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Studies of Small Systems in Quantum Information

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Abstract

In this thesis, I study two topics in quantum information theory from the perspective of algebra and geometry. The first relates to exploring the geometry of unitary operators for small quantum systems, specifically three-level systems. Such an understanding of the space over which quantum systems evolve is central to understanding the detailed dynamics of quantum systems and to understand the correlation properties of subsystems that compose a given quantum system. The geometry of unitary operators also allows for the calculation of path-dependent phases called geometric phases. These geometric phases are central to understanding a variety of experiments. I present a general technique, called unitary integration to handle operator equations[1] and employ it to study various physical systems in quantum optics and quantum information. Unitary integration employs an inductive program to solve for the time-evolution of a system in terms of a unitary integration solution of smaller systems. The solution to the smallest system involving just a phase is easily solved, hence truncating the program and providing a solution to the initial problem. Unitary integration is developed in chapters 2 and 3 and this technique is applied to three-level systems in chapter 4.

The second topic involves quantum systems involving many subsystems[2]. Understanding the correlation properties of the subsystems that compose such systems has been of interest in the recent past. A useful tool in furthering this understanding has been parametrized families of states[3]. Such states depend on a smaller set of parameters than a general state in the system and hence are easier to study

[1] Such equations tell us how a quantum system evolves and hence "where" it travels in this space over which quantum systems evolve.

[2] Each subsystem is made up of "qubits", an object defined later.

[3] Examples of which include Werner states, GHZ states, Dicke states, etc.

and manipulate. I will present an iterative procedure to define such a parametric family of states called X states. I discuss the algebraic characterization for such states and develop a geometric picture for the algebra of such states. This geometric picture involves generalizations of triangles called "simplexes". X states are developed along with their algebraic characterization and connections to geometry in chapters 5 and 6.

The central theme that is common to both topics is the use of algebraic and geometric concepts to solve for various specific problems in quantum information iteratively. While the first topic deals with the iterative decomposition of operator equations, the second topic deals with the iterative definition of parametrized families of quantum states.

Chapter 1
Introduction

"All our knowledge has its origins in our perceptions"

Leonardo di ser Piero da Vinci (1452-1519)

In the last decade, there has been a significant body of work that has involved ideas from both physics and computer science. Much of this work culminated as a result of some important algorithms that pointed out that certain computational tasks can be performed in significantly lesser time on machines that exploit specific rules of quantum mechanics in comparison to machines that do not. Examples of such algorithms include the Deutsch-Josza algorithm[30], Shor's algorithm [85] and Grover's search algorithm [40]. These resulted in not just an effort to build "proof of principle" demonstrations of the algorithmic speedup suggested but an attempt at better understanding the subtle principles of quantum mechanics that give rise to the advantages exploited by these examples. Soon many other instances of tasks that offered this "quantum advantage" were pointed out. Examples of this include metrology [23], imaging [87], cryptography [64], steganography [62] etc. In some of the aforementioned cases, claims of a "quantum advantage" have sparked classical algorithms that have matched their quantum counterparts. As a part of this work, many new concepts have been invented and a plethora of new phenomenon have either been discovered or discussed in a new light.

This thesis details the study of certain geometric and algebraic aspects of quantum mechanics with an eye on applications in this branch of physics named "quantum information theory". This chapter will provide a broad overview of the branch

of physics relevant to understanding the rest of the material in this thesis while being accessible to the reader not versed in quantum information. As a brief introduction to quantum information, we discuss two interrelated themes: quantum mechanics and information. To this effect, section 1.1. will introduce the fields of quantum mechanics and section 1.2. will introduce information. We note that each of these topics considered is very vast and a through account of any one topic is beyond the scope of this thesis. An attempt has been made only to provide a flavor for questions, concepts and techniques employed by each field. In section 1.3 we will present concluding remarks.

1.1 Quantum Mechanics

Quantum theory describes a set of rules obeyed by any modern fundamental theory that describes the interaction of matter with energy and with itself[1]. Since any theory begins by writing down a representation for what is observed, we must write down a representation for what is observed when one considers a given physical system. The representation of a physical system in quantum mechanics is given by a so-called "quantum state". Hence the state of a physical system is described by this quantum state in quantum mechanics in contrast with the position and momentum variables in classical mechanics. These physical quantities are then derived from the quantum state(this will be explained below). For a single particle, such a state is given by a ray in a space called a Hilbert space[2]. The state is represented as $|\psi\rangle$ and the states associated with the dual space (the space that is endowed as a result of having an inner product) are represented by $\langle\psi|$. Such states can be expanded in terms of basis vectors $|i\rangle$. Basis vectors are defined as vectors that decompose the

[1]The only exception to this to date is a consistent quantum theory of gravity.

[2]A complex inner product space that is a Cauchy(Augustin-Louis Cauchy(1789-1857)) metric space induced by the inner product.

identity ($I = |i\rangle\langle i|$) and that are linearly independent($\sum_i c_i|i\rangle = 0 \Rightarrow c_i = 0\ \forall i$). The first condition simply states that there should be enough basis vectors to represent any state in the space and the second condition makes sure that there are not too many. Note that there are an infinite number of choices for the basis vectors in any dimension and that changing the basis changes the coefficients c_i so that the state is unchanged.

From this abstract formalism, predictions are made via Born[3]'s rule. This rule states that the probability of the state $|\psi\rangle$ being in the state $|i\rangle$ is given by $|c_i|^2$. Stated differently, the probability that any quantum state $|\psi\rangle$ is present in a state $|\varphi\rangle$ is given by $|\langle\varphi|\psi\rangle|^2$. Given this and from the conservation of probability, we can see that $\langle\psi|\psi\rangle = 1$. Besides states, two other quantities have to be introduced in quantum mechanics, namely observables and measurements. Observables (such as position and momentum) are represented by self-adjoint operators(operators which equal their Hermitian[4] conjugate). This is because the eigenvalues of Hermitian operators are real. Indeed, there exist a set of self-adjoint operators that represent the unique observations that characterize the representation of the system. Measuring any one of the physical properties associated with one of these observables does not change the other compatible observables that also characterize the system. These set of operators are called a "complete set of commuting observables" and are eigen-operators of the state $|\psi\rangle$. In fact $|\psi\rangle$ is just an eigenvector that is constructed from the eigenvalue labels corresponding to each of these operators that belong in the complete set of commuting observables.

[3]Max Born(1882-1970).
[4]Charles Hermite(1822-1901).

Measurements are represented by a set of operators E_i such that $E_i^\dagger E_i$ is a positive operator[5] and $\sum_i E_i^\dagger E_i = I$. The post-measurement state is given by

$$|\psi'\rangle = \frac{E_i}{\sqrt{||E_i|\psi\rangle||}}|\psi\rangle. \tag{1.1}$$

The time-evolution of this state is given by the so-called Schrödinger[6]'s equation

$$i\hbar|\dot{\psi}\rangle = \mathbf{H}(t)|\psi\rangle. \tag{1.2}$$

Here $\hbar$ is Plank's constant[7] and $\mathbf{H}(t)$ is the called the Hamiltonian[8] and is the self-adjoint operator that corresponds to the energy of the system. Finally, consider a quantum state $|\psi\rangle = \sum_i \psi_i|i\rangle$ being transformed to a state $|\varphi\rangle = \sum_i \varphi_i|i\rangle$. Here we have denoted the expansion coefficients of $|\psi\rangle$ by the functions ψ_i, an overloading of notation that is quite common in linear algebra and quantum mechanics. Such a transformation preserves probability since $\langle\psi|\psi\rangle = \langle\varphi|\varphi\rangle$. This evolution of the system can be represented by a unitary matrix U such that $U^\dagger U = I$ and is known as the "evolution operator". The transformation above is given by the unitary operator $U = \sum_{ij} \psi_i^* \varphi_j$ and corresponds simply to $|\varphi\rangle\langle\psi|$. Thus the problem of discussing the transition between quantum states that represents the change in the properties of a physical system can be restated as a problem of determining the evolution operator. Chapters 2-4 deal with a technique for evaluating the time-evolution operator(the evolution operator that captures the evolution of the physical system in time) for small quantum systems and extract the geometry of the evolution operator involved.

Let us consider an important example that highlights the axioms presented above. Consider a system described by the rules of quantum mechanics which

[5]Strictly speaking only the operators $M_i = E_i^\dagger E_i$ exist for the most general measurement(see [100]).
[6]Erwin Schrödinger(1887-1961).
[7]Max Planck(1858-1947).
[8]William Hamilton(1805-1865).

is represented by a two-dimensional vector. Such a system is called a two-level system or a "qubit"(quantum bit) and is represented by a vector written explicitly as

$$|\psi\rangle = \begin{pmatrix} c_0 \\ c_1 \end{pmatrix}. \tag{1.3}$$

Here $\{c_0, c_1\} \in \mathbb{C}$ and $|c_0|^2 + |c_1|^2 = 1$. $\langle\psi|$ is given by

$$\langle\psi| = \begin{pmatrix} c_0^* & c_1^* \end{pmatrix}. \tag{1.4}$$

A choice of basis that will exemplify the remarks made earlier are given either by

$$|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{1.5}$$

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{1.6}$$

while another choice of basis is given by

$$|+\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}. \tag{1.7}$$

$$|-\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}. \tag{1.8}$$

An example[9] of a measurement performed on this system is given by $M_1 = |\psi\rangle\langle\psi|$ and $M_2 = I - M_1$. Finally, an example of a Hamiltonian that determines the

[9]Note that in this example $M_1.M_2 = 0$ because $M_1^2 = M_1$. Such measurements are called von-Neumann measurements and form a subset of general measurements.

dynamics of this system is given by

$$\mathbf{H}(t) = \begin{pmatrix} E_0(t) & H_{01}(t) \\ H_{10}(t) & E_1(t) \end{pmatrix}. \tag{1.9}$$

Since $\langle\psi|\mathbf{H}(t)|\psi\rangle = |c_0|^2 E_0(t) + |c_1|^2 E_1(t)$, $E_{0,1}$ are the energies associated with the states $\{c_0 = 1, c_1 = 0\}$ and $\{c_0 = 0, c_1 = 1\}$ respectively. The former state is called the "ground state" and the latter the "excited state" because of convention. $H_{01} = H_{10}^*$ is the coupling that induces transitions between the two states.

Until now, we have focused on the representation of the quantum state associated with a single particle. Such states, as was explained above, are represented by a vector $|\psi\rangle$. Let us now consider a generalization of this idea involving a collection of systems whose description is sought. A collection of physical systems, all characterized by the state $|\psi\rangle$ are said to be a "pure ensemble" characterized by $|\psi\rangle$ and hence this state is also called a "pure state". But this is not the only way to prepare a collection of N quantum systems. Indeed, we can prepare $n := pN$ of them in a state $|\psi\rangle$ and $N - n = (1 - p)N$ in a state $|\varphi\rangle$. This can be done for instance by choosing each quantum system and tossing a biased coin (with probability p of yielding "heads") and preparing $|\psi\rangle$ when the outcome is "heads" and likewise $|\varphi\rangle$ when the outcome is "tails". Such a state is now represented not by a state vector but by a Hermitian operator given by

$$\rho = p|\psi\rangle\langle\psi| + (1 - p)|\varphi\rangle\langle\varphi|. \tag{1.10}$$

ρ is called a density matrix and is the most general description of a quantum system. Such an ensemble is called a "mixed ensemble" and the corresponding state of the system is described to be in "a mixed state". Note that $\mathsf{Tr}(\rho) = 1$ and $\mathsf{Tr}(\rho^2) \leq 1$. The value of an observable $\mathbf{A}$ in this state is now given by $\mathsf{Tr}(\mathbf{A}\rho)$. The post-measurement state in the density matrix description of physical systems

is given by

$$\rho' = \frac{1}{\mathsf{Tr}(E_i \rho E_i^\dagger)} E_i \rho E_i^\dagger. \tag{1.11}$$

The analogue of Schrödinger's equation for density matrices is known as the Liouville[10] von-Neumann equation and is given by

$$\dot{\rho} = \frac{-i}{\hbar}[\mathbf{H}(\mathbf{t}), \rho]. \tag{1.12}$$

Here $[A, B] = A.B - B.A$ is the commutator[11] of two matrices and is given by the antisymmetrized product of the two matrices.

This highlights the second theme of this thesis, namely the role of algebra in quantum mechanics. In this case, the algebra involves that of the various operators along with the commutation operation. Clearly the way the commutator works out is central in deciding how the quantum system evolves. If $\rho(0)\mathbf{H}(\delta t) = \mathbf{H}(\delta t)\rho(0)$, then clearly the initial quantum system is unchanged for all times. Having paused to highlight the central role the algebra of operators plays in the evolution of quantum systems, we will postpone a detailed discussion of the role of algebra to later chapters.

Having introduced some of the basic axioms of quantum mechanics, we will take up a brief discussion of the geometry of unitary operators. By "geometry of a quantum state " is meant a representation of all possible quantum states as points (or some other general curves) in some space such that there is a unique point associated with each quantum state. This way quantum operators that transform a quantum system from $|\psi\rangle$ to $|\varphi\rangle$ can be thought of as going from "here" to "there"

[10] Joseph Liouville(1809-1882).

[11] One way to think about why these antisymmetric operators appear in physics is to note that the product of exponents of antisymmetric matrices multiplied by real parameters is the most general way of writing unitary operators. These operators, as we noted above, represent the general evolution of a quantum system subject only to the conservation of probability. We can also infer that since we wish to discuss infinitesimal time evolution, the real parameters that multiply each antisymmetric operator is a continuous function of time.

in this space and hence the dynamics of a quantum system can be "visualized". Since every transformation between quantum states is also captured by a unitary operator, the geometry of quantum states is identical to the geometry of evolution operators in that space. Understanding this geometry of state space had proven very fruitful in the early days of quantum mechanics for the design of simple schemes in spin resonance (for example, the spin-echo scheme[35]). But the ability to visualize dynamics is not the only reason why the geometry of state space is studied. The geometry of a quantum state can have a measurable impact on the quantum state. This point will be explained by considering once more the quantum state associated with a two-level system.

The quantum state of a two-level system can be written as $|\psi\rangle = \psi_0|0\rangle + \psi_1|1\rangle$, where the two levels are labeled 0 and 1 respectively. Since $|\psi_0|^2 + |\psi_1|^2 = 1$, we can rewrite this state as $|\psi\rangle = e^{i\gamma}(\cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle)$ with $0 \leq \theta < \pi$, $0 \leq \phi < 2\pi$ and $0 \leq \gamma < \infty$. Hence we can represent a general quantum state in terms of these three parameters $\{\gamma, \theta, \phi\}$. The two parameters θ and ϕ define a point on a unit sphere in three dimensions while the parameter γ is a line associated with each point on this sphere. This phase γ can be measured experimentally if a general two level system is evolved around a random closed curve and then compared with an identical state that did not traverse this closed path. It can be shown in this example that part of the phase γ is given simply by half the area of the loop traversed by the quantum state. Since this part of the phase depends on the geometry of the path traversed in state space, it is referred to as a "geometric phase" in quantum physics.

We will end this section with an introduction to the correlation among subsystems that compose a quantum system. To study these correlations, consider a quantum system composed of two physically distinct subsystems. Initially(i.e.,

at $t = 0$), if we assume that they are independent systems, then each system is in a physical state and hence is represented by a state vector $|\psi\rangle_A$ and $|\psi\rangle_B$. in fact the consistent thing to do is to write the state of the entire system as $|\Psi\rangle_{AB} = |\psi\rangle_A|\psi\rangle_B$. Such a state is called a "product state". Writing the two representations of the states side by side highlights the fact that each system comes bearing its own quantum labels initially. Mathematically speaking, the state $|\Psi\rangle_{AB}$ is given by the Cartesian[12] product of the two vectors. Similarly, if the observables relating to the two subsystems are given by $\mathbf{A}_A$ and $\mathbf{A}_B$, then the observables for the system are given by the tensor product of the two observables $\mathbf{A}_A \otimes \mathbf{A}_B$. Now consider a case where such a system which is initially in a product state evolves to an (unnormalized) state given by $|\Psi\rangle_{AB} = |\psi\rangle_A|\psi\rangle_B + |\varphi\rangle_A|\varphi\rangle_B$. Then it is unreasonable to assume that each subsystem still retains a representation of "what is observed" independent of the other subsystem. This is because if we measure the first subsystem and find it to be in a state $|\psi\rangle_A$, then the quantum state of the second subsystem is given by $|\psi\rangle_B$. Hence the representation that assigns unique measurable properties to each subsystem does not exist since measuring one subsystem can affect what is observed in the other subsystem. Indeed, this issue is not resolved if one measures the subsystems simultaneously.

There are in fact two "issues" here. Firstly, there is the issue that representations of subsystems in quantum mechanics are no longer assigned independent of the whole system[13] and second is the issue that the state of a subsystem can be affected instantaneously by measuring the other subsystem[14]. We will simply note

[12] René Descartes(1596-1650).

[13] Some thought will clarify that this is never the case in classical physics. For instance, irrespective of the nature of the interaction of a red ball with a green ball, all of the attributes that define each of the two balls are well defined at all times for each ball.

[14] This is an issue if the subsystems are physically separated because it "seems" like one is violating causality.

that the first of these issues is resolved by noting that for most systems[15] in quantum mechanics, subsystems can no longer be assigned representations independent of other subsystems. This is a major departure from classical mechanics and the central reason for this departure lies with the nonlocal superposition implied by the example presented above. Schrödinger famously [81] called this non-local superposition "the hallmark of quantum mechanics" and coined the word "entanglement" to highlight this unique feature of quantum mechanics. A state is considered entangled if it can not be written as a product state in some basis. Separable density matrices are written as

$$\rho = \sum_i p_i |\psi_i\rangle_{AB}\langle\psi_i|, \tag{1.13}$$

with $0 \leq p_i \leq 1$ with $\sum_i p_i = 1$. While for simple examples one might infer if a state is entangled by inspection, the question of whether a state is entangled or not becomes very hard to establish for mixed states in general. We will define a set of measures that distinguish between probability distributions in the next section and present generalizations them to yield functions of the density matrix of a bipartite system that evaluate the amount of entanglement in a given state.

Note that entanglement is not the only kind of "quantum" correlation that is present in a quantum system. Consider a state given by $\rho = |\psi\varphi_0\rangle\langle\psi\varphi_0| + |\psi_\perp\varphi_1\rangle\langle\psi_\perp\varphi_1|$ where $\langle\psi|\psi_\perp\rangle = 0$ but $\langle\varphi_0|\varphi_1\rangle \neq 0$. While it is separable by the criterion stated above, the measurement outcomes on the subsystems of this state are clearly still correlated. Such states are said to have non-zero "quantum discord" [43, 65].

[15] the states for which this is not true are of measure zero.

1.2 Information Theory

1.2.1 Classical Information Theory

Information theory evolved around questions relating to the transmission and reception of messages. Consider a message comprised of a string of letters. It is of interest to know if this message can be compressed(i.e., made into a smaller message with the same amount of information by removing redundancies) so that it maybe transmitted at faster rate and at a lower cost. It is also of interest to know at what rate this message can be communicated over a noisy transmission line(channel) reliably. Questions such as these are the topic of classical information theory. By "information", we mean the knowledge that can be derived from the message. While for simple examples, these questions maybe answered by inspection, notions such as "information" have to be quantified if the intention is to develop a general theory. To this effect, many new concepts were introduced in classical information theory. Classical information theory deals with answers to questions posed about messages that are transmitted via physical systems wherein the laws of quantum mechanics are not required to explain any part of the communication protocol. One of the most important ideas developed in classical information is the idea of Shannon[16] entropy [84]. We will introduce this idea along with some other ideas that will prove fruitful in understanding ideas in quantum information theory.

Let us consider two probability distributions p_i and q_i. These probability distributions may represent two a priori distributions from which letters i are derived to write down two messages respectively. To elaborate, in the limit that we have a very long message, with N letters in it, if the number of times that a letter i is repeated is asymptotically given by n_i, then this message is said to be characterized by $p_i := Lim_{N\to\infty}(n_i/N)$. We wish to know if the messages represented

[16] Claude Shannon(1916-2001)

by p_i and q_i are similar. The answer to this question relates to the "closeness" of the probability distribution, i.e., the closer the two probability distributions are to each other, the more similar the two messages will be.

To further clarify the notion of closeness, assume that we know p_i and are trying to guess q_i. Since we know nothing about q_i, we assume that the probability of each letter being present in the second message is also given by p_i and try to ascertain by how much our guess deviates from the actual probability distribution q_i. This deviation represents our "surprise" about q_i given that we assumed $p_i = q_i$. To quantify our surprise about q_i relative to p_i, we note that a quantity such as p_i/q_i is useful. This is because the closer q_i is to p_i, the closer this ratio is to 1. Hence, if there is a letter k for which say $p_k >> q_k$, then our surprise in not finding as many of the letters k in the message as predicted by p_k is captured by the smallness of the ratio. Hence, we can quantify our surprise by saying that the closer the ratio p_i/q_i is to 1, the less surprised we will be by the actual probability distribution q_i. One problem with using a ratio such as p_i/q_i is that it is not additive. To fix this, we can consider the quantity $log_2(p_i/q_i) = log(p_i/q_i)$ to quantify the surprise with respect to each letter i. Now, the average "surprise" is given by

$$H(p||q) = \sum_i p_i \left(log(\frac{p_i}{q_i}) \right). \tag{1.14}$$

$$H(p||q) = \sum_i p_i log(p_i) - \sum_i p_i log(q_i). \tag{1.15}$$

$$H(p||q) = -H(p) + H_{cr}(p, q). \tag{1.16}$$

This average surprise [31] is known as the "Kullback-Liebler divergence[17]" [53] or the "relative entropy" while the quantity $H(p) = -\sum_i p_i log(p_i)$, known as the Shannon entropy quantifies the average surprise of the probability distribution p_i and hence quantifies the "information" in the message derived from this distribu-

[17] Solomon Kullback(1907-1997) and Richard Liebler(1914-2003)

tion. Note that unlike measures of distance, the Kullback-Liebler divergence is not symmetric in its entries(hence the name "divergence"). The last term $H_{cr}(p,q)$ is called the "cross-entropy" of the distributions p_i and q_i. Thus Shannon entropy and relative entropy can be used to quantify the average surprise associated with a distribution and the average surprise discrepancy between two distributions.

