if we are working in a quantum control setting there is another expression we can use that occasionally simplifies matters a great deal. Writing the evolution for the constraint:

$$\hat{F}(t) = \hat{U}(t,0)\hat{F}(0)\hat{U}^{+}(t,0)$$

(A3.00)

We then right-multiply by $\hat{U}(t,0)$ on both sides to give:

$$\hat{F}(t)\hat{U}(t,0) = \hat{U}(t,0)\hat{F}(0)$$

(A3.01)

Assuming an F-operator that is given by the variation of the isotropic constraint and some linear form we obtain:

$$\hat{F} = \tilde{H} + \hat{F}'$$
$$\tilde{H}(t)\hat{U} + \hat{F}'(t)\hat{U} = \hat{U}\tilde{H}(0) + \hat{U}\hat{F}'(0)$$

(A3.02)

We have the Schrodinger equation for $\hat{U}$, so substitution yields:

$$i\frac{\mathrm{d}\hat{U}}{\mathrm{dt}} = -\hat{F}'(t)\hat{U} + \hat{U}\tilde{H}(0) + \hat{U}\hat{F}'(0)$$

(A3.03)

For which we can formally write a solution as:

$$\hat{U}(t,0) = T_{\rightarrow}[\exp(+i\int_0^t \hat{F}'(s)\mathrm{d}s].\exp(-it(\tilde{H}(0) + \hat{F}'(0))$$

(A3.04)

where the $T_{\rightarrow}$ represents the time ordering operator. For examples with a constant constraint, the operator ordering trivialises and the evolution operator may be immediately evaluated.

A4. Tensor Equation of Open-Loop Quantum Control

Assume we have a Lie Algebra of dimension N that is spanned by a set of constant orthonormal generators $\hat{g}_j$. We then partition the group of generators G_N into two separate groups, which we call G_F and G_H. Defining the Hamiltonian and constraint by the sums:

$$\tilde{H} = \sum_{k \in G_H} \lambda_k(t)\, \hat{g}_k \; ; \qquad \hat{F}' = \sum_{l \in G_F} \lambda_l(t)\, \hat{g}_l$$

(A4.00)

with $G = G_H \oplus G_F$. The algebraic structure is given by the structure constants f_{jkl} :

$$[\hat{g}_k, \hat{g}_l] = i \sum_{j \in G} f_{jkl}\, \hat{g}_j$$

(A4.01)

We now use this expression in the quantum brachistochrone equation to write it in a new form:

$$i \sum_{j \in G} \hat{g}_j\, d\lambda_j/\mathrm{d}t = \sum_{k \in G_H} \sum_{l \in G_F} \lambda_k\, \lambda_l [\hat{g}_k, \hat{g}_l]$$

$$= i \sum_{j \in G} \sum_{k \in G_H} \sum_{l \in G_F} \lambda_k\, \lambda_l f_{jkl} \hat{g}_j$$

(A4.02)

Dropping the sum over the group and the generator $\hat{g}_j$ (which is arbitary) we arrive at the Riemannian form of the quantum brachistochrone equation, which specifies the behaviour for a chosen constraint:

$$\frac{\mathrm{d}\lambda_j}{\mathrm{d}t} - \sum_{k \in G_H} \sum_{l \in G_F} f_{jkl} \lambda_k\, \lambda_l = 0$$

(A4.03)

This equation is non-linear, and it is this difficulty that leads to complexity in analysis. For the analytically solvable examples we have some of the constraint or control variables being constants of the motion, and this allows the evaluation of the tensor equation. To examine a simple non-linear problem, consider two vectors $\vec{m}$ and $\vec{n}$ in $\mathbb{R}^3$ which define the control and constraint in SU(2).

The Hamiltonian and constraint have the form:

$$\hat{H} = \vec{m} \cdot \vec{\sigma} \ , \quad \hat{F}' = \vec{n} \cdot \vec{\sigma} \qquad ; \qquad \vec{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$$

(A4.04)

The algebra in this case is the Pauli spin algebra, with structure:

$$[\hat{\sigma}_j, \hat{\sigma}_k] = i f_{jkl} \hat{\sigma}_l$$

$$f_{jkl} = 2\epsilon_{jkl}$$

(A4.05)

where we have used ϵ_{jkl} to stand for the Levi-Civita symbol. Quantum control theory gives us the isotropic condition and the orthonormality property:

$$|\vec{m}|^2 = \text{const.}$$

$$\vec{m} \cdot \vec{n} = 0$$

(A4.06)

The equations of motion read as:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\vec{m} + \vec{n}) \cdot \vec{\sigma} = \sum_{j \in S} \sum_{k \in S} 2\epsilon_{ljk} m_j n_k \hat{\sigma_l} = 2(\vec{m} \wedge \vec{n}) \cdot \vec{\sigma}; \quad S = \{x, y, z\}$$

(A4.07)

Cancelling the sigma operators yields the concise expression:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\vec{m} + \vec{n}) = 2(\vec{m} \wedge \vec{n}); \qquad \vec{m} \wedge \vec{n} = \sum_{j \in S} \sum_{k \in S} \epsilon_{ljk} m_j n_k$$

However, for more complex constraints, and even some very simple ones on SU(3) and SU(4), there is no obvious constant of the dynamics and the equations which define the constraint and control variables become coupled in a highly non-linear fashion.

A5. Gell-Mann Basis of SU(3)

The SU(3) Lie Algebra is generated by the following matrices:

$$\hat{g}_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \hat{g}_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \hat{g}_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \hat{g}_4 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$\hat{g}_5 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad \hat{g}_6 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}$$

$$\hat{g}_7 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \hat{g}_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

(A5.00)

We may write any hermitean $\hat{M}$ in the 3 x 3 matrix space as a linear combination of these generators and the identity

$$\hat{M} = \alpha \hat{1}_3 + \sum_j \lambda_j \hat{g}_j .$$

(A5.01)

The generators $\hat{g}_j$ have various useful relationships, such as

$$\hat{g}_k^+ = \hat{g}_k \qquad , \qquad \mathrm{Tr}(\hat{g}_k) = 0 \quad , \quad \mathrm{Tr}(\hat{g}_j \hat{g}_k) = 0$$

(A5.02)

as well as the fundamental structure constants:

$$\hat{g}_j \hat{g}_k = (d_{mjk} + i f_{mjk}) \hat{g}_m$$

(A5.03)

where the structure constants are taken in symmetric ($d_{mjk} = d_{mkj}$) and antisymmetric ($f_{mjk} = - f_{mkj}$) parts. Through this formula we may define the commutator on the SU(3) algebra as given by

$$[\hat{g}_j, \hat{g}_k] = 2i f_{mjk} \hat{g}_m$$

(A5.04)

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