These definitions can be generalized in many ways. Firstly, these quantities can be defined for continuous probability distributions in which case all the summation symbols are replaced by integrals. The second generalization involves multivariate distributions. Examples of such distributions involving more than one variable arise in describing a system involving subsystems or a system characterized by more than one attribute. Correlations between such subsystems of a given system are of interest. To this effect, consider a joint probability distribution $P(x_i, y_j) := P_{ij}$. Such a probability distribution can be used to describe a message with two attributes(letters of a certain color, for instance). The probability distribution of the individual subsystems is given by $p(x_i) := p_i = \sum_j P_{ij}$ and $q(y_j) = q_j = \sum_i P_{ij}$. As before, the entropy of the entire system is defined as $H(x,y) = -\sum_{ij} P_{ij} log(P_{ij})$ and the entropies of the subsystems are defined as before as $H(x) = -\sum_i p_i log(p_i)$ and $H(y) = -\sum_j q_j log(q_j)$. Now several questions can be answered immediately. Firstly, the amount of information that is common to both subsystems is given by the "mutual information" and is defined as

$$I(x:y) = H(x) + H(y) - H(x,y). \tag{1.17}$$

On the other hand, the reduction in the uncertainty in x given y is quantified by the "conditional entropy" given by

$$I(x|y) = H(x,y) - H(y). \tag{1.18}$$

These ideas have been generalized to discuss the "surprise" associated with probabilities and measurement outcomes relating to quantum systems. This generalization will be the topic of the next subsection.

1.2.2 Quantum Information Theory

Consider a quantum system characterized by the density matrix ρ. The quantum analogue of the Shannon entropy is given by

$$H(\rho) = -\mathsf{Tr}(\rho log(\rho)). \tag{1.19}$$

and is known as the von-Neumann[18] entropy. Since unitary transformations do not affect the trace of the density matrix, we can unitary transform the above formula to the diagonal representation of the density matrix wherein the formula is given by $H(\rho) = -\sum_i \lambda_i log(\lambda_i)$. Here λ_i are the eigenvalues of the density matrix and the formula is reminiscent of Shannon entropy(and indeed identical to it for a classical system characterized by a diagonal density matrix). This quantity is central to quantum information and to quantum statistical mechanics. Note that this formula for calculating entropy in terms of eigenvalues is relevant only in the diagonal basis.

To discuss correlations between subsystems, consider a bipartite system whose density matrix is given by ρ_{AB}. Each subsystem is characterized by the reduced density matrix given respectively by $\rho_A = \mathsf{Tr}_B(\rho_{AB})$ and $\rho_B = \mathsf{Tr}_A(\rho_{AB})$. Like before, we wish to quantify the correlations between the subsystems. "Quantum mutual information" [64] can be defined analogous to classical mutual information as

$$I(\rho_{AB}) = H(\rho_A) + H(\rho_B) - H(\rho_{AB}), \tag{1.20}$$

[18] John von Neumann(1903-1957)

and represents the information common to both subsystems. For pure states(i.e., $\rho_{AB}^2 = \rho_{AB}$), the entropy of each subsystem is known as the "entropy of entanglement" [64] and is given by

$$E_0(\rho_{AB}) = H(\mathsf{Tr}_B(\rho_{AB})) = H(\mathsf{Tr}_A(\rho_{AB})). \tag{1.21}$$

This quantity is an entanglement measure for pure states. For mixed states, the following trick is used. Consider a mixed bipartite state ρ_{AB}. This density matrix can be written in a pure-state decomposition as

$$\rho_{AB} = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|. \tag{1.22}$$

The generalization of the definition of the entropy of entanglement for mixed states is given by

$$EoF(\rho_{AB}) = \mathsf{Inf}_{p_i} \sum_i p_i E_0(|\Psi_i\rangle\langle\Psi_i|). \tag{1.23}$$

Here, EoF stands for the "entanglement of formation" [12] and Inf_{p_i} stands for minimizing the resulting quantity over all possible pure-state decompositions.

An entanglement measure that is related to EoF is the concurrence of two-qubit systems [101] defined as,

$$C(\rho_{AB}) := \mathsf{Max}\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{1.24}$$

where, λ_i are the eigenvalues of the matrix $\sqrt{\sqrt{\rho_{AB}}(\sigma_2 \otimes \sigma_2)\rho_{AB}^*(\sigma_2 \otimes \sigma_2)\sqrt{\rho_{AB}}}$ arranged in decreasing order of magnitude. Note that EoF is the asymptotic cost per copy of the state ρ_{AB} needed to transform a given Bell[19]-state[20] into the state ρ_{AB} using local operations and classical communication (LOCC). LOCC represents the set of operations wherein local operations are performed on subsystems and the

[19] John Bell(1928-1990).

[20] A maximally entangled two-qubit state. Explicit forms of the four Bell states are given in Section 5.2.

results of that operation is communicated classically to other subsystems [63]. We conclude our discussion on measures of entanglement based on entropy by defining two measures of entanglement based on a generalization of the Kullback-Liebler divergence. The classical relative entropy may be generalized simply to yield,

$$H(\rho||\sigma) = -Tr(\rho log(\rho) - \rho log(\sigma)). \tag{1.25}$$

This quantity is known as the quantum relative entropy and is a measure of the "closeness" of two density matrices. We state without proof that $0 \leq H(\rho||\sigma) \leq \infty$. If we minimize $H(\rho||\sigma)$ for the choice $\rho = \rho_{AB}$ and $\sigma \in \mathcal{S}$, where $\mathcal{S}$ is the space of separable states, then we obtain a measure of the "closeness" of a given state ρ_{AB} to the set of separable states. Clearly this is an entanglement measure and is defined as the relative entropy of entanglement. Likewise if $\sigma \in \mathcal{C}$, where $\mathcal{C}$ is the set of classical states, then we obtain a measure of quantum correlations. This measure is an alternative definition of quantum discord[59].

Finally, we will present one more measure of entanglement that is commonly used[21] in quantum information. This measure of entanglement is called negativity [93] and is defined as

$$N(\rho) = \frac{||\rho^{T_B}|| - 1}{2}. \tag{1.26}$$

Here $||A|| := \mathsf{Tr}(\sqrt{A^\dagger A})$ and ρ^{T_B} is the partial transpose [67] of ρ with respect to the subsystem B[22].

1.3 Conclusions

In the previous sections, we discussed how the geometry of quantum states is defined by considering an example and separately we discussed entanglement. These

[21] In chapter 5, for instance.
[22] defined as $(\rho^{T_B})_{ijkl} := \rho_{kjil}$

topics are closely related. As we noted in the previous section, many measures of entanglement are geometric measures that measure the "closest distance" of a given quantum state to the set of all separable states. Likewise, we stated briefly that quantum discord, a measure of non-classical correlations can also be defined in terms of a distance measure. Hence entanglement and quantum discord are related to "how close" a given quantum state is to other states, an intrinsically geometric idea. Likewise the geometry of the space of observables and of the measurement operators have a profound influence on various properties of quantum algorithms. The fact that the algebra of the operators involved plays a crucial role can readily be ascertained by looking at the definition of the different measures of entanglement and discord provided.

This thesis is roughly separated into two parts. In chapters 2-4, we will discuss in detail the geometry of time evolution operators for N-level systems with an emphasis on small quantum systems ($N = 2, 3, 4$). This will be done by introducing a new technique to handle Schrödinger's equation . In chapters 5,6 we will take up the study of a class of N-qubit states and highlight how the algebra of these quantum states makes some hard calculations easy to perform. We will present a scheme of "visualizing" the operator algebra and present connections to various fields of physics and mathematics.

Chapter 2
Unitary Integration I

"Problems worthy of
attack prove their worth
by fighting back"

Paul Erdös(1913-1996)

2.1 Introduction

In classical probability theory, the properties of a system are captured by the probability distribution. Important questions of interest like the dynamical behavior of the system and correlation properties of subsystems can be inferred from this probability distribution. For quantum systems, the probability distribution is replaced by the density operator $\rho(t)$. For a closed system, the evolution of this density operator is governed by the Heisenberg equation of motion, given by

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H(t), \rho(t)] = -\frac{i}{\hbar}(H(t)\rho(t) - \rho(t)H(t)). \tag{2.1}$$

Here H stands for the Hamiltonian of the system. Since probability is conserved, the dynamics of a closed system can be described in terms of a unitary operator $U(t)$. Such an operator satisfies $U(t)U^\dagger(t) = U^\dagger(t)U(t) = I$. Here I is the unit operator and $U^\dagger$ stands for the conjugate transpose of U. Operators such as the density operator are transformed by the rule $\rho(t) = U(t)\rho(0)U^\dagger(t)$ and the equation of motion is written as

$$\dot{U}(t) = -\frac{i}{\hbar}H(t)U(t). \tag{2.2}$$

The equation above captures two aspects of quantum systems that are essential. The first aspect is the dynamical nature of quantum systems. The second is the notion of incompatibility of observables. This refers to the fact that the order in

which certain observations are performed greatly influence the outcomes on the state being observed.

Some special cases of this equation of motion are easy to solve. If the Hamiltonian does not change in time, then the integration can be done formally and we obtain

$$U(t) = e^{-\frac{i}{\hbar}Ht}U(0). \tag{2.3}$$

It is customary to assume that the $U(0) = I$, though not necessary. For this choice of initial conditions, the general evolution of the eigenstate of the Hamiltonian can be written as $|n(t)\rangle = e^{-\frac{i}{\hbar}E_n t}|n\rangle$. hence the general element of the density matrix evolves according to $\rho_{nm}(t) = e^{-\frac{i}{\hbar}(E_n - E_m)t}\rho_{nm}(0)$, which completes the solution.

Another class of problems of physical interest involve Hamiltonians that neither commute with the unitary operator, nor have trivial time dependance. We will briefly mention a technique often employed to deal with problems like this in the next section. We will then present the unitary integration solution and discuss the solution for various small quantum systems.

2.2 Time-dependent Perturbation Theory

In this section we will briefly mention time-dependent perturbation theory, the technique used to handle time-dependent Hamiltonians when the perturbations involved are small. Perturbation theory deals with obtaining the solution of Schrödinger's equation when a Hamiltonian which can be exactly diagonalized is perturbed by a small time dependent Hamiltonian. Let us discuss this approximation technique from the standpoint of Schrödinger's equation written for a wavefunction and given by (in units where $\hbar = 1$)

$$i|\dot{\Psi}(t)\rangle = H(t)|\Psi(t)\rangle. \tag{2.4}$$

Let us assume that the Hamiltonian is written as $H = H_0 + H_1(t)$ and that the eigenvectors for the unperturbed Hamiltonian are given by the equation $H_0|n\rangle = E_n|n\rangle$. The eigenvectors $|\Psi(t)\rangle$ for the full Hamiltonian $H(t)$ is expanded in the unperturbed eigenbasis and is written as $|\Psi(t)\rangle = \sum_n C_n(t)e^{-iE_nt}|n\rangle$. Substituting this into Schrödinger's equation above gives

$$\begin{aligned} i\sum_n \dot{C}_n(t)e^{-iE_nt}|n\rangle &= \sum_n C_n(t)e^{-iE_nt}H_1(t)|n\rangle, \Rightarrow \\ i\dot{C}_m(t) &= \sum \langle m|H_1(t)|n\rangle e^{-i(E_n-E_m)t}C_n(t). \end{aligned} \tag{2.5}$$

Assuming that the initial state of the system is in one of the eigenstates of the unperturbed Hamiltonian, say $|i\rangle$, we get $C_n(0) = \delta_{ni}$. Here δ_{ni} stands for the Kronecker symbol. Substituting this into the right hand side of the above equation gives the first order equation namely.

$$i\dot{C}_m(t) = \langle m|H_1(t)|i\rangle e^{-i(E_i-E_m)t}. \tag{2.6}$$

This can be formally integrated to yield

$$C_m(t) = -i\int_0^t dt'\langle m|H_1(t')|i\rangle e^{-i(E_i-E_m)t'}. \tag{2.7}$$

Assuming different forms of the perturbation Hamiltonian $H_1(t)$ allows us to solve for the coefficients which determine the eigenvector at all times. In the next section, we will introduce a technique that does not rely on the relative magnitude of the perturbation and is a general technique to handle arbitrary time-dependence.

2.3 Basic Theory of Unitary Integration

Consider again the Liouville equation,

$$\dot{U}(t) = -iH(t)U(t). \tag{2.8}$$

for a two-level system. We can write an arbitrary time dependent Hamiltonian in terms of the unit matrix in two dimensions and the three Pauli matrices as

$H(t) = \sum_{j=0}^{3} h_j(t)\sigma_j$ with $\sigma_0 = I$ and $h_j(t) = Tr(H(t)\sigma_j)$. Such Hamiltonians are often written while discussing physical systems such as spin resonance. Hence, we can write Schrödinger's equation as

$$\dot{U}(t) = -i(\sum_{j=0}^{3} h_j(t)\sigma_j)U(t). \tag{2.9}$$

Now let us choose an ansatz whereby we write

$$U = e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3}. \tag{2.10}$$

Such an ansatz is justified not only by the completeness of the su(2) algebra, but further justification will be provided by explicit construction of time-evolution operator for arbitrary Hamiltonians. Unitarity implies that μ_i are real and if the Hamiltonian is traceless then there are only three real parameters needed to define $U(t)$. This is commensurate with the fact that the density matrix for a two level system is characterized by three parameters: the population difference(which is one real number) and the coherence(which is one complex or two real numbers). The derivative of $U(t)$ with respect to time has four terms and is given by

$$\begin{aligned}\dot{U}(t) = -i\dot{\mu}_0(t)U(t) - i\dot{\mu}_1(t)\sigma_1 U(t) - ie^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}\dot{\mu}_2(t)\sigma_2 e^{-i\mu_3(t)\sigma_3} \\ -i\dot{\mu}_3(t)e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}e^{-i\mu_2(t)\sigma_2}\sigma_3 e^{-i\mu_3(t)\sigma_3}.\end{aligned} \tag{2.11}$$

This means that Eq. (2.8) can be written as

$$\begin{aligned}\dot{\mu}_0(t)U(t) + \dot{\mu}_1(t)\sigma_1 U(t) + e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}\dot{\mu}_2(t)\sigma_2 e^{-i\mu_3(t)\sigma_3} \\ +\dot{\mu}_3(t)e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}e^{-i\mu_2(t)\sigma_2}\sigma_3 e^{-i\mu_3(t)\sigma_3} = (\sum_{j=0}^{3} h_j(t)\sigma_j)U(t).\end{aligned} \tag{2.12}$$

As it stands, the equation above does not seem to be any more revealing than the original Schrödinger's equation. To complete the solution, we wish to collect all of the exponential factors together in the equation above so that $U(t)$ is made

the last factor on the right hand side of all terms. This way, we can compare the terms attached to different Pauli matrices to reduce the matrix equation above to a set of differential equations. Hence we recall the Baker-Campbell-Hausdorff (BCH) lemma [76] given by

$$e^X Y e^{-X} = Y + [X,Y] + \frac{1}{2!}[X,[X,Y]] + \frac{1}{3!}[X,[X,[X,Y]]] + \cdots . \tag{2.13}$$

This formula relates the transformation $e^X Y e^{-X}$ of an operator Y by another operator X that it does not commute with to a series of nested commutators.

To use this, consider the third term in Eq. (2.12). This term is given by

$$e^{-i\mu_0(t)\sigma_0} e^{-i\mu_1(t)\sigma_1} \dot{\mu}_2(t) \sigma_2 e^{-i\mu_3(t)\sigma_3}.$$

Noting that σ_0 commutes with all operators and that $e^{i\mu_1(t)\sigma_1} e^{-i\mu_1(t)\sigma_1} = I$, we can insert the identity element after σ_2 to get,

$$\dot{\mu}_2(t) \{ e^{-i\mu_1(t)\sigma_1} \sigma_2 e^{i\mu_1(t)\sigma_1} \} e^{-i\mu_0(t)\sigma_0} e^{-i\mu_1(t)\sigma_1} e^{-i\mu_3(t)\sigma_3}. \tag{2.14}$$

Now we can apply the BCH lemma to the term in the curly braces. This will yield

$$e^{-i\mu_1(t)\sigma_1} \sigma_2 e^{i\mu_1(t)\sigma_1} = \sigma_2 - i\mu_1(t)\,[\sigma_1,\sigma_2] - \frac{\mu_1^2(t)}{2!}[\sigma_1,[\sigma_1,\sigma_2]] + \cdots \tag{2.15}$$

Using $[\sigma_l, \sigma_m] = 2i\varepsilon_{lmn}\sigma_n$, we get,

$$e^{-i\mu_1(t)\sigma_1} \sigma_2 e^{i\mu_1(t)\sigma_1} = \sigma_2 + 2\mu_1(t)\sigma_3 - 2^2 \frac{\mu_1^2(t)}{2!}\sigma_2 + \cdots \tag{2.16}$$

Collecting terms, we can write,

$$e^{-i\mu_1(t)\sigma_1} \sigma_2 e^{i\mu_1(t)\sigma_1} = \sigma_2 \left(1 - \frac{(2\mu_1(t))^2}{2!} + \frac{(2\mu_1(t))^4}{4!} \cdots \right) + \sigma_3 \left((2\mu_1(t)) - \frac{(2\mu_1(t))^3}{3!} \cdots \right)$$

We can sum the infinite series in the above equation to write

$$e^{-i\mu_1(t)\sigma_1} \sigma_2 e^{i\mu_1(t)\sigma_1} = \sigma_2 \cos(2\mu_1(t)) + \sigma_3 \sin(2\mu_1(t)). \tag{2.17}$$

Hence, noting that $e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}e^{-i\mu_3(t)\sigma_3} = U(t)$, we can write Eq. (2.14) as

$$\dot{\mu}_2(t)\{\sigma_2\cos(2\mu_1(t)) + \sigma_3\sin(2\mu_1(t))\}U(t) \tag{2.18}$$

The last term on the LHS of Eq. (2.12) can be handled in a similar way, which we shall present here for completeness. This term is given by

$$\begin{aligned}
\dot{\mu}_3(t)e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}e^{-i\mu_2(t)\sigma_2}\sigma_3 e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}\{e^{-i\mu_2(t)\sigma_2}\sigma_3\}e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}\{e^{-i\mu_2(t)\sigma_2}\sigma_3 e^{i\mu_2(t)\sigma_2}\}e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}\{\sigma_3\cos(2\mu_2(t)) - \sigma_1\sin(2\mu_2(t))\}e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}\sigma_3\cos(2\mu_2(t))e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} & \\
-\dot{\mu}_3(t)e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}\sigma_1\sin(2\mu_2(t))e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} &
\end{aligned} \tag{2.19}$$

Thus the term under consideration is the sum of two terms. The second of these terms is easily rearranged to yield

$$\begin{aligned}
\dot{\mu}_3(t)e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}\sigma_1\sin(2\mu_2(t))e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)\sin(2\mu_2(t))\sigma_1 e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)\sin(2\mu_2(t))\sigma_1 U(t) &
\end{aligned} \tag{2.20}$$

The first term is also computed by this "inductive" procedure whereby

$$
\begin{aligned}
\dot{\mu}_3(t)e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}\sigma_3\cos\left(2\mu_2(t)\right)e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)\cos\left(2\mu_2(t)\right)\{e^{-i\mu_1(t)\sigma_1}\sigma_3\}e^{-i\mu_0(t)\sigma_0}e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)\cos\left(2\mu_2(t)\right)\{e^{-i\mu_1(t)\sigma_1}\sigma_3 e^{i\mu_1(t)\sigma_1}\}e^{-i\mu_1(t)\sigma_1}e^{-i\mu_0(t)\sigma_0}e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)\cos\left(2\mu_2(t)\right)\{\sigma_3\cos\left(2\mu_1(t)\right)-\sigma_2\sin\left(2\mu_1(t)\right)\}e^{-i\mu_1(t)\sigma_1}e^{-i\mu_0(t)\sigma_0}e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)\cos\left(2\mu_2(t)\right)\{\sigma_3\cos\left(2\mu_1(t)\right)-\sigma_2\sin\left(2\mu_1(t)\right)\}e^{-i\mu_0(t)\sigma_0}e^{-i\mu_1(t)\sigma_1}e^{-i\mu_2(t)\sigma_2}e^{-i\mu_3(t)\sigma_3} &= \\
\dot{\mu}_3(t)\cos\left(2\mu_2(t)\right)\{\sigma_3\cos\left(2\mu_1(t)\right)-\sigma_2\sin\left(2\mu_1(t)\right)\}U(t). &
\end{aligned}
\tag{2.21}
$$

To further simplify, we collect the terms simplified in Eqs. (2.18,2.20,2.21) and write Eq. (2.12) as

$$\dot{\mu}_0(t) = h_0(t) \tag{2.22}$$

$$\dot{\mu}_1(t) + \dot{\mu}_3(t)\sin\left(2\mu_2(t)\right) = h_1(t) \tag{2.23}$$

$$\dot{\mu}_2(t)\cos\left(2\mu_1(t)\right) - \dot{\mu}_3(t)\cos\left(2\mu_2(t)\right)\sin\left(2\mu_1(t)\right) = h_2(t) \tag{2.24}$$

$$\dot{\mu}_2(t)\sin\left(2\mu_1(t)\right) + \dot{\mu}_3(t)\cos\left(2\mu_1(t)\right)\cos\left(2\mu_2(t)\right) = h_3(t) \tag{2.25}$$

Note that the initial condition $U(0) = I$ implies $\mu_i(0) = 0$. Thus the problem of solving Schródinger's equation with a Hamiltonian with arbitrary time dependence has been reduced to solving a set of coupled equations. Substituting the solutions into Eq. (2.9) will yield the time evolution operator for all times and completes the solution. Without loss of generality, let us assume that the Hamiltonian is traceless $h_0(t) = 0$ from now on. Then, we have captured all of the dynamics of this general two-level system in terms of three coordinates $\mu_i(t)$. Hence we can "visualize" the dynamics of two-level systems in terms of a coordinate in three dimensions, governed by the equations of motion for $\mu_i(t)$. As we will show in Section 3.2, the

first two angles $\mu_1(t)$ and $\mu_2(t)$ can be mapped onto points on a sphere (using a technique called "inverse stereographic projection") and hence can be thought of as a point traversing the surface of a sphere. The third coordinate $\mu_3(t)$ will be visualized as an infinite line attached to each point on this sphere.

2.4 Choice of Basis in Unitary Integration

Before we discuss solving for the unitary operator, let us look at Eq. (2.22) more closely. Though Schrödinger's equation is a linear equation, the final differential equations have high non-linearities. This is due to our choice of exponential transformation implied by the ansatz for the unitary operator and the basis $\{\sigma_1, \sigma_2, \sigma_3\}$. The reason for this is because all terms in the BCH lemma survive and hence the resulting equations have all powers of $\mu_i(t)$. Note that this level of non-linearity is not a problem (i.e., does not give rise to "chaotic behavior" in unitary dynamics) since we know the initial condition $\mu_i(0) = 0$ with infinite precision. This being the case, this exponential non-linearity has two implications: first, outside the most trivial example, the equations in Eq. (2.22) are not solvable analytically and second, the numerical solution for a given choice of $h_i(t)$ is governed not by the infinite precision of the initial condition but the machine precision with which that initial condition is recorded. This means that for long times, one might expect the numerical solution to deviate from the actual solution. Hence it is useful to consider other choices of basis whereby the non-linearity of the subsequent equations of motion is as small as possible. We will consider one such choice of basis below.

Consider the alternative basis $\{J_+ = \sigma_+/2, J_- = \sigma_-/2, J_3 = \sigma_3/2\}$, where $\sigma_\pm = \sigma_1 \pm i\sigma_2$. The Lie algebra of these operators is given by $[\sigma_+, \sigma_-] = 4i\sigma_3 \Rightarrow [J_+, J_-] = 2iJ_3$ and $[\sigma_\pm, \sigma_3] = \mp 2i\sigma_\pm \Rightarrow [J_\pm, J_3] = \mp iJ_\pm$. In this basis, let us

write $H(t) = h_+(t)J_+ + h_-(t)J_- + h_3(t)J_3$. Since $J_\pm$ are not Hermitian matrices, $h_\pm(t)$ are complex functions of time and $h_3(t)$ is real because J_3 is Hermitian. Since $H(t)$ is Hermitian, it follows that $h_+^*(t) = h_-(t)$. Thus there are again only three real parameters that are needed to define a traceless Hamiltonian operator. Now, following our ansatz, let us write

$$U = e^{-i\mu_+(t)J_+} e^{-i\mu_-(t)J_-} e^{-i\mu_3(t)J_3}. \tag{2.26}$$

Since $J_+^2 = J_-^2 = 0$, we can write this ansatz explicitly as

$$U(t) = \begin{pmatrix} 1 & -i\mu_+(t) \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -i\mu_-(t) & 1 \end{pmatrix} \begin{pmatrix} e^{-i\mu_3(t)} & 0 \\ 0 & e^{i\mu_3(t)} \end{pmatrix} \tag{2.27}$$

$U(t)U^\dagger(t) = I$ implies that

$$\begin{pmatrix} 1 & -i\mu_+(t) \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -i\mu_-(t) & 1 \end{pmatrix} \begin{pmatrix} 1 & i\mu_-^*(t) \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ i\mu_+^*(t) & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{2.28}$$

The choice $\mu_- = \mu_+^*/(1+|\mu_+|^2)$ and $e^{\mathcal{I}(\mu_3(t))} = 1+|\mu_+|^2$ satisfies the above equation. Hence the number of independent coefficients is reduced from the six of three complex numbers to three, $\mathbf{z}(t)$ and $\mathcal{R}(\mu_3(t))$.

Let us see how the structure of commutators affects the non-linearity of the equations governing the evolution of $\{\mu_\pm(t), \mu_3(t)\}$. The derivative of Eq. (2.26) with respect to time yields

$$\begin{aligned} \dot{U}(t) = -i\dot{\mu}_+(t)J_+U(t) - i\dot{\mu}_-(t)e^{-i\mu_+(t)J_+}J_-e^{-i\mu_-(t)J_-}e^{-i\mu_3(t)J_3} \\ -i\dot{\mu}_3(t)e^{-i\mu_+(t)J_+}e^{-i\mu_-(t)J_-}J_3e^{-i\mu_3(t)J_3}. \end{aligned} \tag{2.29}$$

To simplify the second term on the right hand side of the above equation, we have to consider

$$e^{-i\mu_+(t)J_+}J_-e^{-i\mu_+(t)J_+} = J_- - i\mu_+(t)\,[J_+, J_-] - \frac{\mu_+^2}{2!}\,[J_+, [J_+, J_-]] + \cdots \tag{2.30}$$

Since the commutator $[J_+, J_-] \approx J_3$, this means that $[J_+, [J_+, J_-]] \approx [J_+, J_3] \approx J_+$. This means that the next term in the BCH lemma $[J_+, [J_+, [J_+, J_-]]] = 0$ and hence the infinite series terminates after the quadratic term in $\mu_+(t)$. Thus the nonlinearity of the final evolution equations is greatly reduced and is never more than quadratic. Applying the BCH lemma as outlined above yields the following equations,

$$\dot{\mu}_+(t) + i\mu_+(t)h_3(t) - \frac{1}{2}h_+(t)\mu_+^2(t) = \frac{1}{2}h_-(t), \tag{2.31}$$

$$\dot{\mu}_-(t) - i\mu_-(t)\dot{\mu}_3(t) = \frac{1}{2}h_+(t), \tag{2.32}$$

$$\dot{\mu}_3(t) - i\mu_+(t)h_+(t) = h_3(t). \tag{2.33}$$

Along with the initial conditions $\mu_\pm(0) = \mu_3(0) = 0$, these differential equations represent a recasting of Schrödinger's equation. The solution to these equations when substituted into the expression in Eq. (2.26) yields the time evolution operator at arbitrary times. Note that this reduced(quadratic) non-linearity is desirable to the equations obtained for the parameters at the end of the previous section. This quadratic non-linearity owes itself to the algebra of the matrices $\{\sigma_\pm, \sigma_3\}$. We will show in the next chapter that this algebraic characteristic of yielding quadratically non-linear equations can be generalized to N-level systems to yield equations similar to Eq. (2.31). Returning to the case of two-level systems, let us now look at some examples of unitary integration solutions to physical problems.

2.5 Solution for Some Specific Systems

2.5.1 Constant Hamiltonian

Let us start by considering the simplest case wherein the Hamiltonian is time independent. In this case, we can write $h_i(t) = h_i(0) = h_i$. Substituting this into

Eq. (2.31) yields

$$\dot{\mu}_+(t) + i\mu_+(t)h_3 - \frac{1}{2}h_+(t)\mu_+^2(t) = \frac{1}{2}h_-, \tag{2.34}$$

$$\dot{\mu}_-(t) - i\mu_-(t)\dot{\mu}_3(t) = \frac{1}{2}h_+, \tag{2.35}$$

$$\dot{\mu}_3(t) - i\mu_+(t)h_+ = h_3. \tag{2.36}$$

Let us consider the first of these equations. This equation

$$\dot{\mu}_+(t) + i\mu_+(t)h_3 - \frac{1}{2}h_+\mu_+^2(t) = \frac{1}{2}h_-. \tag{2.37}$$

is known as a Ricatti equation and is solved as follows. Written in its canonical form, the Ricatti equation is given by

$$\dot{\mu}_+(t) = \frac{1}{2}h_- - ih_3\mu_+(t) + \frac{1}{2}h_+\mu_+^2(t). \tag{2.38}$$

$\tau(t) = \frac{1}{2}h_+\mu_+(t)$ obeys the equation

$$\dot{\tau}(t) = \tau^2(t) + i\Delta\tau(t) + \frac{A^2}{4}, \tag{2.39}$$

where $\Delta = -h_3$ and $A^2 = h_+h_-$. Substituting $\tau(t) = -\frac{\dot{\lambda}(t)}{\lambda(t)}$ yields

$$\ddot{\lambda}(t) + i\Delta\dot{\lambda}(t) + \frac{A^2}{4}\lambda(t) = 0. \tag{2.40}$$

For the trial solution $\lambda(t) = e^{i\kappa t}$, we get two solutions

$$\kappa_\pm = \frac{1}{2}(\Delta \pm \sqrt{\Delta^2 + A^2}). \tag{2.41}$$

This means that

$$\lambda(t) = c_+e^{i\kappa_+ t} + c_-e^{i\kappa_- t}. \tag{2.42}$$

2.5.2 Rabi Oscillations

Let us now look at a Hamiltonian of the form

$$H(t) = \frac{\Omega_0}{2}\sigma_3 - A\cos(\Omega t)\sigma_1 = \frac{\hbar\Omega_0}{2}\sigma_3 - \frac{A}{2}\cos(\Omega t)\sigma_+ - \frac{A}{2}\cos(\Omega t)\sigma_-. \tag{2.43}$$

This Hamiltonian represents a two-level system whose energy levels are separated by Ω_0 and which is driven by a transverse sinusoidal field whose amplitude is given by A and frequency is Ω. Eq. (2.31) for this case is given by

$$\dot{\mu}_+(t) + i\frac{\Omega_0}{2}\mu_+(t) - \frac{A}{4}\cos(\Omega t)\mu_+^2(t) = \frac{A}{4}\cos(\Omega t), \tag{2.44}$$

$$\dot{\mu}_-(t) - i\mu_-(t)\dot{\mu}_3(t) = \frac{A}{4}\cos(\Omega t), \tag{2.45}$$

$$\dot{\mu}_3(t) - i\mu_+(t)\frac{A}{2}\cos(\Omega t) = \frac{\Omega_0}{2}. \tag{2.46}$$

Again, let us consider the first of the above equations. The transformation $\mu_+(t) = e^{-i\Omega_0 t/2}\nu_+(t)$ yields,

$$e^{-i\Omega_0 t/2}\dot{\nu}(t) - \frac{A}{4}\cos(\Omega t)e^{-i\Omega_0 t}\nu_+^2(t) = e^{-i\Omega_0 t/2}\frac{A}{4}\cos(\Omega t) \Rightarrow \tag{2.47}$$

$$\dot{\nu}(t) - \frac{A}{4}\cos(\Omega t)e^{-i\Omega_0 t/2}\nu_+^2(t) = \frac{A}{4}\cos(\Omega t) \Rightarrow \tag{2.48}$$

$$\dot{\nu}(t) = \frac{A}{4}\cos(\Omega t)(1 - e^{-i\Omega_0 t/2}\nu^2(t)). \tag{2.49}$$

Upon solving these differential equations and substituting into the ansatz discussed, one can obtain the familiar Rabi oscillation solution of the two-level system.

2.6 Unitary Integration in Higher Dimensions

In the previous section, we outlined the basic technique of unitary integration within the context of two-level systems. In this section, we will discuss how this technique can be extended to N-level systems. Let us begin by considering three-level systems. A general Hamiltonian for three-level systems can be written as

$$H(t) = \sum_{j=1}^{8} h_j(t)\lambda_j. \tag{2.50}$$

Here λ_j are the Gell-Mann matrices detailed in the Appendix(see appendix for details). Written explicitly, this Hamiltonian is given by

$$H(t) = \begin{pmatrix} h_3(t) + \frac{h_8(t)}{\sqrt{3}} & h_1(t) - ih_2(t) & h_4(t) - ih_5(t) \\ h_1(t) + ih_2(t) & -h_3(t) + \frac{h_8(t)}{\sqrt{3}} & h_6(t) - ih_7(t) \\ h_4(t) + ih_5(t) & h_6(t) + ih_7(t) & -2\frac{h_8(t)}{\sqrt{3}} \end{pmatrix}. \tag{2.51}$$

The time-evolution operator corresponding to three-level systems is closed under the SU(3) group, characterized by $3^2 - 1 = 8$ operators. Again, we can proceed as before by writing the time evolution operator as

$$U(t) = \Pi_{i=1}^{8} e^{-\mu_i \lambda_i}. \tag{2.52}$$

This allows us to use the BCH lemma as outlined in the previous section and derive a set of differential equations that govern the evolution of $\mu_i(t)$. Before we attempt this, let us consider a special case where

$$H(t) = \begin{pmatrix} h_3(t) & h_1(t) - ih_2(t) & 0 \\ h_1(t) + ih_2(t) & -h_3(t) & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{2.53}$$

This Hamiltonian suggests a general two level system accompanied by an uncoupled third level(the column and row of zeros). As we concluded in the previous section, from the standpoint of numerical stability, the choice of basis $\sigma_{1,2,3}$ (or alternatively $\lambda_{1,2,3}$) involves high non-linearities in $\mu_i(t)$. A better choice of basis is given by $b_\pm = 1/2(\lambda_1 \pm i\lambda_2)$, $b_3 = \lambda_3/2$. This choice of basis can be generalized to the entire algebra by the choice of the eight operators $a_\pm = 1/2(\lambda_6 \pm i\lambda_7)$, $b_\pm = 1/2(\lambda_1 \pm i\lambda_2)$, $c_\pm = 1/2(\lambda_4 \pm i\lambda_5)$, $a_3 = 1/2(\sqrt{3}\lambda_8 - \lambda_3)$ and $c_3 = 1/2(\sqrt{3}\lambda_8 + \lambda_3)$. This basis is related to the "spherical representation" of SU(3) given by $T_\pm = b_\pm$, $V_\pm = c_\pm$, $U_\pm = a_\pm$, $T_3 = \frac{1}{2}\lambda_3$ and $Y = \frac{1}{\sqrt{3}}\lambda_8$.

The choice of this alternative basis is not the only choice that has to be made before we present the unitary integration solution. We must also specify the order in which the operators defined above appear in the time evolution operator in order to derive the equations whose solutions determine the time evolution operator for three-level systems driven by arbitrary time dependent Hamiltonians. Since $[c_\pm, c_3] = \mp 2c_\pm$, we would like to arrange c_3 to be to the right of $c_\pm$. This is done so that the infinite series given by the BCH lemma terminates after the quadratic term in this case. Since the operator c_3 acts similarly on $a_\pm$ and $b_\pm$, we should choose to place c_3 to the right of all of these operators. One can conclude similarly that a_3 should be placed to the right hand side of $\{a_\pm, b_\pm, c_\pm\}$ as well. Since $[a_3, c_3] = 0$, either of these operators can be placed to the right of the other operator. Thus, motivated by the algebraic structure of the operators, we can now choose the ansatz for the unitary operator as

$$U(t) = e^{i\delta} e^{-i\mu_8 b_+} e^{-i\mu_7 b_-} e^{-i\mu_6 c_+} e^{-i\mu_5 c_-} e^{-i\mu_3 a_+} e^{-i\mu_2 a_-} e^{-i\mu_1 a_3} e^{-i\mu_4 c_3}. \tag{2.54}$$

As outlined in the previous section, differentiation by parts followed by repeated application of the BCH lemma can be used to solve for the dynamics of an arbitrary time dependent Hamiltonian driving a three-level system. The coefficients of the operators $I, b_+, b_-, c_+, c_-, a_+, a_-, a_3, c_3$ in the operator sum upon repeated

application of the BCH lemma are given by

$$
\begin{aligned}
&\dot{\delta} \\
&\dot{\mu}_8 + i\mu_5 s + \mu_8^2 w + i\mu_8(-i\mu_3 r + \dot{m}u_1 - 2\mu_5\mu_7 s - \dot{\mu}_4 + i\mu_6 v), \\
&w = \dot{\mu}_7 - i\mu_6 r + i\mu_5\mu_7^2 - i\mu_7(-i\mu_3 r + \dot{m}u_1 + i\mu_6 v - \dot{\mu}_4), \\
&u = \dot{m}u_6 + \mu_6^2 v + i\mu_6(-i\mu_3 r + \dot{\mu}_1 + 2\dot{\mu}_4) - i\mu_7(1 - \mu_5\mu_6)s, \\
&v + i\mu_8(r + i\mu_7 v), \\
&-i\mu_8 u + (1 - \mu_5\mu_6)s, \\
&r + i\mu_7 v, \\
&\dot{\mu}_1 - i\mu_8 w - i\mu_3 r - \mu_5\mu_7 s, \\
&\dot{\mu}_4 + i\mu_8 w - i\mu_6 v + \mu_5\mu_7 s
\end{aligned}
\tag{2.55}
$$

respectively. Here $r = \dot{\mu}_2 - i\mu_2(\dot{\mu}_4) + 2\dot{\mu}_1$, $s = \dot{\mu}_3 + \mu_3^2 r + i\mu_3(\dot{\mu}_4 + 2\dot{\mu}_1)$ and $v = \dot{\mu}_5 - i\mu_5(-i\mu_3 r + \dot{\mu}_1 + 2\dot{\mu}_4)$. Like before, each of the rows above is equated to the term in the Hamiltonian corresponding to the operator whose coefficients each term is to yield a set of nine differential equations.

As a final example of extending unitary integration to higher dimensions, let us discuss the choice of basis in the extension of unitary integration to four-level systems. Let us again choose the tensor Pauli basis for four-level systems O_i defined as $\sigma \otimes I, I \otimes \tau, \sigma \otimes \tau$(for details see appendix). A general four-level Hamiltonian is now written as $H(t) = \sum_{i=1}^{15} h_i(t)O_i$. Such a system is characterized by $4^2 - 1 = 15$ operators and the evolution is closed in the SU(4) group. The unitary integration solution proceeds as before by differentiation of the time-evolution operator written as a product of the 15 linearly independent operators O_i written in the exponent accompanied by functions $\mu_i(t)$. For the rest of this section, we will consider two important special cases of the su(4) unitary integration procedure outlined above.

The two special cases relate to two non-trivial sub-algebras of the su(4) namely su(2)⊗u(1)⊗su(2) and so(5). The first of these sub-algebras is characterized by seven operators and the second is characterized by ten operators. The operators that define the su(2)⊗u(1)⊗su(2) algebra[1] are given by $\{O_{13} = \sigma_1 \otimes \tau_1/4, O_{15} = \sigma_1 \otimes \tau_2/2, O_{16} = \sigma_2 \otimes \tau_1/2, O_{14} = \sigma_2 \otimes \tau_2/4, O_3 = I \otimes \tau_3/2, O_2 = \sigma_3 \otimes I/2, O_4 = \sigma_3 \otimes \tau_3/2\}$. Note that this set is not unique(there are fifteen different such subgroups in SU(4). For details please see the appendix). Note also that if a Hamiltonian obeys a certain symmetry and the initial density matrix belongs in that symmetry group, subsequent unitary evolution will keep the density matrix in the subspace defined by that symmetry. This means that if we consider a Hamiltonian written as a sum of the operators that define the su(2)⊗u(1)⊗su(2) algebra, then given that $U(0) = I$ trivially belongs in the same algebra, we can conclude that the unitary operator at all times belongs in the given sub-algebra too. Similar to the unitary integration solution for two-level and three-level systems, we anticipate that the non-linearities involved in using the basis noted above is exponential and instead choose the basis $S_\pm = (\sigma_1 \pm i\sigma_2)(\tau_1 \pm i\tau_2)/2$, $s_\pm = (\sigma_1 \pm i\sigma_2)(\tau_1 \mp i\tau_2)/2$, $S_3 = (\sigma_3 + \tau_3)/2$, $s_3 = (\sigma_3 - \tau_3)/2$ and $\sigma_3\tau_3$. The relevant commutation relations are given by

$$[S_\pm, S_3] = \mp 2S_\pm \tag{2.56}$$

$$[s_\pm, s_3] = \mp 2s_\pm \tag{2.57}$$

$$[S_+, S_-] = 4S_3 \tag{2.58}$$

$$[s_+, s_-] = 4s_3. \tag{2.59}$$

[1]We will follow the usual convention of denoting algebras in lowercase and groups in uppercase letters.

Each member of the triplet $\{S_\pm, S_3\}$ commutes with each member of $\{s_\pm, s_3\}$. For this reason, the solution is similar to two copies of the unitary integration solution for the two-level system outlined before.

Finally, consider the so(5) subalgebra of su(4). An example of the ten operators that close under such a sub-algebra are given by $\{O_2, O_3, O_5, O_6, O_{11}, O_{13}, O_{14}, O_{15}, O_{16}\}$. Once again, a unitary integration solution can be built analogous to the technique outlined above.

2.7 Including Dissipation and Decoherence

Dissipation and decoherence are introduced within the framework of the Liouville equation by writing a master equation for the density matrix namely

$$i\dot{\rho} = [H(t), \rho] + \frac{i}{2}\sum_m \gamma_m (A_m^\dagger A_m \rho + \rho A_m^\dagger A_m - 2A_m \rho A_m^\dagger). \tag{2.60}$$

The operators A_m are called Lindblad operators and the coefficients γ_m are positive. This equation preserves the trace of the density matrix and the positivity of the eigenvalues and is called the Liouville von-Neumann Lindblad (LvNL) equation. The LvNL equation is a generalization of Schrödinger's equation and incorporates a given quantum system along with the environment that it is interacting with. The equation hence simulates the evolution of a quantum system wherein it interacts with an "external" environment. We will discuss in this section how to obtain the unitary integration solution for the evolution operator(which is no longer unitary) for arbitrary time dependence of both the Hamiltonian and the Lindblad operators. For a detailed derivation of Lindblad equations, see [20].

Let us illustrate the procedure to apply the unitary integration procedure to solve the LvNL equation by considering a two-level system subject to phase decoherence. The Hamiltonian for a such a system was studied in the context of clarifying

dynamics in the presence of Landau[2]-Zener[3]-Stueckelberg[4] transitions [54, 88, 103] and is given by $H(t) = \epsilon(t)\sigma_3/2 + J\sigma_1$. There is only one Lindblad operator in this case and is given by σ_3. γ determines the rate of decoherence in this case. The LvNL equation can now be written as

$$i\dot{\rho} = [\epsilon(t)\sigma_3/2 + J\sigma_1, \rho] + i\gamma(\rho - \sigma_3\rho\sigma_3). \tag{2.61}$$

The solution for this full master equation is obtained by writing an evolution equation for the population difference and the coherence of the density matrix from Eq. (2.61). This equation is given by

$$i\frac{d}{dt}\begin{pmatrix} \rho_{21}+\rho_{12} \\ \rho_{21}-\rho_{12} \\ \rho_{11}-\rho_{22} \end{pmatrix} = \begin{pmatrix} -i\gamma & -\epsilon(t) & 0 \\ -\epsilon(t) & -i\gamma & 2J \\ 0 & 2J & 0 \end{pmatrix}\begin{pmatrix} \rho_{21}+\rho_{12} \\ \rho_{21}-\rho_{12} \\ \rho_{11}-\rho_{22} \end{pmatrix} \tag{2.62}$$

This equation represents the evolution of the elements of the density matrix, albeit the "Hamiltonian" is non-Hermitian. This does not pose an issue as the coefficients can be assumed to be complex and linearly independent. For instance,in the two qubit example μ_- was determined by μ_+ due to the Hermiticity of the Hamiltonian. Since this is no longer the case, all coefficients in the exponents are independent and to be determined from the evolution equations. The solution for the above LvNL equation maybe obtained by writing a time-evolution operator in the form presented in Eq.(2.54) and solving the subsequent set of differential equations. Note that arbitrary time dependence in the Hamiltonian in Eq. (2.62) can be handled in this way

Furthermore, this method can be extended to N-level systems. First, the LvNL equation is written for the given system. Next, this evolution is recast in terms of

[2]Lev Landau(1908-1968)
[3]Clarence Zener(1905-1993)
[4]Ernst Stueckelberg(1905-1984)

the $N-1$ diagonals and $N(N-1)$ real off-diagonal terms (real and imaginary parts of the $N(N-1)/2$ coherences) to obtain a Schrödinger-like equation in N^2-1 dimensions. This evolution equation is then solved by writing the (non-unitary) time-evolution matrix as a product of exponents of coefficients multiplied by operators that form a basis and the resulting equations are solved. This technique of solving the LvNL equation for a N-level system by embedding it in a (N^2-1) dimensions is called "dimensional embedding".

Note that dimensional embedding is not a recasting of the "Steinspring dilation theorem" [86]. Consider any positive and trace preserving map $\Phi : S(H) \rightarrow S(H)$ acting on a density matrix in finite dimensional Hilbert space H. The Steinspring dilation theorem states that this map is equivalent to unitary operations in a higher dimensional Hilbert space $H \otimes K$ such that $\Phi(\rho) = Tr_k\{U^\dagger(\rho \otimes |0\rangle\langle 0|)U\}\ \forall \rho$ such that $dim(k) < dim^2(H)$. This means that general positive maps acting on density matrices of N-level systems can be thought of as unitary operations on atmost N more ancillary modes, followed by the ancillary modes being traced over. On the other hand, dimensional embedding is an algebraic technique that facilitates obtaining the unitary integration solution of LvNL equations.

2.8 Conclusions

In this chapter we presented a semi-analytic method to solve time-dependent problems in quantum mechanics. While techniques such as perturbation theory provide very good approximate solutions when the perturbing Hamiltonian is small, a more general technique such as variational principle has to be employed for solving non-perturbative problems in physics. Such problems have been of interest in recent years because of the availability of strong lasers that can subject atomic systems to very strong fields. The technique of unitary integration presented here separates the

non-commutativity of the operators involved from the dynamics to provide "classical" equations that can be visualized. We also presented a systematic method to include dissipation and decoherence to a general N-level system's dynamics and obtain unitary integration solutions for the same, though the evolution operator is no longer unitary. In the next chapter, we will provide a further generalization of this technique that allows us to visualize dynamics on curved manifolds.

Chapter 3
Unitary Integration II

"We defend ourself with descriptions and tame the world by generalizing."

Iris Murdoch (1919-1999)

3.1 Introduction

In the previous chapter we introduced a semi-analytic technique to handle the evolution of arbitrary time-dependent Hamiltonians of N-level systems. We will briefly recall that procedure to solve for the evolution operator since we will modify it in this chapter. The solution is obtained by introducing N^2 linearly independent operators that form a basis to describe $su(N)$ operators. The evolution operator is written as a product of exponents each of which involves one of the basis operators and a time-dependent parameter. The solution is then obtained using repeated application of the BCH lemma so that the original Schrödinger's equation is reduced to N^2 differential equations in the time dependent parameters.

This procedure, though capable of solving for the time-evolution operator of an N-level system, grows quadratically in N. This quadratic growth in the number of coupled non-linear differential equations is undesirable in practice. In this chapter, we will outline an alternative procedure to handle arbitrary time-dependent Hamiltonians for a N-level system. Though the final number of coupled differential equations cannot be reduced from $N^2 - 1$, the procedure outlined in this chapter will be shown to be fruitful in other ways. Firstly, the technique introduced in this chapter will allow us to solve for the evolution operator by a bootstrapping process that requires solving a smaller set of differential equations at each step in

the process. Secondly, we will show how a geometric picture of unitary dynamics can be built up from this procedure. Since the new procedure is a variant of the one presented in the previous chapter, we will retain the use of the phrase "unitary integration" to describe this new procedure.

We will begin by briefly discussing the technique for two-level systems. The next section will outline how the technique can be generalized to N-level systems. We will present some technical details in the next section and will present some analysis relating this work to geometric phases. We will conclude the chapter with some important remarks relating to the SU(4) group.

3.2 su(2) Solution as a Prelude to su(N).

Let us, once again, consider an arbitrary two-level Hamiltonian written as $H(t) = -B_+\sigma_+ - B_-\sigma_- - B_3\sigma_3$. The Schrödinger's equation for such a system is written as

$$\dot{\mathbf{U}}(t) = -i\mathbf{H}(t)\mathbf{U}(t). \tag{3.1}$$

The evolution operator, as described in the previous chapter was written as

$$\mathbf{U} = e^{-i\mu_+(t)\sigma_+}e^{-i\mu_-(t)\sigma_-}e^{-i\mu_3(t)\sigma_3}, \tag{3.2}$$

and the solution was obtained by the repeated application of the BCH lemma. Before we proceed any further, with an eye to generalizing the solution to $su(N)$, we will rename $-i\mu_+$ as $\mathbf{z}(t)$, $-i\mu_-$ as $\mathbf{w}^*(t)$. Note that though the functions $\mathbf{z}(t)$ and $\mathbf{w}^*(t)$ are scalar functions of time, they will be generalized to matrices eventually. With this in mind, the two functions have been written in boldface.

With this change in notation , noting that $\sigma_{\pm}^2 = 0$, we can write the above time-evolution operator explicitly as

$$\mathbf{U}(t) = \begin{pmatrix} 1 & \mathbf{z}(t) \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ \mathbf{w}^*(t) & 1 \end{pmatrix} \begin{pmatrix} e^{-i\mu_3(t)} & 0 \\ 0 & e^{i\mu_3(t)} \end{pmatrix}. \tag{3.3}$$

Again, one can verify that $UU^\dagger = I$ implies that $\mathbf{w}^*(t) = -\mathbf{z}^*(t)/(1+|\mathbf{z}(t)|^2)$ and $\mathsf{exp}(\mathcal{I}(\mu_3(t))) = 1+|\mathbf{z}(t)|^2$. This completes the unitary integration solution, as detailed in the previous chapter. Before we present the generalization of this to N-level systems, we note that the above solution can be transformed into the so-called "Bloch [1]-sphere" representation of $su(2)$ dynamics. This is done by defining the vector $\vec{m}$ such that $m_1 + im_2 = -2\mathbf{w}^*(t)$ and $m_3 = \sqrt{1-|m_1+im_2|^2}$. m_3 can be shown to be equal to $(1-|\mathbf{z}(t)|^2)/(1+|\mathbf{z}(t)|^2)$. Note that we arranged for $|\vec{m}|^2 = 1$. Thus $\vec{m}$ is a unit vector whose dynamics is determined by the dynamics of $\mathbf{z}(t)$ and vice versa. The dynamics of $\vec{m}$ can be derived by using the form of the Hamiltonian $H(t) = -\vec{\sigma}.\vec{B}$ and using the differential equations that govern the dynamics of $\mathbf{z}(t)$ and $\mathcal{R}(\mu_3(t))$. It can be verified that this dynamical equation is given by $\dot{\vec{m}} = -2\vec{B} \times \vec{m}$. We emphasize that exploring the geometry of the time evolution operator for two-level systems thus involves what amounts to an inverse-stereographic projection of the complex matrix $\mathbf{z}(t)$ onto the surface of a three-dimensional sphere. In the next chapter, we will generalize this "Bloch-sphere" representation by a similar inverse stereographic projection technique for larger N.

Note that the dynamics of the two-level system is now given by two angles corresponding to the position of the unit vector $\vec{m}$ on the "Bloch-sphere" and an additional phase given by $\mathcal{R}(\mu_3(t))$. This is depicted in Fig. (3.1). While the unit

[1] Felix Bloch(1905-1983)

vector on the Bloch-sphere is familiar in the description of a two-level system, the phase $\mathcal{R}(\mu_3(t))$ is an additional $u(1)$ phase that is usually not accessible in experiments since it is a "global phase". This global phase is accessible only if the there is a phase reference relative to which one can measure it.

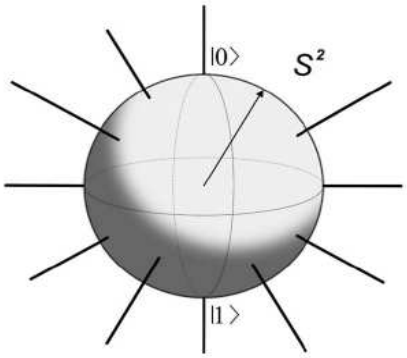

FIGURE 3.1. Bloch or Poincare sphere representation for SU(2). The base manifold is the S^2 sphere while the fiber is given by the U(1) phase at each point on that sphere. Together, we have the fiber bundle SU(2) $\simeq$ S$^2\times$U(1).

With an eye towards generalizing the derivation to N dimensions, let us write the Hamiltonian as

$$\mathbf{H}(t) = \begin{pmatrix} \widetilde{\mathbf{H}}^{(2-1)}(t) & \mathbf{V}(t) \\ \mathbf{Y}^*(t) & \widetilde{\mathbf{H}}^{(1)}(t) \end{pmatrix}. \tag{3.4}$$

Here $\widetilde{\mathbf{H}}^{(2-1)}(t)$ refers to the fact that we are partitioning a two-dimensional Hamiltonian into a $(2-1)$-dimensional(i.e., one-dimensional) upper diagonal block and a (1)-dimensional lower diagonal block, which is given by $\widetilde{\mathbf{H}}^{(1)}(t)$. The overhead tilde denotes that $\mathbf{H}(t)$ can be non-Hermitian, a further generalization we will discuss in the future, and likewise $\mathbf{V}(t)$ and $\mathbf{Y}^\dagger(t)$ reflect the possibility that the off-diagonal terms are not related for a general non-Hermitian Hamiltonian. Note once again that though all the elements of this 2×2 Hamiltonian written above are scalar functions of time, they have been written in boldface in anticipation of the generalization to N-dimensions.

Likewise let us write the unitary operator as $\mathbf{U}(t) = \widetilde{U}_1(t)\widetilde{U}_2(t)$, where

$$\widetilde{U}_1(t) = \begin{pmatrix} \mathbf{I}^{(2-1)} & \mathbf{z}(t) \\ 0 & \mathbf{I}^{(1)} \end{pmatrix} \begin{pmatrix} \mathbf{I}^{(2-1)} & 0 \\ \mathbf{w}^*(t) & \mathbf{I}^{(1)} \end{pmatrix}, \tag{3.5}$$

and

$$\widetilde{U}_2(t) = \begin{pmatrix} \widetilde{U}^{(2-1)}(t) & 0 \\ 0 & \widetilde{U}^{(1)}(t) \end{pmatrix}. \tag{3.6}$$

Here, the matrices $\widetilde{U}^{(2-1)}(t)$ and $\widetilde{U}^{(1)}(t)$ have an overhead tilde to denote that they are individually not unitary operators, while their product is guaranteed[2] to be unitary for Hermitian Hamiltonians. Substituting $U(t) = \widetilde{U}_1(t)\widetilde{U}_2(t)$ into Schrödinger's equation yields

$$i(\dot{\widetilde{U}}_1(t)\widetilde{U}_2(t) + \widetilde{U}_1(t)\dot{\widetilde{U}}_2(t)) = \mathbf{H}(t)\widetilde{U}_1(t)\widetilde{U}_2(t). \tag{3.7}$$

This can be rearranged to yield

$$i\dot{\widetilde{U}}_2(t) = \mathbf{H}_{\mathsf{eff}}(t)\widetilde{U}_2(t), \tag{3.8}$$

where $\mathbf{H}_{\mathsf{eff}}(t) = \widetilde{U}_1^{(-1)}(t)\mathbf{H}(t)\widetilde{U}_1(t) - i\widetilde{U}_1^{(-1)}(t)\dot{\widetilde{U}}_1(t)$ is the effective Hamiltonian that describes the dynamics of $\widetilde{U}_2(t)$. Since $\widetilde{U}_2(t)$ was assumed to be block-diagonal, the off-diagonal blocks of Eq. (3.8) can be set to be equal to zero. This equation is given by

$$i\dot{\mathbf{z}}(t) = \widetilde{\mathbf{H}}^{(2-1)}(t)\mathbf{z}(t) + \mathbf{V}(t) - \mathbf{z}(t)(\mathbf{Y}^\dagger(t)\mathbf{z}(t) + \widetilde{\mathbf{H}}^{(1)}(t)). \tag{3.9}$$

Note that this equation depends only on the Hamiltonian and $\mathbf{z}(t)$ and hence solving this equation yields $\mathbf{z}(t)$(and $\mathbf{w}(t)$, which is related to $\mathbf{z}(t)$ for Hermitian Hamiltonians). This solution can hence be substituted into the diagonal blocks of

[2]It follows from Schrödinger's equation.

Eq. (3.8), which is given by

$$i\dot{\widetilde{U}}_2(t) = \begin{pmatrix} \widetilde{\mathbf{H}}^{(2-1)}(t) - \mathbf{z}(t)\mathbf{Y}^\dagger(t) & 0 \\ 0 & \widetilde{\mathbf{H}}^{(1)}(t) + \mathbf{Y}^\dagger(t)\mathbf{z}(t) \end{pmatrix} \widetilde{U}_2(t). \tag{3.10}$$

Finally, let us combine the equations relating $\mathbf{z}(t)$ and $\mathbf{w}(t)$ and assume that $H(t) = -B_+\sigma_+ - B_-\sigma_- - B_3\sigma_3$ to write the two terms whose product is the unitary operator explicitly [73] as

$$\widetilde{U}_1(t) = \begin{pmatrix} \frac{1}{1+|\mathbf{z}(t)|^2} & \mathbf{z}(t) \\ \frac{\mathbf{z}^*(t)}{1+|\mathbf{z}(t)|^2} & 1 \end{pmatrix} \tag{3.11}$$

and

$$\widetilde{U}_2(t) = \begin{pmatrix} \widetilde{U}^{(2-1)}(t) & 0 \\ 0 & \widetilde{U}^{(1)}(t) \end{pmatrix}. \tag{3.12}$$

Similarly, $\mathbf{H}_{\mathsf{eff}}(t)$ is given by the difference of $\widetilde{U}_1^{-1}(t)\mathbf{H}(t)\widetilde{U}_1(t)$ and $i\widetilde{U}_1^{-1}(t)\dot{\widetilde{U}}_1(t)$, where the first term is given explicitly in terms of $\mathbf{z}(t)$ by,

$$\begin{pmatrix} \frac{\mathbf{z}^*(t)B_- + \mathbf{z}(t)B_+ - (1-|\mathbf{z}(t)|^2)B_3}{2(1+|\mathbf{z}(t)|^2)} & -\mathbf{z}(t)B_3 - \frac{1}{2}B_- + \frac{1}{2}\mathbf{z}^2(t)B_+ \\ \frac{-2\mathbf{z}^*(t)B_3 - B_+ - |\mathbf{z}(t)|^2 B_-}{2(1+|\mathbf{z}(t)|^2)} & \frac{-2(1+|\mathbf{z}(t)|^2)B_+ - \mathbf{z}^*(t)B_- + (1-|\mathbf{z}(t)|^2)B_3}{2(1+|\mathbf{z}(t)|^2)} \end{pmatrix}, \tag{3.13}$$

and $i\widetilde{U}_1^{-1}(t)\dot{\widetilde{U}}_1(t)$ is given by

$$\begin{pmatrix} \frac{\mathbf{z}^*(t)B_- - \mathbf{z}^*(t)|\mathbf{z}(t)|^2 B_+ + 2|\mathbf{z}(t)|^2 B_3}{2(1+|\mathbf{z}(t)|^2)} & -\mathbf{z}(t)B_3 - \frac{1}{2}B_- + \frac{1}{2}\mathbf{z}^2(t)B_+ \\ \frac{-2\mathbf{z}^*(t)B_3 - B_+ - |\mathbf{z}(t)|^2 B_-}{2(1+|\mathbf{z}(t)|^2)} & \frac{\mathbf{z}^*(t)(\mathbf{z}^*(t)^2 B_+ + iB_- - 2i\mathbf{z}^*(t)B_3)}{2(1+|\mathbf{z}(t)|^2)} \end{pmatrix}. \tag{3.14}$$

The difference of the above two matrices leaves the effective Hamiltonian as a diagonal matrix given by $\mathbf{H}_{\mathsf{eff}} = (-B_3 + \mathbf{z}B_+)\sigma_3/2$.

Solving for $\widetilde{U}_2(t)$ given the effective Hamiltonian above yields the unitary operator for arbitrary Hamiltonians. Note that this formalism lends itself to two kinds of generalizations. The first generalization allows us to extend this solution to non-Hermitian Hamiltonians. In this case, $\mathbf{z}(t)$ and $\mathbf{w}(t)$ are unrelated. In this case,

along with Eq. (3.9), the equation that governs $\mathbf{w}(t)$ is independently derived, and is given by

$$i\dot{\mathbf{w}}^\dagger = \mathbf{w}^\dagger(\mathbf{z}\mathbf{Y}^\dagger - \widetilde{\mathbf{H}}^{(2-1)}) + (\widetilde{\mathbf{H}}^{(1)} + \mathbf{Y}^\dagger\mathbf{z})\mathbf{w}^\dagger + \mathbf{Y}^\dagger. \tag{3.15}$$

Since $\mathbf{V}^\dagger(t) \neq \mathbf{Y}(t)$, the form of the effective Hamiltonian is more complicated. Furthermore, the imaginary part of $\widetilde{U}_2(t)$ is no longer related to $\mathbf{z}(t)$. The four complex scalar functions $\mathbf{z}(t)$, $\mathbf{w}(t)$, $\widetilde{U}^{(2-1)}(t)$ and $\widetilde{U}^{(1)}(t)$ parametrize the non-Hermitian evolution of a general two-level system.

The second generalization involves solving for the time-evolution operator for a general su(N) Hamiltonian. This will be the topic of the next section.

3.3 Unitary Integration Solution for su(N) Hamiltonians

Consider the N-dimensional Hamiltonian $\mathbf{H}^{(N)}$ given by

$$\mathbf{H}^{(N)} = \begin{pmatrix} \mathbf{H}^{(N-n)} & \mathbf{V} \\ \mathbf{V}^\dagger & \mathbf{H}^{(n)} \end{pmatrix}. \tag{3.16}$$

The diagonal blocks are (N−n)- and (n)-dimensional square matrices, respectively, while $\mathbf{V}$ is an $(N-n)\times(n)$-dimensional matrix.

The evolution operator $\mathbf{U}^{(N)}(t)$ for such a $\mathbf{H}^{(N)}$ is written as a product of two operators $\mathbf{U}^{(N)}(t) = \widetilde{U}_1\widetilde{U}_2$, where

$$\widetilde{U}_1 = \begin{pmatrix} \mathbf{I}^{(N-n)} & \mathbf{z}(t) \\ \mathbf{0}^\dagger & \mathbf{I}^{(n)} \end{pmatrix} \begin{pmatrix} \mathbf{I}^{(N-n)} & \mathbf{0} \\ \mathbf{w}^\dagger(t) & \mathbf{I}^{(n)} \end{pmatrix}, \tag{3.17}$$

$$\widetilde{U}_2 = \begin{pmatrix} \widetilde{\mathbf{U}}^{(N-n)} & \mathbf{0} \\ \mathbf{0}^\dagger & \widetilde{\mathbf{U}}^{n} \end{pmatrix}.$$

For any N, n is arbitrary with $1 \leq n < N$, and tilde denotes that the matrices need not be unitary. The product of three factors parallels the product of exponentials in three Pauli matrices. Note that the structure of the unitary operator is a generalization of the unitary operator ansatz presented for two-level systems. Equations defining the rectangular matrices $\mathbf{z}(t)$ and $\mathbf{w}^\dagger(t)$ are developed and the problem is reduced to the two residual $(N-n)$- and (n) dimensional evolution problems sitting as diagonal blocks of $\widetilde{U}_2$. $\mathbf{z}(t)$ and $\mathbf{w}^\dagger(t)$ are related to each other through the unitarity of $\mathbf{U}^{(N)}(t)$ [90, 91]:

$$\mathbf{z} = -\gamma_1 \mathbf{w} = -\mathbf{w}\gamma_2, \tag{3.18}$$

with $\gamma_1 = \hat{\mathbf{I}}^{(N-n)} + \mathbf{z}.\mathbf{z}^\dagger$ and $\gamma_2 = \hat{\mathbf{I}}^{(n)} + \mathbf{z}^\dagger.\mathbf{z}$.

With $\mathbf{U}^{(N)}(t)$ in such a product form, the Schrödinger equation is written as

$$\begin{aligned} i\dot{\widetilde{U}}_2(t) &= \mathbf{H}_{\mathtt{eff}}\widetilde{U}_2, \\ \mathbf{H}_{\mathtt{eff}} &= \widetilde{U}_1^{-1}\mathbf{H}^{(N)}\widetilde{U}_1 - i\widetilde{U}_1^{-1}\dot{\widetilde{U}}_1. \end{aligned} \tag{3.19}$$

Since $\widetilde{U}_2$ is block diagonal, the off-diagonal blocks of Eq. (3.19) define the equation satisfied by $\mathbf{z}$ given by

$$i\dot{\mathbf{z}} = \mathbf{H}^{(N-n)}\mathbf{z} + \mathbf{V} - \mathbf{z}(\mathbf{V}^\dagger\mathbf{z} + \mathbf{H}^{(n)}). \tag{3.20}$$

Note that the initial condition $U^N(0) = \mathbf{I}^N$ implies that $\widetilde{U}_1(0) = \mathbf{I}^{(N-n)}$, $\widetilde{U}_2(0) = \mathbf{I}^{(n)}$ and $\mathbf{z}(0) = \mathbf{0}^{(N-n)}$. Eq. (3.20), along with the initial condition can be solved to determine $\mathbf{z}$ and thereby $\widetilde{U}_1$ and $\mathbf{H}_{\mathtt{eff}}$ for subsequent solution of Eq. (3.19) for $\widetilde{U}_2$. In this manner, the procedure iteratively determines $U^{(N)}(t)$.

Before discussing the geometry of the time evolution operators for this unitary case, we briefly mention the procedure to deal with non-Hermitian Hamiltonians.

For such a non-Hermitian Hamiltonian,

$$\mathbf{H}^{(N)} = \begin{pmatrix} \widetilde{\mathbf{H}}^{(N-n)} & \mathbf{V} \\ \mathbf{Y}^{\dagger} & \widetilde{\mathbf{H}}^{(n)} \end{pmatrix}, \tag{3.21}$$

where tilde denotes possibly non-Hermitian character, and the off-diagonal components $\mathbf{V}$ and $\mathbf{Y}$ are independent. In this case, Eq. (3.20) is replaced by

$$i\dot{\mathbf{z}} = \widetilde{\mathbf{H}}^{(N-n)}\mathbf{z} + \mathbf{V} - \mathbf{z}(\mathbf{Y}^{\dagger}\mathbf{z} + \widetilde{\mathbf{H}}^{(n)}), \tag{3.22}$$

and there is a separate equation governing the evolution of $\mathbf{w}$ given by

$$i\dot{\mathbf{w}}^{\dagger} = \mathbf{w}^{\dagger}(\mathbf{z}\mathbf{Y}^{\dagger} - \widetilde{\mathbf{H}}^{(N-n)}) + (\widetilde{\mathbf{H}}^{(n)} + \mathbf{Y}^{\dagger}\mathbf{z})\mathbf{w}^{\dagger} + \mathbf{Y}^{\dagger}. \tag{3.23}$$

The diagonal terms of the time-evolution operators are governed by

$$i\dot{\widetilde{U}}_2(t) = \begin{pmatrix} \widetilde{\mathbf{H}}^{(N-n)} - \mathbf{z}\mathbf{Y}^{\dagger} & 0 \\ 0 & \widetilde{\mathbf{H}}^{(n)} + \mathbf{Y}^{\dagger}\mathbf{z} \end{pmatrix} \widetilde{U}_2. \tag{3.24}$$

Returning to the case where the Hamiltonian is Hermitian, it is convenient to render the two matrices $\widetilde{U}_1$ and $\widetilde{U}_2$ themselves unitary [90, 91]. For this purpose, a "gauge factor" b is chosen such that the unitary counterparts of $\widetilde{U}_1$ and $\widetilde{U}_2$ are defined via $U_1 = \widetilde{U}_1 b$ and $U_2 = b^{-1}\widetilde{U}_1$. Since $\widetilde{U}_1^{\dagger}\widetilde{U}_1 = diag(\gamma_1^{(-1)}, \gamma_2)$, this would imply that b is the "Hermitian square-root" of $diag(\gamma_1^{(-1)}, \gamma_2)$. This "Hermitian square-root" is defined by the relation $(b^{(-1)})^{\dagger}b^{(-1)} = diag(\gamma_1^{(-1)}, \gamma_2)$. Inspection of the power series expansion of $\gamma_1^{(\pm\frac{1}{2})} = (\hat{\mathbf{I}} + \mathbf{z}.\mathbf{z}^{\dagger})^{(\pm\frac{1}{2})}$ and $\gamma_2^{(\pm\frac{1}{2})} = (\hat{\mathbf{I}} + \mathbf{z}^{\dagger}.\mathbf{z})^{(\pm\frac{1}{2})}$ show that since each term in the expansion is Hermitian, matrices $\gamma_1^{\pm\frac{1}{2}}$ and $\gamma_2^{\pm\frac{1}{2}}$ are Hermitian and have non-negative eigenvalues. Because of this, it is sufficient to define b as the inverse square root via $b^{(-2)} = diag(\gamma_1^{(-1)}, \gamma_2)$.

Furthermore, $H_{\mathtt{eff}}$ in Eq. (3.19) is Hermitian for the unitary counterpart U_1. The upper diagonal block of this Hermitian Hamiltonian accompanying the decomposition $U = U_1U_2$ is given by

$$\frac{i}{2}[\frac{d(\gamma_1^{-\frac{1}{2}})}{dt}, \gamma_1^{\frac{1}{2}}] + \frac{1}{2}\left(\gamma_1^{-\frac{1}{2}}(\widetilde{\mathbf{H}}^{(N-n)} - \mathbf{z}\mathbf{V}^{\dagger})\gamma_1^{\frac{1}{2}} + H.c.\right), \tag{3.25}$$

where [,] represents the commutator and $H.c.$ stands for the Hermitian conjugate. The lower diagonal block is similarly given by

$$\frac{i}{2}[\frac{d(\gamma_2^{-\frac{1}{2}})}{dt}, \gamma_2^{\frac{1}{2}}] + \frac{1}{2}\left(\gamma_2^{-\frac{1}{2}}(\widetilde{\mathbf{H}}^{(n)} + \mathbf{z}^\dagger \mathbf{V})\gamma_2^{\frac{1}{2}} + H.c.\right). \tag{3.26}$$

In this section, we outlined a general technique to solve for the time-evolution of an N-level system driven by an arbitrary time-dependent Hamiltonian. The solution involved successive partitioning of the problem into smaller blocks and solving for the matrix $\mathbf{z}(t)$ at each stage. This solution is then used to write the effective Hamiltonian that determines the time-evolution of $\widetilde{U}_2(t)$. Each block of the $\widetilde{U}_2(t)$ equation is now solved according to the same technique.

For example, consider a general seven-level problem. This can be broken up using a $N = 7$, $n = 1$ decomposition. $\mathbf{z}(t)$ is now a 6×1 matrix and $\widetilde{U}_2(t)$ is a block diagonal matrix with a 6×6 block and a 1×1 block. Furthermore, the effective Hamiltonian also has a block structure similar to that of $\widetilde{U}_2(t)$. Having obtained the solution for $\mathbf{z}(t)$, we can substitute the solution to obtain the effective Hamiltonian. The 1×1 part of the $\widetilde{U}_2(t)$ solution is now easily solved and the 6×6 part of the $\widetilde{U}_2(t)$ is handled as a "new" unitary integration problem with $N = 6$ and $n < 6$ problem. This bootstrapping method hence provides a solution to the problem. The choice of the dimensionality of the decomposition is made at each step of the bootstrapping algorithm based on either special symmetries the problem affords or based on a simplification afforded in solving for $\widetilde{U}_2(t)$, given a choice of n. In the next section, we will expand upon the $n = 1$ case of the unitary integration solution and state some simplifications that arise in the gauge factor γ_2 for this choice of decomposition.

3.4 Simplification of "Gauge Factors" for $n = 1$

For $n = 1$, the SU(N) problem is decomposed into SU($N-1$) and U(1). This U(1) sector of the solution provides a simplification in evaluating the corresponding gauge factor γ_2 since it is a scalar given by $\gamma_2 = 1 + \mathbf{z}^\dagger\mathbf{z}($ in fact γ_1 can also be simplified significantly by using the fact that $\mathbf{z}^\dagger(t)\mathbf{z}(t)$ is a scalar). This yields $\dot{\gamma}_2 = \dot{\mathbf{z}}^\dagger\mathbf{z} + \mathbf{z}^\dagger\dot{\mathbf{z}}$. Substituting for $\dot{\mathbf{z}}(t)$ from Eq. (3.20), we can verify the relation $\dot{\gamma}_2 = i\gamma_2(\mathbf{V}^\dagger\mathbf{z}(t) - \mathbf{z}^\dagger(t)\mathbf{V})$. Furthermore, this equation can be used to evaluate the lower-diagonal block of the effective Hamiltonian that governs the dynamics the unitary matrix $U_2(t)$ defined in Eq. (3.26). This one-dimensional equation is given by $\widetilde{\mathbf{H}}^{(1)} + \frac{1}{2}(\mathbf{z}^\dagger(t)\mathbf{V} + \mathbf{V}^\dagger\mathbf{z}(t))$. Thus the lower block of the unitary operator $U_2(t)$ is given by

$$U^{(1)}(t) = \mathsf{Exp}\left(-i\int_{t'=0}^{t} dt'\{\widetilde{\mathbf{H}}^{(1)} + \frac{1}{2}(\mathbf{z}^\dagger(t')\mathbf{V} + \mathbf{V}^\dagger\mathbf{z}(t'))\}\right). \tag{3.27}$$

In this way, the dynamics of the N-level system can be decomposed into a series of phases. The dynamics of these phases is governed by an effective Hamiltonian, transformed by a gauge factor when the time evolution operator is decomposed into the product of unitary matrices. This effective Hamiltonian is the difference of two terms, which will be discussed in the next section.

3.5 Effective Hamiltonian and Geometric Phase

As outlined in the previous section, the equation that governs the dynamics of $\tilde{U}_2(t)$ is given by Eq. (3.19), where

$$\mathbf{H}_{\mathtt{eff}} = \widetilde{U}_1^{-1}\mathbf{H}^{(N)}\widetilde{U}_1 - i\widetilde{U}_1^{-1}\dot{\widetilde{U}}_1. \tag{3.28}$$

This equation has two terms, the second of which does not depend on the Hamiltonian explicitly. This term records the geometric (i.e., path dependent) effect on the

time-evolution matrix and is hence significant in recording the geometric phases acquired by the physical system as it traverses state space. We will present a detailed derivation of the geometric phase part of the time-evolution matrix for three-level systems in the next chapter. For the rest of this section, we will try to understand the significance of the form of Eq. (3.28) by presenting two related derivations.

To understand the significance of this equation, let us look at the solution to Schrödinger's equation involving a Hamiltonian $\mathbf{H}(\vec{\lambda})$ which depend continuously on a set of parameters that is varied adiabatically [99]. Assume the existence of an m-fold degenerate subspace whose energy is equal to zero, and which evolves as the parameters $\vec{\lambda}$ are varied from $\vec{\lambda}_i$ at $t = 0$ to $\vec{\lambda}_f$ at $t = T$. Assume furthermore that these degenerate levels do not cross other levels. In the limit of adiabatic variation, the solutions of

$$\mathbf{H}(\vec{\lambda}_i)|\psi\rangle = 0, \tag{3.29}$$

adiabatically transform into the solutions of

$$\mathbf{H}(\vec{\lambda}_f)|\eta\rangle = 0. \tag{3.30}$$

If the adiabatic variation of the parameter is done over a closed path such that $\vec{\lambda}_i = \vec{\lambda}_f$, then the initial solutions are mapped onto themselves. Now since we assumed an m-fold degeneracy to begin with, these m-states can be mapped onto themselves not trivially (i.e. $|\eta_i\rangle = |\psi_i\rangle$) but rather non-trivially. This non-trivial transformation can be written as

$$|\eta_i\rangle = \sum_j U_{ij}|\psi_j\rangle. \tag{3.31}$$

Since Schrödinger's equation implies that $|\dot{\eta}_i\rangle = -i\mathbf{H}(\vec{\lambda}_f)|\eta_i\rangle = 0$, we get

$$0 = |\dot{\eta}_i\rangle = \sum_j \dot{U}_{ij}|\psi_j\rangle + \sum_j U_{ij}|\dot{\psi}_j\rangle. \tag{3.32}$$

This implies

$$0 = \langle \eta_k | \dot{\eta}_i \rangle = \sum_j \langle \eta_k | \dot{U}_{ij} | \psi_j \rangle + \sum_j \langle \eta_k | U_{ij} | \dot{\psi}_j \rangle. \tag{3.33}$$

This equation can be written as

$$\langle \eta_k | U^{-1} \dot{U} | \eta_i \rangle = \langle \psi_k | \dot{\psi}_i \rangle := \mathsf{A}_{ki}, \tag{3.34}$$

and solved formally,

$$U(t) = P\{\mathsf{Exp}(\int_0^t dt' \mathsf{A}(t'))\}. \tag{3.35}$$

In the equation above, P refers to path ordering.

If we now imagine that $|\psi_i\rangle$ is transformed according to $|\psi_i'\rangle = \mathcal{U}(t)|\psi_i\rangle$, then A transforms to

$$\mathsf{A}'(t) = \dot{\mathcal{U}}(t)\, \mathcal{U}^{-1}(t) + \mathcal{U}(t)\, \mathsf{A}\, \mathcal{U}^{-1}(t). \tag{3.36}$$

This transformation has the same form as Eq. (3.28) and A is said to transform like a "gauge potential".

This name derives from the following argument relating to preserving the equations of motion under local gauge transformations, which is a generalization of the example presented above. Suppose that we have a Lagrangian of a scalar complex field written in the form $\mathcal{L} = \partial_\mu \varphi \partial^\mu \varphi - F(\varphi^\dagger \varphi)$. Then if we transform the "coordinate system" such that $\varphi \to \mathcal{U}\varphi$, the Lagrangian is preserved. But if we consider a transformation of the type $\varphi \to \mathcal{U}(x_\mu)\varphi$, the kinetic energy term is no longer invariant. The relevant transformation is given by $\partial_\mu(\mathcal{U}(x_\mu\varphi)) = \mathcal{U}(x_\mu)\{\partial_\mu\varphi + (\mathcal{U}^\dagger(x_\mu)\partial_\mu\mathcal{U}(x_\mu))\varphi\}$. If we now define a "new" derivative D_μ called a covariant derivative such that $D_\mu\varphi = \partial_\mu\varphi - i\mathsf{A}_\mu(x_\mu)\varphi$ and demand that $D_\mu\mathcal{U}(x_\mu)\varphi \to \mathcal{U}(x_\mu)D_\mu\varphi$, then the transformation equation for A_μ can be worked out to be exactly equal to Eq. (3.36). A_μ is called a gauge potential since it preserves the

equations of motion under a "gauge transformation" (i.e., Rescaling the coordinate system at each point in spacetime x_μ). This notion of the gauge invariance of the Lagrangian and hence the equations of motion is a central feature of all modern field theories.

Thus we understand the effective Hamiltonian as being composed of two terms. The first is a "dynamic term" that relates the Hamiltonian to the evolution of $\tilde{U}_2(t)$ while the second term is a "geometric term" that records path dependent phases acquired as the system evolves.

3.6 Conclusions

In the previous sections, we presented a bootstrapping approach to solve for the dynamics of N-level systems and illustrated how the technique can be used to derive the Bloch sphere representation for a single qubit. We note that such a procedure has been implemented for various other subgroups of SU(4) [90, 91]. We also presented in this chapter, important remarks relating the technique of unitary integration to geometric phases.

In the next chapter, we will use much of the technology developed here to solve for the time evolution operator of three-level systems. We will present detailed applications and present connections to geometric phases in physics.

Chapter 4

Bloch Sphere Like Representations for su(3) Hamiltonians

"What is the use of a book, thought Alice, 'without pictures or conversations?""

Lewis Carroll(1832-1898)

4.1 Introduction

[1] Three-level systems are of fundamental importance in many branches of physics. While two levels give the simplest model for the dynamics of discrete systems, three levels illustrate the role that an intermediate state can play in inducing transitions between the other two. Canonical examples of this include applications in quantum optics that use three-level atoms to control quantum state evolution [82]. Such laser control is used, for instance, to transfer population between two states using stimulated Raman[2] adiabatic passage (STIRAP) [52, 66] and chirped adiabatic passage (CARP) [26]. In some of these systems, the interaction of the radiation with the atom is represented as a time-dependent Hamiltonian inducing an energy separation between the two states that varies with time. For a non-zero sweep rate, it can be shown that there is finite transition probability between the states [54, 88, 103]. The study of Landau-Zener-Stueckelberg transitions in multilevel systems is of interest to understand the interplay between various level crossings [46]. Particle physics represents another example where three-level systems play a central role as, for example, the oscillations of neutrino flavor eigenstates [51].

[1] This chapter is based on [95].

[2] Chandrasekhara Venkata Raman(1988-1970).

The general Hamiltonian of a three-level system involves 8 independent operators. Such a set can also naturally arise as a subgroup of higher level systems where there is some degeneracy involved. Thus, several important two-qubit problems in quantum computing and quantum information can be so written in terms of eight operators that form a subalgebra of the full fifteen operators that describe two spins. The Hamiltonian describing anisotropic spin exchange is an example of one such important physical problem. While isotropic spin exchange has been explored to design two-qubit gates in quantum computing, anisotropic spin exchange has been studied as a possible impediment to two-qubit gate operations [17, 48]. Such a SU(3) Hamiltonian is given by

$$\mathbf{H}(t) = J(t)(\vec{\sigma}.\vec{\tau} + \vec{\beta}(t).(\vec{\sigma} \times \vec{\tau}) + \vec{\sigma}.\mathbf{\Gamma}(t).\vec{\tau}), \tag{4.1}$$

when written in terms of a scalar, a vector and a symmetric tensor operator expressed in terms of two Pauli spins. Here, $\vec{\beta}(t)$ is the Dzyaloshinksii-Moriya vector [33, 60] and $\mathbf{\Gamma}(t)$ is the (traceless) symmetric interaction term. While the first term is the familiar Ising interaction Hamiltonian [25], the last two terms are due to spin-orbit coupling.

Given this wide applicability, a geometrical picture of the dynamics of three-level systems can be useful. For a two-level system, the geometry of the evolution operator is well known. Any density matrix can be written as $\rho = (I^{(2)} + \vec{n}.\vec{\sigma})/2$, where $\vec{\sigma}$ are the Pauli matrices. Unitary evolution of ρ is represented as the vector $\vec{n}$ rotating on the surface of the three dimensional unit sphere called the Bloch sphere [37] discussed in chapter 3. This vector, along with a phase, accounts for the three parameters describing the time evolution operator of a two-level system. The vector $\vec{n}$, along with the phase factor, is shown again in Fig. (4.1) for convenience. The vector $\vec{n}$ shown traces out the "base manifold" and together with

the global phase factor or "fiber" at each point on that manifold is referred to as a "fiber bundle" [11]. While the density matrix is independent of it, the complete description of the system requires this phase as well. The aim of this chapter is to provide an analogous geometrical picture for a three-level system with appropriate generalizations of the base and fiber.

Some work already exists regarding the geometry of SU(3). Following Wei and Norman [97], Dattoli and Torre have constructed the "Rabi matrix" for a general SU(3) unitary evolution in [29]. Mosseri and Dandoloff in [61] described the generalization of the Bloch sphere construction of single qubits to two qubits via the Hopf fibration description. This method relies upon the homomorphism between the SU(2) and SO(3) groups and likewise between the SU(4) and SO(6) groups. In [89], the authors propose a generalized Euler angle parameterization for SU(4). This decomposition is similar to the work in [68, 69, 72, 74, 75, 83, 104] into which fits our treatment of SU(3) in this chapter.

Another well known choice of the (N^2-1) generators $\mathbf{s}_j$ of the SU(N) group was studied in [28, 45]. Consider $\mathbf{s}_j$, chosen to be traceless and Hermitian such that $[\mathbf{s}_i, \mathbf{s}_j] = 2if_{ijk}\mathbf{s}_k$ and $Tr\{\mathbf{s}_i\mathbf{s}_j\} = 2\delta_{jk}$. Here, f_{ijk} is the completely antisymmetric symbol which for a two-level system is the Levi-Civita symbol ϵ_{ijk}, and a repeated index is summed over. In this basis, the Hamiltonian is written as $\mathbf{H}(t) = \Gamma_i\mathbf{s}_i$. With this choice, the Liouville-Von Neumann equation for the density matrix $\rho = \mathbf{I}/N + S_j\mathbf{s}_j/2$ becomes $\dot{S}_i = f_{ijk}\Gamma_j S_k$. Note that for the N=2 case, this is the familiar Bloch sphere representation. But, for SU(3), this representation differs from the one we present in two aspects. Firstly, the "coherence vector", whose elements are real and are given by S_j, experiences rotations in a (N^2-1) dimensional space. For instance, for SU(3), the coherence vector undergoes rotations in an eight-dimensional space. Arbitrary rotations in eight dimensions are

characterized by 28 parameters. But since a three-level Hamiltonian is only characterized by 8 real quantities, this means that the coherence vector is not permitted arbitrary rotations and is instead constrained. Secondly, the coherence vector representation does not differentiate between local and non-local operations. Our decomposition of the time evolution operator into a diagonal and an off-diagonal term in this chapter is more suited for this differentiation. Such a parameterization of the time evolution operator in terms of local and non-local operations can be useful in understanding quantum entanglement discussed in chapter 1. The aim of this chapter is to discuss the geometry of two-qubit time evolution operators in terms of such a decomposition. The authors in [34] discuss an alternative decomposition of two-qubit states in terms of two three-vectors and a 3×3 dyadic to discuss entanglement.

A series of papers presented a systematic approach to studying N-level systems using a program of unitary integration [68, 69, 72, 74, 75, 83, 90, 91, 104] as discussed in chapter 3. Continuing this program, we present a complete analytical solution to the three-level problem that generalizes the Bloch sphere approach to three levels in this chapter. Below, we define the fiber bundle via two different decompositions which allows us to extract the geometric phases associated with a three-level system (for a discussion on the quantum phases of three-level systems, see [10, 49]). These fiber bundles are $\{\mathrm{SU(3)/SU(2)}\times \mathrm{U(1)}\} \times \{\mathrm{SU(2)}\times\mathrm{U(1)}\}$ and $\{\mathrm{SU(4)/[SU(2)}\times\mathrm{SU(2)]}\} \times \{\mathrm{SU(2)}\times\mathrm{SU(2)}\}$. The structure of this chapter is as follows: Section 4.2 outlines the unitary integration program to solve time-dependent operator equations. Section 4.3 uses this technique for the solution of a general time-dependent SU(3) Hamiltonian completely analytically. Section 4.4 presents the geometry of the time evolution operator for SU(3) with some applications. Section 4.5 presents a coordinate description that is useful to define the geometric

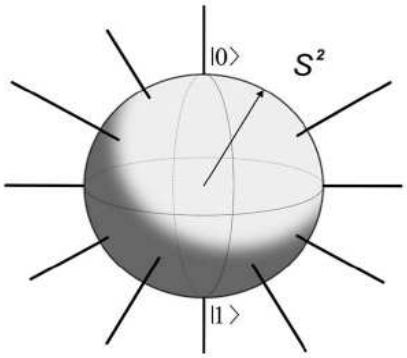

FIGURE 4.1. Bloch or Poincare sphere representation for SU(2). The base manifold is the S^2 sphere while the fiber is given by the U(1) phase at each point on that sphere. Together, we have the fiber bundle SU(2) $\simeq$ S$^2\times$U(1).

phase for three-level systems, and Section 4.6 will present an alternative analytical solution to the three-level problem by exploiting the natural embedding of SU(3) in SU(4). Section 4.7 presents the conclusions.

4.2 Unitary Integration

In the previous chapter, we discussed in detail the basic technique of unitary integration. We presented the unitary integration solution in terms of a product of two operators, namely $\tilde{U}_1$ and $\tilde{U}_2$ and presented a gauge transformation that rendered each matrix unitary. While the first matrix $\tilde{U}_1$ consisted of off-diagonal elements, the second matrix $\tilde{U}_2$ was diagonal. For $N = 3$, $n = 1$, these diagonal blocks define an SU(2)- and a U(1) Hamiltonian and $\mathbf{z}$ is a pair of complex numbers.The SU(2) Hamiltonian is in turn rendered in terms of its fiber bundle in Fig.(4.1) and the U(1) Hamiltonian corresponds to a phase. Together, they describe a four-dimensional fiber for SU(3) over the base manifold, also four dimensional, of $\mathbf{z}$.

Alternatively, $N = 3$ SU(3) problems may be conveniently seen as a part of $N = 4$ SU(4) problems, making contact with two-qubit systems that are extensively studied. In this case, for $N = 4$, $n = 2$, these diagonal blocks define two SU(2) Hamiltonians and $\mathbf{z}$ is a 2×2 matrix representable in terms of Pauli spinors.

Generally, it is 8-dimensional while the fiber has seven dimensions (two SU(2) and a mutual phase) but for the SU(3) subgroup of SU(4),both the base and manifold again reduce to four dimensions each. With $\mathbf{z}$ a pair of complex numbers, the non-trivial part of geometrizing SU(3) is thereby reduced to describing this four-dimensional manifold. Exploring this for the $N = 3$, $n = 1$ decomposition will be the content of the next section whereas Section 4.6 gives the alternative SU(4) rendering.

4.3 Geometry of General SU(3) Time Evolution Operator

A general time-dependent three-level Hamiltonian may be written in terms of eight linearly independent operators of a three-level system. Such a Hamiltonian can also be written in terms of a subgroup of 15 operators of a four-level system. Before the time evolution operator is presented in the SU(3) basis in terms of a $N = 3$, $n = 1$ decomposition, we will note that it can be rendered in a few alternative ways.

First, a general time-dependent four-level Hamiltonian may be written as $H(t) = \sum_i c_i \mathbf{O}_i$. Here c_i are time-dependent and $\mathbf{O}_i$ are the unit matrix and 15 linearly independent operators of a 4-level system that may be chosen in a variety of matrix representations. One choice used in particle physics are the so called Greiner matrices [39, 68, 74, 75, 83]. Another choice consists of using $\vec{\sigma}$, $\vec{\tau}$, $\vec{\sigma} \otimes \vec{\tau}$ and the 4×4 unit matrix. Such a choice was discussed in [69, 72] and will be used throughout this chapter. As it stands, the above Hamiltonian describes a general four-level atom with 4 energies and 6 complex couplings. Note that only the three differences in energies are important. Restricting the 15 coefficients c_i to a smaller number allows this Hamiltonian to describe various physical Hamiltonians, forming different subalgebras of the su(4) algebra [72]. For example, if two of the six complex cou-

plings are zero (levels 1 and 4 and levels 2 and 3 of a four-level atom not coupled), then the Hamiltonian may be recast such that the operators involved belong to an so(5) subalgebra [72]. On the other hand, if levels 2 and 3 are degenerate and level 4 is uncoupled from the rest, then the problem may be recast in terms of only eight operators belonging to the su(3) subalgebra of su(4). This is illustrated in Fig. 4.2 and is one of the systems of interest in this chapter.

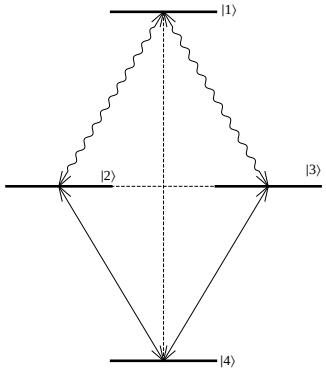

FIGURE 4.2. Levels $|2\rangle$ and $|3\rangle$ couple equally to $|1\rangle$ and to $|4\rangle$, which are themselves coupled. The three complex coupling matrix elements and two energy positions define such an SU(3) system.

Alternatively, after one arrives at the linear equation for the $N = 4$, $n = 2$ decomposition, one can represent the resulting vector in terms of six homogeneous coordinates. This is the so-called "Plücker coordinate" representation for the SU(3) Hamiltonian. These coordinates as well as the alternative derivation are presented in Section 4.6. The $N = 3$, $n = 1$ decomposition will be the content of the rest of this section.

Consider the Hamiltonian in the basis of the Gell-Mann lambda matrices [36] $H(t) = \sum_i a_i \lambda_i$. The $N = 3$, $n = 1$ decomposition consists of writing the time evolution operator in terms of a product of two matrices $U = \widetilde{U}_1 \widetilde{U}_2$ where $\widetilde{U}_1$ is composed of a (2×1)-dimensional $\mathbf{z}$, as explained in Sec. II. The equation that

governs the evolution of $\mathbf{z}$, equation (3.20), can be written in this case as

$$\dot{z}_\mu = -iV_\mu - iF_{\mu\nu}z_\nu + iV^*_\nu z_\nu z_\mu;\ \mu,\nu = 1,2. \tag{4.2}$$

Here, the symbols used in defining $\dot{\mathbf{z}}$ are defined as $V = (a_4 - ia_5, a_6 - ia_7)$, and

$$F = \begin{pmatrix} a_3 + \sqrt{3}a_8 & a_1 - ia_2 \\ a_1 + ia_2 & -a_3 + \sqrt{3}a_8 \end{pmatrix}.$$

Using the transformation equations $m_{1,2} = -z_{1,2}(De^{i\phi})^{-1}$, $m_3 = (De^{i\phi})^{-1}$ and $|m_1|^2+|m_2|^2+|m_3|^2 = 1$ leads to the evolution equation for $\vec{m} = (m_{1r}, m_{2r}, m_{3r}, m_{1i}, m_{2i}, m_{3i})^T$:

$$\dot{\vec{m}} = \begin{pmatrix} 0 & -a_2 & a_5 & a_3 + \sqrt{3}a_8 & a_1 & -a_4 \\ a_2 & 0 & a_7 & a_1 & -a_3 + \sqrt{3}a_8 & -a_6 \\ -a_5 & -a_7 & 0 & -a_4 & -a_6 & 0 \\ -a_3 - \sqrt{3}a_8 & -a_1 & a_4 & 0 & -a_2 & a_5 \\ -a_1 & a_3 - \sqrt{3}a_8 & a_6 & a_2 & 0 & a_7 \\ a_4 & a_6 & 0 & -a_5 & -a_7 & 0 \end{pmatrix} \vec{m}, \tag{4.3}$$

which describes the rotation of a unit vector in a six dimensional space of the real and imaginary parts of $\vec{m}$ defined by $m_\mu = m_{\mu r} + im_{\mu i}$. In the above equations, $D = (1 + |z_1|^2 + |z_2|^2)^{1/2}$ and $i\dot{\phi} = i(V^*_\nu z_\nu + V_\nu z^*_\nu)$. The phase ϕ is real and determined only up to a constant factor. Since the real and imaginary parts of m_3 are not independently defined, the geometrical description of the base manifold for the $N = 3$, $n = 1$ decomposition may be thought of as a point on the surface of a constrained six-dimensional unit sphere.

The two constraints, namely $|m_1|^2 + |m_2|^2 + |m_3|^2 = 1$ and the "phase arbitrariness" of ϕ, reduce the 6-dimensional manifold of the three-dimensional complex vector $\vec{m}$ to a four-dimensional manifold in agreement with there being only four independent parameters in $\mathbf{z}$.The first condition defines the base as a vector on

an S^5 sphere while the phase arbitrariness serves as an additional constraint. The fiber, on the other hand, is an SU(2) block, evolving as a vector on S^2 Poincare-like sphere with a phase at each point, and a U(1) block that amounts to an extra phase.This is presented schematically in Fig.(4.3), as the product of three matrices of the evolution operator.

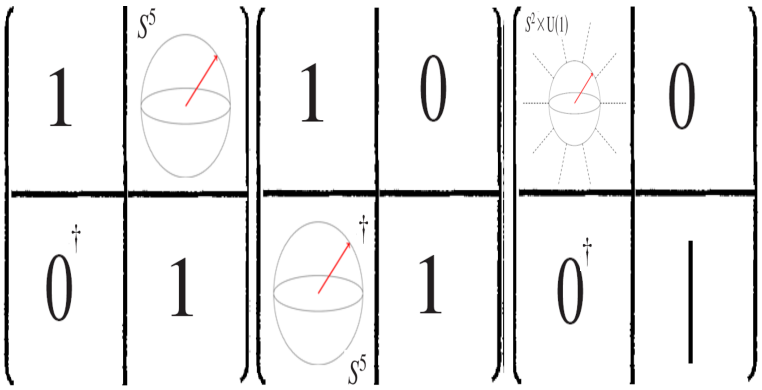

FIGURE 4.3. The base and fiber for the SU(3) group. The first two factors give the base manifold, an S^5 sphere with a phase arbitrariness defined in the text. The fiber, described by the third matrix, is composed of a Bloch sphere and a phase associated with each of its points, and the second an extra phase represented by a vertical line.

The alternative $N = 4$, $n = 2$ decomposition in the appendix yields the equation of motion for $m_\mu = -z_\mu/De^{i\phi}$ in Eq. (4.30). Following Eq. (3.25) and Eq. (3.26), we see that for this case, the two remaining blocks of the time evolution operator, namely $\widetilde{U}^{(4-2)}$ and $\widetilde{U}^{(2)}$, can be transformed into unitary matrices for SU(2). The fiber evolves as vectors on two identical S^2 Bloch-like spheres with a mutual phase, whose evolution is coupled to the base that evolves as a vector on an S^5 sphere. This is illustrated in Fig. (4.4). Either decomposition can be used to study various physical processes as will be discussed in the next section.

4.4 Applications

It is often desirable to control the time evolution of quantum states to manipulate an input state into a desirable output state. In [57, 58], the authors considered a

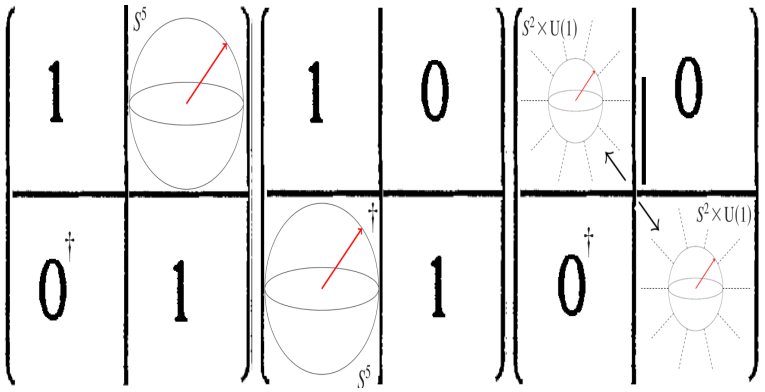

FIGURE 4.4. The base and fiber for the SU(3) group via the $N = 4, n = 2$ decomposition. The base again is given by an S^5 sphere as in Fig. (4.3). The fiber is composed of two identical SU(2) Bloch spheres plus phase, and an extra mutual phase between them. The four parameters each of base and fiber again account for all eight parameters of the SU(3).

Hamiltonian of the form $\mathbf{H}_0 - \mu\mathcal{E}(t)$, where $\mathbf{H}_0$ is a free-field Hamiltonian and $\mu\mathcal{E}(t)$ is a control field. To illustrate the "Hamiltonian encoding" scheme to control quantum systems, the authors considered a three-level system and studied stimulated Raman adiabatic passage (STIRAP), an atomic coherence effect that employs interference between quantum states to transfer population completely from a given initial state to a specific final state. This is done through a "counterintuitive" pulse sequence. Consider the Hamiltonian

$$\mathbf{H}(t) = \begin{pmatrix} 0 & G_1(t) & 0 \\ G_1(t) & 2\Delta & G_2(t) \\ 0 & G_2(t) & 0 \end{pmatrix}. \tag{4.4}$$

Here $G_{1,2}(t) = 2.5\exp[-(t - t_{1,2})^2/\tau^2]$ and $\Delta = 0.1$. The initial population is in the upper state. For $t_1 = \tau$, $t_2 = 0$ and $\tau = 3$, it is seen that the two empty states are coupled first via $G_2(t)$ and then the levels $|1\rangle$ and $|2\rangle$ are coupled through G_1. The dynamics of the populations reveal complete population transfer. A complete solution as per Section 4.3 was constructed for this model and the results are presented in Fig. 4.5 in total agreement with the results of [58].

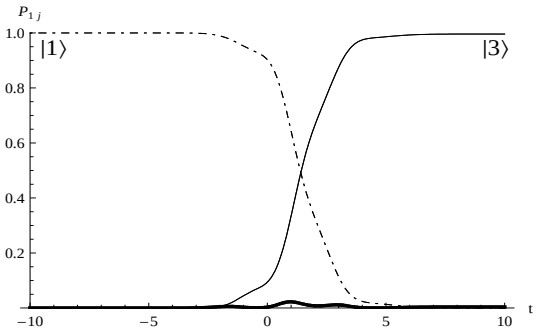

FIGURE 4.5. Population $P_{1j} = |\langle 1|j\rangle|^2$ plotted as a function of time. The initial population in state $|1\rangle$ is completely transferred to $|3\rangle$. Both the unitary integration solution and the direct numerical solution [58] are plotted and they coincide at all times.

Quantum control can also be achieved by understanding the nature of tunneling. The famous Landau-Zener-Stueckelberg formula [54, 103, 88] predicts the transition probability of the ground state of a two-level system when the energy levels adiabatically undergo a crossing. The study of level crossings has since been extended to multi-level systems. For example, in [42], the authors considered a three-level atom to study population trapping by manipulating the phase acquired as a three-level system evolves under the influence of frequency modulated fields [4]. Such a frequency modulated field is given by

$$\mathbf{E}(t) = \mathbf{E}_1 e^{-i[\omega_1 t + \varphi_1(t)]} + \mathbf{E}_2 e^{-i[\omega_2 t + \varphi_2(t)]} + c.c. \tag{4.5}$$

$$\varphi_i(t) = M_i \sin \Omega_i t. \tag{4.6}$$

Here, *c.c.* stands for complex conjugation. The phase $\varphi_i(t)$ in the exponent can be written in terms of Bessel functions as [1]

$$e^{M_j \sin \Omega_j t} = \sum_{k=-\infty}^{\infty} J_k(M_j) e^{ik\Omega_j t}. \tag{4.7}$$

For large values of Ω_j, the leading contribution for slow time scales would come from $J_0(M_j)$. Hence, for large Ω_j, the interaction Hamiltonian can be written as

$$\mathbf{H}_{int}(t) = -\mathbf{d}.(\mathbf{E}_1 J_0(M_1) + \mathbf{E}_2 J_0(M_2). \tag{4.8}$$

Hence, for values of $M_{1,2}$ that are zeros of the zeroth-order Bessel functions, the interaction Hamiltonian is zero and population trapping is observed. Under this assumption, consider the full Hamiltonian under the rotating-wave approximation,

$$\mathbf{H}(t) = \begin{pmatrix} E_1(t) & G_1(t) & 0 \\ G_1^*(t) & 0 & G_2(t) \\ 0 & G_2^*(t) & E_3(t) \end{pmatrix}.$$

Here, $E_1(t) = \Delta_1 - M_1\Omega_1\cos(\Omega_1 t + \theta)$ and $E_3(t) = -\Delta_2 + M_2\Omega_2\cos(\Omega_2 t)$. Results are presented in Fig. 4.6, and for the parameter values $\Omega_{1,2} = 1$, $\Delta_1 = -\Delta_2 = 10$, $\theta = 0$ and $G_{1,2} = 6$, demonstrate the phenomenon of population localization discussed in [42].

As a final illustration of the unitary integration technique applied to three-level systems, let us consider the example discussed in [47]. Here, a three-level system is subject to strong fields and the correlation between the scattered light spectrum and the atom dynamics is discussed. The authors consider the Hamiltonian

$$\mathbf{H}(t) = \begin{pmatrix} 0 & 0 & G_1(t) \\ 0 & 0 & G_2(t) \\ G_1^*(t) & G_2^*(t) & 0 \end{pmatrix}. \tag{4.9}$$

Here, $G_{1,2}(t) = -V_{1,2}e^{-i\delta t}$. The time evolution of the states calculated as per our procedure in Section 4.3 is plotted in Fig. 4.7 for different values of the parameters. All of these results agree with those given in [47]. Further features of the base and fiber will be presented at the end of the next section.

4.5 Geometric Phase for SU(3) Group

Many physical systems give rise to a measurable phase that does not depend directly on the dynamical equations that govern the evolution of the system, but depends only on the geometry of the path traversed by vectors characterizing the

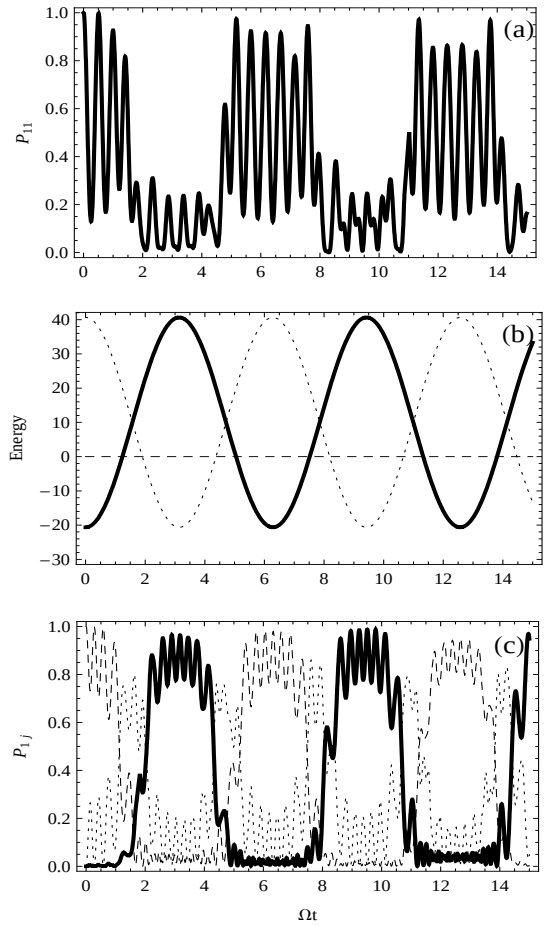

FIGURE 4.6. (a) For $M_{1,2} = 7$ and the other parameter values given in the text, there is no population trapping observed. (b) The energy landscape for $M_{1,2} = 30.6346$ showing energy level crossing. (c) Population trapping is observed with $M_{1,2} = 30.6346$ which corresponds to the tenth zero of the zeroth-order Bessel function. Note that the thick line is P_{11} and the thin line corresponds to P_{12}. The results agree completely with [42].

state of the system. This geometric phase is denoted by γ_g and is given by the integral [14],

$$\gamma_g = \int d\mathbf{R} \,.\langle n(\mathbf{R}(t))|i\nabla_{\mathbf{R}}|n(\mathbf{R}(t))\rangle, \tag{4.10}$$

where the state evolution is governed by a set of internal coordinates that parameterize the Hamiltonian $\mathbf{R}(t)$, and $\nabla_{\mathbf{R}}$ is the gradient in the space of these internal coordinates. This phase has been generalized to non-cyclic non-adiabatic evolution of quantum systems [5, 78, 99]. The purpose of this section is to present this phase

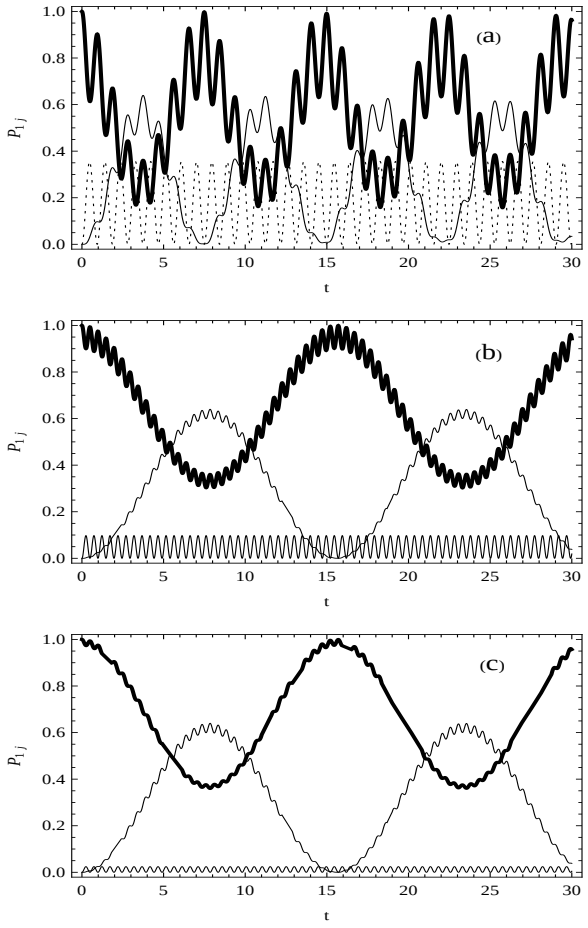

FIGURE 4.7. (a) Populations $P_{1j} = |\langle 1|j\rangle|^2$ for $\delta = 5$, $V_1 = 2$ and $V_2 = 1$. P_{11} is given by the solid line and P_{12} is given by the thin line. (b) Same as (a), for $\delta = 12$. Note that P_{13} oscillates close to zero at all times. (c) P_{1j} for $\delta = 12$, $V_1 = 1$ and $V_2 = 2$.

in terms of coordinates on the Bloch sphere for two-level systems and extend it to three-level systems.

In two-level systems, the time evolution operator is described by three parameters as described in Section 4.1. Two of these parameters describe a point on the Bloch sphere. Traversing closed loops on this Bloch sphere returns the quantum system to its initial state as described by the two parameters on the Bloch sphere but not the third parameter of an overall phase. Hence, general closed loops on the Bloch sphere do not correspond to closed loops in the space of the full unitary operator. This discrepancy in the phase between the initial and final state corresponds to the geometric phase given above and amounts to changes along the fiber at each point on the sphere. To formalize this, consider U_1, given by Eq. (3.17) as unitarized through the matrix b in Section 4.2, which for $N = 2$, $n = 1$ takes the form

$$U_1 = \frac{1}{\sqrt{1+|\mathbf{z}|^2}} \begin{pmatrix} 1 & \mathbf{z} \\ -\mathbf{z}^* & 1 \end{pmatrix}. \tag{4.11}$$

By identifying $\cos\frac{\theta}{2} = (1+|\mathbf{z}|^2)^{-\frac{1}{2}}$ and $\sin\frac{\theta}{2}e^{-i\epsilon} = -\mathbf{z}(1+|\mathbf{z}|^2)^{-\frac{1}{2}}$, we get the usual description of the base manifold in terms of the angles $0 \leq \theta < \pi$ and $0 \leq \epsilon < 2\pi$ that are associated with the Bloch sphere, namely,

$$U_1 = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2}e^{-i\epsilon} \\ \sin\frac{\theta}{2}e^{i\epsilon} & \cos\frac{\theta}{2} \end{pmatrix}. \tag{4.12}$$

In terms of the parameters θ and ϵ, the Hamiltonian $H(t) = -\vec{a}.\vec{\sigma}$ is given by

$$H(t) = \begin{pmatrix} -\cos\theta & -\sin\theta e^{-i\epsilon} \\ -\sin\theta e^{i\epsilon} & \cos\theta \end{pmatrix}. \tag{4.13}$$

Eq. (3.19) governing the evolution of the fiber U_2 has two terms. The first term is evaluated as

$$U_1^\dagger H(t) U_1 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.14}$$

which corresponds to the eigenvalues of the Hamiltonian. To evaluate the second term, consider the case whereby the vector on the Bloch sphere traverses a closed path defined by a constant θ. The second term is then given by

$$U_1^\dagger \frac{\partial U_1}{\partial(-i\epsilon)} = \begin{pmatrix} -\sin^2\frac{\theta}{2} & -\frac{1}{2}\sin\theta e^{-i\epsilon} \\ -\frac{1}{2}\sin\theta e^{i\epsilon} & \sin^2\frac{\theta}{2} \end{pmatrix}. \tag{4.15}$$

Integrating ϵ from 0 to 2π yields

$$\int_0^{2\pi} d\epsilon U_1^\dagger \frac{\partial U_1}{\partial(-i\epsilon)} = \begin{pmatrix} \pi(1-\cos\theta) & 0 \\ 0 & -\pi(1-\cos\theta) \end{pmatrix},$$

which is the correct agrees with the geometric phase of a two-level system [14].

To extend this analysis to three-level systems, we consider the $N = 3$, $n = 1$ decomposition. The matrix $U_1 = \widetilde{U}_1.b$ is now given by

$$U_1 = \begin{pmatrix} I^{(2)} - \frac{1}{D(D+1)}\mathbf{z}\mathbf{z}^\dagger & \frac{\mathbf{z}}{D} \\ -\frac{\mathbf{z}^\dagger}{D} & \frac{1}{D} \end{pmatrix}, \tag{4.16}$$

where $\mathbf{z}$ is a complex column vector $(z_1, z_2)^T$ and $D = \sqrt{1+|\mathbf{z}|^2}$. Care has to be taken in assigning angles to elements of this matrix such that the transformation satisfies two conditions: the U_1 matrix should not depend on ϕ and the transformation must be commensurate with the definition of $\vec{m}$. To this effect, we transform $\mathbf{z}$ into polar coordinates: $z_1 = -\tan\frac{\theta_1}{2}\cos\frac{\theta_2}{2}e^{i\epsilon_1}$, $z_2 = -\tan\frac{\theta_1}{2}\sin\frac{\theta_2}{2}e^{i\epsilon_2}$. These transformation equations imply that $D = \sqrt{1+|\mathbf{z}|^2} = \sec\frac{\theta_1}{2}$, $m_1 = \sin\frac{\theta_1}{2}\cos\frac{\theta_2}{2}e^{i(\epsilon_1-\phi)}$,

$m_2 = \sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}e^{i(\epsilon_2-\phi)}$ and $m_3 = \cos\frac{\theta_2}{2}e^{-i\phi}$. The U_1 matrix is given by

$$U_1 = \begin{pmatrix} 1-2\sin^2\frac{\theta_1}{4}\cos^2\frac{\theta_2}{2} & -\sin^2\frac{\theta_1}{4}\sin\theta_2 e^{i(\epsilon_1-\epsilon_2)} & -\sin\frac{\theta_1}{2}\cos\frac{\theta_2}{2}e^{i\epsilon_1} \\ -\sin^2\frac{\theta_1}{4}\sin\theta_2 e^{-i(\epsilon_1-\epsilon_2)} & 1-2\sin^2\frac{\theta_1}{4}\sin^2\frac{\theta_2}{2} & -\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}e^{i\epsilon_2} \\ \sin\frac{\theta_1}{2}\cos\frac{\theta_2}{2}e^{-i\epsilon_1} & \sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}e^{-i\epsilon_2} & \cos\frac{\theta_1}{2} \end{pmatrix} \quad (4.17)$$

In the above equation, the range on the angles $0 \leq \theta_i < \pi$ and $0 \leq \epsilon_i < 2\pi$ are chosen so that the absolute value of each element of the time-evolution operator is positive [8]. Hence U_1 can be represented as two vectors on a sphere, at angles (θ_1, ϵ_1) and (θ_2, ϵ_2) respectively. This is represented in Fig. (4.8). Since the columns

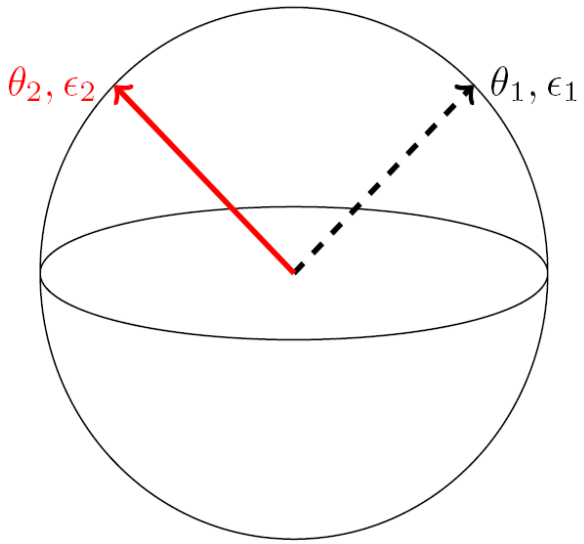

FIGURE 4.8. The base manifold U_1 is characterized by two sets of angles $0 \leq \theta_i < \pi$, $0 \leq \epsilon_i < 2\pi$ which can be represented as two vectors with polar angles (θ_1, ϵ_1) and (θ_2, ϵ_2).

of a unitary operator correspond to normalized eigenvectors, we can consider the last column of the matrix above, $|\psi\rangle = (-\sin\frac{\theta_1}{2}\cos\frac{\theta_2}{2}e^{i\epsilon_1}, -\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}e^{i\epsilon_2}, \cos\frac{\theta_1}{2})^T$, and evaluate the so-called connection 1-form given by [16]

$$\mathcal{A} = -i\langle\psi|d|\psi\rangle. \quad (4.18)$$

The Abelian geometric phase, given by $\gamma_g = \int \mathcal{A}$ is evaluated to be

$$\gamma_g = -\frac{1}{2}\int \sin^2\frac{\theta_1}{2}\left((d\epsilon_1 + d\epsilon_2) + \cos\theta_2(d\epsilon_1 - d\epsilon_2)\right). \tag{4.19}$$

If the various angles are relabelled $\epsilon_1 \rightarrow -\gamma - \alpha$, $\epsilon_2 \rightarrow -\gamma + \alpha$, $\theta_1 \rightarrow 2\theta$ and $\theta_2 \rightarrow 2\beta$, the formula above agrees with [21] and [8]. The time-evolution operator above can now be used as in the case of SU(2) to evaluate the dynamic contribution $\int U_1^\dagger H(t) U_1$ and the geometric contribution to the time evolution operator which is given by $-i\int U_1^\dagger dU_1$, where $dU_1 = \frac{dU_1}{d\theta_i}d\theta_i + \frac{dU_1}{d\epsilon_i}d\epsilon_i$, $i = 1, 2$.

This description of the base manifold in terms of (θ_i, ϵ_i) can now be used to describe the dynamics of various physical processes. Fig. (4.9) represents the base manifold corresponding to the results in Fig. (4.7). (θ_1, ϵ_1) depend on all the parameters that define the system while (θ_2, ϵ_2) depend only on the ratio V_1/V_2. Also note that the maximum value of ϵ_2, corresponding to the maximum latitude traversed by the black curve, is inversely proportional to δ. Such observations can be used to control the dynamics of this system.

4.6 Alternative Derivations for a General SU(3) Hamiltonian.

Consider a three-level Hamiltonian written in terms of the Gell-Mann matrices [36] as $H(t) = \sum_{i=1}^{8} a_i\lambda_i$. To exploit the fact that this Hamiltonian is a subgroup of four-level problems, it is represented in terms of the O matrices [72] as

$$2\frac{a_8}{\sqrt{3}}\mathbf{O}_2 + (a_3 - \frac{a_8}{\sqrt{3}})\mathbf{O}_3 + (2a_3 + 2\frac{a_8}{\sqrt{3}})\mathbf{O}_4 + a_4\mathbf{O}_5 + a_5\mathbf{O}_6 + 2a_4\mathbf{O}_7 + 2a_5\mathbf{O}_8 + a_1\mathbf{O}_9 + a_2\mathbf{O}_{10} + 2a_1\mathbf{O}_{11} + 2a_2\mathbf{O}_{12} + 2a_6\mathbf{O}_{13} + 2a_6\mathbf{O}_{14} - 2a_7\mathbf{O}_{15} + 2a_7\mathbf{O}_{16}. \tag{4.20}$$

This embeds the Hamiltonian $H(t) = \sum_i a_i\lambda_i$ as a 4×4 matrix with zeros along the last row and column. In such a representation, the various entries of the Hamil-

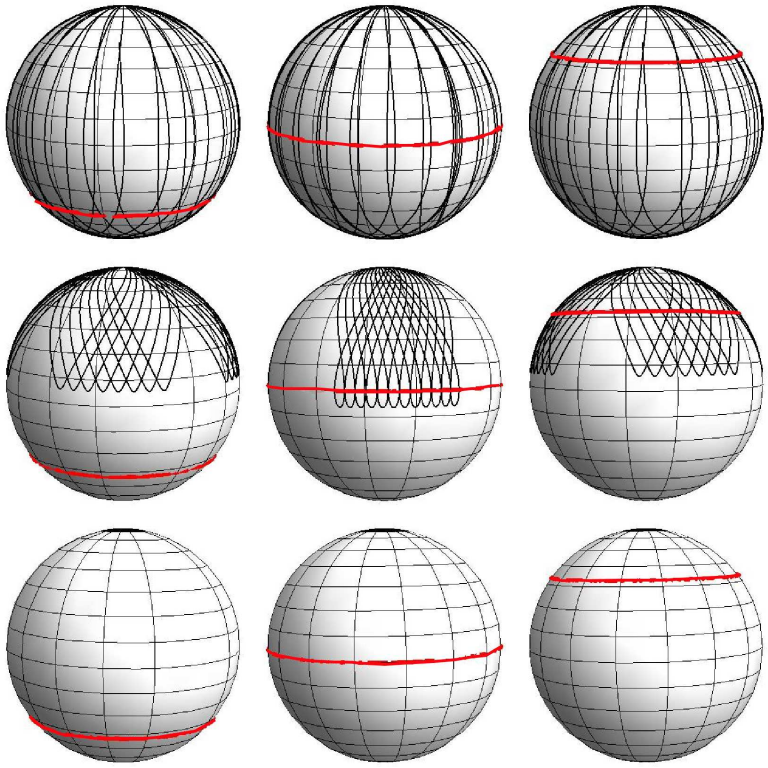

FIGURE 4.9. The base manifold corresponding to the results in Fig. (4.7) for the three--level system of [47]. For the first column, $V_1 = 1$, $V_2 = 2$. The second column corresponds to $V_1 = 2$, $V_2 = 2$ and the third to $V_1 = 2$, $V_2 = 1$. The rows correspond to $\delta = 1$, $\delta = 5$ and $\delta = 50$. The thin black curve describes (θ_1, ϵ_1) and the thick red curve the set (θ_2, ϵ_2).

tonian in Eq. (3.16) are given by

$$H^{(4-2)} = \frac{1}{\sqrt{3}} a_8 \mathbf{I}^{(2)} + a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3, \tag{4.21}$$

$$H^{(2)} = -\frac{1}{\sqrt{3}} a_8 \mathbf{I}^{(2)} - \frac{1}{\sqrt{3}} a_8\sigma_1, \tag{4.22}$$

$$\begin{aligned} \mathbf{V} = \frac{1}{2}(a_4 - ia_5)\mathbf{I}^{(2)} + \frac{1}{2}(a_6 - ia_7)\sigma_1 \\ -i\frac{1}{2}(a_6 - ia_7)\sigma_2 + \frac{1}{2}(a_4 - ia_5)\sigma_3. \end{aligned} \tag{4.23}$$

Writing $\mathbf{z}$ in the standard Clifford basis as $\mathbf{z} = \frac{1}{2} z_4 \mathbf{I}^{(2)} - \frac{i}{2} \sum_i z_i \sigma_i$, it follows from equation (3.20) that $z_1 = iz_2$ and $z_3 = iz_4$ and the equation reduces precisely to Eq. (4.2). The geometry described in Section 4.3 can thus be derived from either of these decompositions of the time evolution operator.

The SU(3) subgroup in Eq. (4.20) is one among many SU(3) subgroups embedded in SU(4). Another choice corresponds to the Dzyaloshinskii-Moriya interaction Hamiltonian [33, 60] and is also of interest because the 4×4 matrices now do not have a trivial row and column of zeros. In the two-spin basis, this Hamiltonian is given by

$$H(t) = a_1(\mathbf{O}_2 + \mathbf{O}_3) + 2a_2(\mathbf{O}_{15} + \mathbf{O}_{16}) + 2a_3(\mathbf{O}_{14} - \mathbf{O}_{13}) + 2a_4(\mathbf{O}_7 + \mathbf{O}_{11})$$
$$+a_5(\mathbf{O}_6 + \mathbf{O}_{10}) + a_6(\mathbf{O}_5 + \mathbf{O}_9) + 2a_7(\mathbf{O}_8 + \mathbf{O}_{12}) + \frac{2a_8}{\sqrt{3}}(2\mathbf{O}_4 - \mathbf{O}_{13} - \mathbf{O}_{14}). \quad (4.24)$$

The correspondence between the coefficients in terms of $\mathbf{O}$ and in terms of the λ matrices is : $c_1 = 0$, $c_2 = a_1$, $c_3 = a_1$, $c_4 = 4a_8/\sqrt{3}$, $c_5 = a_6$, $c_6 = a_5$, $c_7 = 2a_4$, $c_8 = 2a_7$, $c_9 = a_6$, $c_{10} = a_5$, $c_{11} = 2a_4$, $c_{12} = 2a_7$, $c_{13} = -2a_3 - 2a_8/\sqrt{3}$, $c_{14} = 2a_3 - 2a_8/\sqrt{3}$, $c_{15} = 2a_2$ and $c_{16} = 2a_2$. Relabeling of the states $1 \to 2$, $2 \to 3$, $3 \to 4$ and $4 \to 1$ expresses the Hamiltonian as

$$H^{(4-2)} = \frac{1}{\sqrt{3}}a_8\mathbf{I}^{(2)} - a_3\sigma_1 - a_2\sigma_2 - a_1\sigma_3, \quad (4.25)$$

$$H^{(2)} = -\frac{1}{\sqrt{3}}a_8\mathbf{I}^{(2)} - \frac{1}{\sqrt{3}}a_8\sigma_1, \quad (4.26)$$

$$\mathbf{V} = \frac{1}{2}(a_6 - ia_7)\mathbf{I}^{(2)} + \frac{1}{2}(a_6 - ia_7)\sigma_1 \quad (4.27)$$
$$-\frac{1}{2}(a_5 + ia_4)\sigma_2 - \frac{1}{2}(a_4 - ia_5)\sigma_3.$$

If $\mathbf{z}$ is written in terms of the standard Clifford basis $(\hat{\mathbf{I}}, -i\vec{\sigma})$ as $\mathbf{z} = \frac{1}{2}z_4\mathbf{I}^{(2)} - \frac{i}{2}\sum_{i=1}^{3} z_i\sigma_i$, it follows from Eq. (3.20) that $z_1 = iz_4$ and $z_2 = iz_3$. This is consistent with the parameter count that since the inhomogeneity $\mathbf{V}$ has only two free complex parameters (namely $V_1 = a_6 - ia_7$ and $V_2 = a_4 - ia_5$), the complex $\mathbf{z}$ matrix should be composed only of two independent complex parameters, z_1 and z_2. With the above analysis, equation (3.20) becomes for the pair of complex numbers

$$\frac{1}{2}\dot{z}_\mu = \frac{1}{2}X_\mu - iF_{\mu\nu}z_\nu + 2G_\nu z_\nu z_\mu;\ \mu, \nu = 1, 2. \quad (4.28)$$

Here $X = (V_1/2, -iV_2/2)$, $G = (2V_1^*, 2iV_2^*)$ and

$$-iF = \begin{pmatrix} ia_3 - \sqrt{3}ia_8 & a_1 + ia_2 \\ -a_1 + ia_2 & -ia_3 - \sqrt{3}ia_8 \end{pmatrix}.$$

Paralleling the technique employed to solve an SO(5) Hamiltonian in [90, 91], we transform $\mathbf{z}$ into a complex vector $\vec{m}$: $m_\mu = \frac{-2z_\mu e^{i\phi}}{D}$ and $m_3 = \frac{e^{i\phi}}{D}$ such that $|m_1|^2 + |m_2|^2 + |m_3|^2 = 1$,with $D = (1 + 4(|z_1|^2 + |z_2|^2))^{1/2}$. This leads to the new set of evolution equations

$$\dot{\vec{m}} = \begin{pmatrix} ia_3 - \sqrt{3}ia_8 & a_1 + ia_2 & -a_6 + ia_7 \\ -a_1 + ia_2 & -ia_3 - \sqrt{3}ia_8 & a_5 + ia_4 \\ a_6 + ia_7 & -a_5 + ia_4 & 0 \end{pmatrix} \vec{m}. \tag{4.29}$$

This can be written as an equation describing the rotation of the real and imaginary components of the vector $\vec{m} = (m_{1r}, m_{2r}, m_{3r}, m_{1i}, m_{2i}, m_{3i})^T$,

$$\dot{\vec{m}} = \begin{pmatrix} 0 & a_1 & -a_6 & -a_3 + \sqrt{3}a_8 & -a_2 & -a_7 \\ -a_1 & 0 & a_5 & -a_2 & a_3 + \sqrt{3}a_8 & -a_4 \\ a_6 & -a_5 & 0 & -a_7 & -a_4 & 0 \\ a_3 - \sqrt{3}a_8 & a_2 & a_7 & 0 & a_1 & -a_6 \\ a_2 & -a_3 - \sqrt{3}a_8 & a_4 & -a_1 & 0 & a_5 \\ a_7 & a_4 & 0 & a_6 & -a_5 & 0 \end{pmatrix} \vec{m}. \tag{4.30}$$

Here, the coefficients c_i are written in terms of the coefficients a_i, whose correspondence was given earlier in this section. Also note that $m_\mu = m_{\mu r} + i m_{\mu i}$, $D = (1+|z_1|^2+|z_2|^2)^{\frac{1}{2}}$ and $\dot{\phi} = (V_\nu^* z_\nu + V_\nu z_\nu^*)$. Simplifying this leads to the equation $i\dot{\phi} = -2(X_\mu z_\mu^* - X_\mu^* z_\mu)$ for the evolution of ϕ which is clearly real but determined only to within a constant. A little algebra yields for the effective Hamiltonian given by equation (3.25),

$$H^{(4-2)} - \frac{1}{(D+1)}(\mathbf{z}\mathbf{V}^\dagger + \mathbf{V}\mathbf{z}^\dagger) - \frac{1}{2(D+1)^2}(\mathbf{z}\mathbf{V}^\dagger\mathbf{z}\mathbf{z}^\dagger + \mathbf{z}\mathbf{z}^\dagger\mathbf{V}\mathbf{z}^\dagger),$$

and for the effective Hamiltonian given by equation (3.26), the expression $H^{(2)} + (\mathbf{z}^\dagger\mathbf{V} + \mathbf{V}^\dagger\mathbf{z})/2$.

Another representation of the SU(3) subgroup of SU(4) Hamiltonians is given by the so called "Plücker coordinate" representation of the SU(4) group discussed in

[90, 91]. For an arbitrary SU(4) matrix, the Plücker coordinates are defined as a set of six parameters $(P_{12}, P_{13}, P_{14}, P_{23}, P_{24}, P_{34})$ such that $P_{12}P_{34} - P_{13}P_{24} + P_{14}P_{23} = 0$ and $\sum |P_{ij}|^2 = 1$. They can be written in terms of the unit vector $\vec{m}$ and are given by

$$\begin{pmatrix} P_{12} \\ P_{13} \\ P_{14} \\ P_{23} \\ P_{24} \\ P_{34} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} im_6 - m_5 \\ im_1 + m_2 \\ -im_3 + m_4 \\ -im_3 - m_4 \\ -im_1 + m_2 \\ im_6 + m_5 \end{pmatrix}. \tag{4.31}$$

The linear equation of motion for $\vec{m}$ translates into an evolution equation for $\mathbf{P} = (P_{12}, -P_{13}, P_{14}, P_{23}, P_{24}, P_{34})$ of the form $i\dot{\mathbf{P}} = \mathbf{H}_P\mathbf{P}$. Here, $\mathbf{H}_P$ is given by

$$\mathbf{H}_P = \begin{pmatrix} \mathbf{H}_{P1} & \mathbf{V}_P \\ \mathbf{V}_P^\dagger & \mathbf{H}_{P2} \end{pmatrix}, \tag{4.32}$$

where

$$\mathbf{H}_{P1} = \begin{pmatrix} 2a_8/\sqrt{3} & a_{64-} + ia_{75-} & a_{64-} + ia_{75-} \\ a_{64-} - ia_{75-} & -a_1 & a_8/\sqrt{3} \\ a_{64-} - ia_{75-} & a_8/\sqrt{3} & -a_1 \end{pmatrix},$$

$$\mathbf{H}_{P2} = \begin{pmatrix} a_1 & -a_8/\sqrt{3} & -a_{64-} - ia_{75-} \\ -a_8/\sqrt{3} & a_1 & -a_{64-} - ia_{75-} \\ -a_{64-} + ia_{75-} & -a_{64-} + ia_{75-} & -2a_8/\sqrt{3} \end{pmatrix},$$

$$\mathbf{V}_P = \begin{pmatrix} -a_{64+} - ia_{75+} & a_{64+} + ia_{75+} & 0 \\ a_{32-} & 0 & -a_{64+} - ia_{75+} \\ 0 & -a_{32-} & a_{64+} - ia_{75+} \end{pmatrix}.$$

In the above equation, $a_{ij\pm}$ denotes $a_i \pm a_j$.

4.7 Conclusions

The ability to decouple the time dependence of operator equations from the non-commuting nature of the operators is the central feature of unitary integration and also characterizes the Bloch sphere representation for the evolution of a single spin. By doing so, the quantum-mechanical evolution is rendered a "classical" picture of a rotating unit vector. For a two-level atom, the Bloch sphere representation along with a phase completely determines the time evolution operator. In this chapter, we have extended this program to deal with the time evolution operator belonging to the SU(3) group. This complements the work in [90] for SU(4) Hamiltonians of two-qubit systems. We have also extended the analysis of geometric phase to three-level systems by providing an explicit coordinate representation for the SU(3) time evolution operator.

Chapter 5
X States for Two Qubits

"There is no royal road to geometry."

Euclid of Alexandria
(325BCE-265BCE)

5.1 Introduction

In Chapters 2-4, we focused on a technique to solve for the evolution operator for N-level systems with a special emphasis on three-level systems. This technique focussed only on operators (specifically, the evolution operator) and the states were evolved from an initial state to a final state according to the prescription outlined in Chapter 4.1. The algebra of the operators played an important role in establishing the unitary integration solution. The geometry of the operators involved the parameters that defined a general unitary operator. In this chapter, we will study a special class of two-qubit quantum states called X states. We will present some motivation and discuss some earlier work that exists relating to the calculation of entanglement in these states. Then, we will analyze these states in terms of their algebraic properties and present an algebraic characterization of X states. Furthermore, we will discuss a geometric representation of the operator algebra that characterizes two-qubit X states. Finally we present some connections to octonions and some concluding remarks.

5.2 Two Qubit X States

Consider a two-qubit system given in Fig. (5.1). Besides the three energy differences that define the relative energy scales of the four states, there are six complex

couplings that determine the Hamiltonian. Since a quantum state is strongly influ-

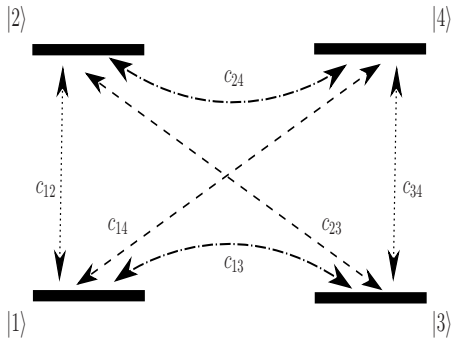

FIGURE 5.1. Diagram representing the different couplings for two interacting qubits. Three non-zero energies along with six complex couplings presented in the diagram define the fifteen real parameters that define an arbitrary two-qubit Hamiltonian. Note that some of these couplings are always zero because of selection rules.

enced by the symmetry of the Hamiltonian that drives it, let us consider these six complex couplings. Quantum mechanical selection rules are a set of rules derived from symmetry that constrain transitions between quantum states. These selection rules can be used to infer that some of these six couplings are always zero. To explain this, assume that the Hamiltonian physically represents a set of magnetic fields coupling to magnetic dipoles and that we consider two identical physical systems as qubits. The selection rule for such magnetic dipole transitions state that a transition is only allowed when the states involved differ in their parity. Let us also assume that states $|1\rangle$ and $|2\rangle$ differ in their parity and likewise $|3\rangle$ and $|4\rangle$. Under these assumptions, the transitions related to the coefficients c_{12}, c_{34}, c_{14} and c_{41} are non-zero. But now this means that $|1\rangle$ and $|3\rangle$ share the same parity and likewise $|2\rangle$ and $|4\rangle$.The corresponding coefficients c_{13} and c_{24} are hence zero. Finally, we assume that $c_{12} = c_{34} = 0$[1]. This simple argument based on selection rules implies

[1]in fact this too is not the most general case. General symmetry conditions would imply that $c_{12} = c_{34}$ and $c_{14} = c_{23}$. The parameter count then adds up to seven for a general non-degenrate two-qubit system.

that a fairly general two-qubit state is characterized by three energy differences and two complex couplings, a total of seven parameters. Such a Hamiltonian can be written as

$$\mathbf{H}(t) = \begin{pmatrix} E_{11} & 0 & 0 & c_{14} \\ 0 & E_{22} & c_{23} & 0 \\ 0 & c_{23}^* & E_{33} & 0 \\ c_{14}^* & 0 & 0 & E_{44} \end{pmatrix}. \tag{5.1}$$

If the initial density matrix is a product state[2], then the most general density matrix that describes the state of this system is given by

$$\rho = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{14} \\ 0 & \rho_{22} & \rho_{23} & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} \end{pmatrix}, \tag{5.2}$$

with $\rho_{ij} = \rho_{ji}^*$, $\mathsf{Tr}(\rho) = 1$ and $\mathsf{Tr}(\rho) \leq 1$. This density matrix is determined by seven parameters and the structure of the density matrix is related to the fact that a Hamiltonian's symmetry group strongly influences the symmetry group of the density matrix at all times[3]. Since the density matrix resembles the letter X, such a state is called an X state.

Let us consider another example which gives rise to X states. Consider a spin chain [79] evolving under some generic Hamiltonian. Let the symmetric ground state of this system, which has the same symmetry as the Hamiltonian, be given by the density matrix ρ. Now, if we wish to study any two spins with labels i and j, and if the reduced density matrix of these two spins is given by ρ_{ij}, then this

[2]this is a special case of a more general condition that we will discuss below.

[3]Indeed these symmetry groups are identical if the initial density matrix belongs in the same symmetry group as the Hamiltonian.

density matrix can be written as

$$\rho_{ij} = \begin{pmatrix} \langle P_i^+ P_j^+ \rangle & \langle P_i^+ \sigma_j^- \rangle & \langle \sigma_i^- P_j^+ \rangle & \langle \sigma_i^- \sigma_j^- \rangle \\ \langle P_i^+ \sigma_j^+ \rangle & \langle P_i^+ P_j^- \rangle & \langle \sigma_i^- \sigma_j^+ \rangle & \langle \sigma_i^- P_j^- \rangle \\ \langle \sigma_i^+ P_j^+ \rangle & \langle \sigma_i^+ \sigma_j^- \rangle & \langle P_i^- P_j^+ \rangle & \langle P_i^- \sigma_j^- \rangle \\ \langle \sigma_i^+ \sigma_j^+ \rangle & \langle \sigma_i^+ P_j^- \rangle & \langle P_i^- \sigma_j^+ \rangle & \langle P_i^- P_j^- \rangle \end{pmatrix}. \tag{5.3}$$

Here $P_i^{\pm} = (I \pm \sigma_{3,i})/2$, $\sigma_i^{\pm} = (\sigma_{1,i} \pm \sigma_{2,i})/2$ and each element of the density matrix represents the expectation value of of the operator indicated. For instance, $\langle \sigma_i^- P_j^- \rangle$ is given by

$$\langle \sigma_i^- P_j^- \rangle = \mathsf{Tr}\{\rho I \otimes I \cdots \sigma_i^- \otimes I \cdots P_j^- \otimes I \cdots\}. \tag{5.4}$$

Now assuming that the Hamiltonian under which the system evolves is symmetric under the transformation $\sigma_{1,2} \to -\sigma_{1,2}$, which amounts to a π rotation about the z-axis, we see that $P_i^{\pm} \to P_j^{\pm}$ and $\sigma_j^{\pm} \to -\sigma_j^{\pm}$. Since the reduced density matrix is also invariant under this transformation, the off-diagonal terms with a single $\sigma_{i,j}^{\pm}$ are zero and we get,

$$\rho_{ij} = \begin{pmatrix} \langle P_i^+ P_j^+ \rangle & 0 & 0 & \langle \sigma_i^- \sigma_j^- \rangle \\ 0 & \langle P_i^+ P_j^- \rangle & \langle \sigma_i^- \sigma_j^+ \rangle & 0 \\ 0 & \langle \sigma_i^+ \sigma_j^- \rangle & \langle P_i^- P_j^+ \rangle & 0 \\ \langle \sigma_i^+ \sigma_j^+ \rangle & 0 & 0 & \langle P_i^- P_j^- \rangle \end{pmatrix}. \tag{5.5}$$

Examples of Hamiltonians invariant under such transformations include

$$\mathbf{H}(t) = -\sum_{\langle i,j \rangle} (\sigma_{1,i}\sigma_{1,j}) + h_z \sum_i \sigma_{3,i} \tag{5.6}$$

$$\mathbf{H}(t) = -\sum_{\langle i,j \rangle} (\sigma_{1,i}\sigma_{1,j} + \sigma_{2,i}\sigma_{2,j}) + \Delta\sigma_{3,i}\sigma_{3,j}. \tag{5.7}$$

The first is the Hamiltonian of the so-called transverse Ising model and the second is the Hamiltonian for the XXZ model [77]. We note that $\langle i, j \rangle$ stands for summation over nearest neighbors.

Having motivated the density matrix, let us look at some correlation properties of Eq. (5.2) by looking at specific examples. An example of two-qubit X states are the Bell states. These states are maximally entangled states and are given by

$$|\Phi^+\rangle\langle\Phi^+| = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 1 \end{pmatrix}, \tag{5.8}$$

$$|\Phi^-\rangle\langle\Phi^-| = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}, \tag{5.9}$$

$$|\Psi^+\rangle\langle\Psi^+| = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & +1 & 0 \\ 0 & +1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{5.10}$$

$$|\Psi^-\rangle\langle\Psi^-| = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{5.11}$$

The maximally mixed state $\rho = I/4$ is also an example of an X state. Werner states, a single parameter family of states are defined as $\rho = (1-p)I/4+p|\Psi^+\rangle\langle\Psi^+|$. These states are known to be entangled for $p > 1/3$. Furthermore, a measure of quantum correlations that is different than entanglement, namely discord, varies smoothly from 0 to 1 as p is varied from 0 to 1 [6]. Bell diagonal states, defined as $\rho = x|\Psi^+\rangle\langle\Psi^+| + y|\Psi^-\rangle\langle\Psi^-| + z|\Phi^+\rangle\langle\Phi^+| + (1-x-y-z)|\Phi^-\rangle\langle\Phi^-|$, is a three-

parameter family of states whose correlation properties have been studied before. These are clearly a three-parameter subset of X states.

Hence X states serve to describe fairly general correlation properties. When entanglement is studied, X states vary from maximally entangled states to maximally mixed states. X states also have been shown to exhibit fairly general behavior in terms of quantum discord.

5.3 Algebraic Characterization of Two-Qubit X States

Once again, let us consider the two qubit X state, given by Eq. (5.2). Such a state can be written in terms of the standard two-qubit Pauli basis as

$$\rho = \frac{1}{4}(I + \sum_{i=1}^{7} g_i \mathbf{X}_i). \tag{5.12}$$

Here, the operators $\mathbf{X}_1 = \sigma_3\tau_3$, $\mathbf{X}_2 = \sigma_2\tau_1$, $\mathbf{X}_3 = \tau_3$, $\mathbf{X}_4 = -\sigma_2\tau_2$, $\mathbf{X}_5 = \sigma_1\tau_2$, $\mathbf{X}_6 = \sigma_3$ and $\mathbf{X}_7 = \sigma_1\tau_1$. It is convenient to also define $\mathbf{X}_0 = I$. The coefficients g_i are related to the elements of the density matrix ρ_{ij} and are explicitly given by

$$g_1 = (\rho_{11} + \rho_{44}) - (\rho_{22} + \rho_{33}), \tag{5.13}$$

$$g_2 = 2i(\rho_{14} - \rho_{41}) + 2i(\rho_{32} - \rho_{23}), \tag{5.14}$$

$$g_3 = (\rho_{11} - \rho_{44}) - (\rho_{22} - \rho_{33}), \tag{5.15}$$

$$g_4 = 2(\rho_{14} + \rho_{41}) - 2(\rho_{32} + \rho_{23}), \tag{5.16}$$

$$g_5 = 2i(\rho_{14} - \rho_{41}) - 2i(\rho_{32} - \rho_{23}), \tag{5.17}$$

$$g_6 = (\rho_{11} - \rho_{44}) + (\rho_{22} - \rho_{33}), \tag{5.18}$$

$$g_7 = 2(\rho_{14} + \rho_{41}) + 2(\rho_{32} + \rho_{23}). \tag{5.19}$$

These seven operators are closed both under multiplication and commutation. The multiplication(Clifford[4]) table is given by table (5.1),

[4]William Clifford(1845-1879)

TABLE 5.1. Multiplication (Clifford) table for su(2)×u(1)×su(2).

$*$	$\mathbf{X}_0$	$\mathbf{X}_1$	$\mathbf{X}_2$	$\mathbf{X}_3$	$\mathbf{X}_4$	$\mathbf{X}_5$	$\mathbf{X}_6$	$\mathbf{X}_7$
$\mathbf{X}_0$	$\mathbf{X}_0$	$\mathbf{X}_1$	$\mathbf{X}_2$	$\mathbf{X}_3$	$\mathbf{X}_4$	$\mathbf{X}_5$	$\mathbf{X}_6$	$\mathbf{X}_7$
$\mathbf{X}_1$	$\mathbf{X}_1$	$\mathbf{X}_0$	$\mathbf{X}_5$	$\mathbf{X}_6$	$\mathbf{X}_7$	$\mathbf{X}_2$	$\mathbf{X}_3$	$\mathbf{X}_4$
$\mathbf{X}_2$	$\mathbf{X}_2$	$\mathbf{X}_5$	$\mathbf{X}_0$	$i\mathbf{X}_4$	$-i\mathbf{X}_3$	$\mathbf{X}_1$	$i\mathbf{X}_7$	$-i\mathbf{X}_6$
$\mathbf{X}_3$	$\mathbf{X}_3$	$\mathbf{X}_6$	$-i\mathbf{X}_4$	$\mathbf{X}_0$	$i\mathbf{X}_2$	$-i\mathbf{X}_7$	$\mathbf{X}_1$	$i\mathbf{X}_5$
$\mathbf{X}_4$	$\mathbf{X}_4$	$\mathbf{X}_7$	$i\mathbf{X}_3$	$-i\mathbf{X}_2$	$\mathbf{X}_0$	$i\mathbf{X}_6$	$-i\mathbf{X}_5$	$\mathbf{X}_1$
$\mathbf{X}_5$	$\mathbf{X}_5$	$\mathbf{X}_2$	$\mathbf{X}_1$	$i\mathbf{X}_7$	$-i\mathbf{X}_6$	$\mathbf{X}_0$	$i\mathbf{X}_4$	$-i\mathbf{X}_3$
$\mathbf{X}_6$	$\mathbf{X}_6$	$\mathbf{X}_3$	$-i\mathbf{X}_7$	$\mathbf{X}_1$	$i\mathbf{X}_5$	$-i\mathbf{X}_4$	$\mathbf{X}_0$	$i\mathbf{X}_2$
$\mathbf{X}_7$	$\mathbf{X}_7$	$\mathbf{X}_4$	$i\mathbf{X}_6$	$-i\mathbf{X}_5$	$\mathbf{X}_1$	$i\mathbf{X}_3$	$-i\mathbf{X}_2$	$\mathbf{X}_0$

while the commutator (Lie) table is given by table (5.2).

TABLE 5.2. Commutation (Lie) table for su(2)×u(1)×su(2).

$[\ ,\ ]$	$\mathbf{X}_0$	$\mathbf{X}_1$	$\mathbf{X}_2$	$\mathbf{X}_3$	$\mathbf{X}_4$	$\mathbf{X}_5$	$\mathbf{X}_6$	$\mathbf{X}_7$
$\mathbf{X}_0$	0	0	0	0	0	0	0	0
$\mathbf{X}_1$	0	0	0	0	0	0	0	0
$\mathbf{X}_2$	0	0	0	$2i\mathbf{X}_4$	$-2i\mathbf{X}_3$	0	$2i\mathbf{X}_7$	$-2i\mathbf{X}_6$
$\mathbf{X}_3$	0	0	$-2i\mathbf{X}_4$	0	$2i\mathbf{X}_2$	$-2i\mathbf{X}_7$	0	$2i\mathbf{X}_5$
$\mathbf{X}_4$	0	0	$2i\mathbf{X}_3$	$-2i\mathbf{X}_2$	0	$2i\mathbf{X}_6$	$-2i\mathbf{X}_5$	0
$\mathbf{X}_5$	0	0	0	$2i\mathbf{X}_7$	$-2i\mathbf{X}_6$	0	$2i\mathbf{X}_4$	$-2i\mathbf{X}_3$
$\mathbf{X}_6$	0	0	$-2i\mathbf{X}_7$	0	$2i\mathbf{X}_5$	$-2i\mathbf{X}_4$	0	$2i\mathbf{X}_2$
$\mathbf{X}_7$	0	0	$2i\mathbf{X}_6$	$-2i\mathbf{X}_5$	0	$2i\mathbf{X}_3$	$-2i\mathbf{X}_2$	0

Besides $\mathbf{X}_0 = I($ which commutes trivially with any operator), one operator namely $\mathbf{X}_1$ commutes with all other operators. This implies that the seven operators that characterize the two-qubit X state are closed under a su(2)×u(1)×su(2) algebra with $\mathbf{X}_1$ serving as the u(1) element. Once we have understood the algebraic characterization of the operators that define the X state, we can generalize the definition of two-qubit X state as a state characterized not by these seven specific operators, but by the sub-algebra of su(4) namely su(2)×u(1)×su(2). Each family of X states is now characterized by the commuting element. This definition yields many different types of X states with distinct correlation properties. In fact, each of the fifteen operators that form the two-qubit Pauli basis commutes with

six other operators. Thus, there are fifteen distinct su(2)×u(1)×su(2) sub-algebras in su(4), each characterized by the operator that forms the commuting element. For the reminder of this section, we will consider examples of two-qubit X states that differ from the one presented in Eq. (5.2).

An alternative set of seven operators that close under the su(2)×u(1)×su(2) sub-algebra of su(4) are given by $\mathbf{X}_1 = \sigma_1\tau_1$, $\mathbf{X}_2 = \sigma_3\tau_2$, $\mathbf{X}_3 = \tau_1$, $\mathbf{X}_4 = -\sigma_3\tau_3$, $\mathbf{X}_5 = \sigma_2\tau_3$, $\mathbf{X}_6 = \sigma_1$ and $\mathbf{X}_7 = \sigma_2\tau_2$. This sub-algebra is characterized by $\mathbf{X}_1$ as the commuting element and represents another X state, given by Eq. (5.12), written explicitly as

$$\rho = \frac{1}{4}\begin{pmatrix} 1-g_4 & g_3-ig_2 & g_6-ig_5 & g_1-g_7 \\ g_3+ig_2 & 1+g_4 & g_1+g_7 & g_6+ig_5 \\ g_6+ig_5 & g_1+g_7 & 1+g_4 & g_3+ig_2 \\ g_1-g_7 & g_6-ig_5 & g_3-ig_2 & 1-g_4 \end{pmatrix}. \tag{5.20}$$

Another example is given by the set of operators σ_3, $\vec{\tau}$ and $\sigma_3 \otimes \vec{\tau}$. These seven operators yield a density matrix that is block diagonal and looks explicitly like

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} & 0 & 0 \\ \rho_{21} & \rho_{22} & 0 & 0 \\ 0 & 0 & \rho_{33} & \rho_{34} \\ 0 & 0 & \rho_{43} & \rho_{44} \end{pmatrix}. \tag{5.21}$$

Hence X states can have either all of the elements of the density matrix being non-zero or can have their non-zero elements present not just along the diagonal and the anti-diagonal of the density matrix.

We will conclude this section by briefly presenting an abstract interferometric scheme to generate two-qubit X states from two copies of arbitrary density matrix ρ. In the above examples, the commuting element was given by $\mathbf{X}_1$. This

operator commutes with the seven operators (including itself) that are in the su(2)×u(1)×su(2) sub-algebra and anticommutes with the other 8. This means that the operation $\mathbf{X}\rho\mathbf{X}^\dagger$ will switch the sign of those elements of the density matrix that are not in the sub-algebra. Hence the combination $(\rho + \mathbf{X}\rho\mathbf{X}^\dagger)/2$ represents a prescription that adds to ρ, a unitarily transformed copy of itself to yield an X state.

5.4 Algebra of X States and Projective Geometry

Consider once more, the sub-algebra su(2)×u(1)×su(2) of su(4). The seven operators involved close both under commutation and multiplication and the corresponding tables were presented in the last section. In this section, we will present a compact way to represent this algebra in terms of seven points and seven lines. These seven points correspond to the seven operators in the sub-algebra whereas each of the seven lines connect three operators and represent both their multiplication and commutation tables in a compact way. Such a diagram is presented in Fig. (5.2) below. Note that the circle inscribed in the triangle is taken to be a "line" as well. Each line with an arrow is used to represent the rule that product of any two operators is the third operator, while if the order of the product is taken against the arrow, the third operator is accompanied by a minus sign. The figure represented above, without the arrows, is the finite projective plane with the smallest number of points and lines possible and is called a Fano[5] plane. A projective plane is a set of lines and points such that any two lines meet at a point, any two points are connected by a unique line and that there exist at least four points, no three of them that belong on the same line. The number of points equals

[5]Gino Fano(1871-1952)

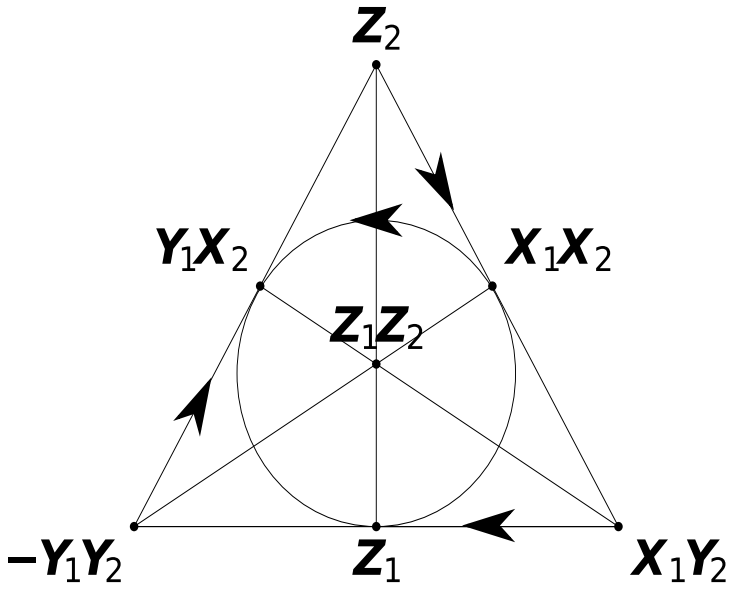

FIGURE 5.2. The multiplication and commutation table of the su(2)×u(1)×su(2) sub--algebra represented diagrammatically using seven points and seven lines.The product of any two operators connected by a line is the third operator. When the line is arrowed, the product of any two operators is represented by ±1 times the third operator, +1 being assigned along the arrow. The commutator is simply worked out from this rule. The order of operation does not matter when the lines are not arrowed. Hence, these operators commute and the commutator of any two operators is zero. The figure with seven lines and seven points presented is called a Fano plane. Note that $\sigma_1\tau_2$ is represented as $\mathbf{X}_1\mathbf{Y}_2$ in the diagram for clarity.

the number of lines for a finite projective plane geometry. This number is given by $1 + n + n^2$ where n is called the order of the finite projective plane geometry [24]. The smallest such diagram has seven lines and points and is said to be a finite projective plane of order 2(since $1 + 2 + 2^2 = 7$). This figure allows calculations such as partial transposition (used to compute negativity) and the product $\rho\sigma_2\tau_2\rho^*$ (used to compute concurrence) to be performed by inspection. We emphasize again that the diagram represents multiplication and commutation relations of a set of seven operators that are closed under the su(2)×u(1)×su(2) and hence represents many families of X states, each characterized by their commuting elements.

Finally, we note that the connection between finite geometry and algebra is a well established one. For instance, the non-associative non-commuting extension

TABLE 5.3. Multiplication (Clifford) table for octonions.

$*$	$\mathbf{e}_1$	$\mathbf{e}_2$	$\mathbf{e}_3$	$\mathbf{e}_4$	$\mathbf{e}_5$	$\mathbf{e}_6$	$\mathbf{e}_7$
$\mathbf{e}_1$	-1	$\mathbf{e}_4$	$\mathbf{e}_7$	$-\mathbf{e}_2$	$\mathbf{e}_6$	$-\mathbf{e}_5$	$-\mathbf{e}_3$
$\mathbf{e}_2$	$-\mathbf{e}_4$	-1	$\mathbf{e}_5$	$\mathbf{e}_1$	$-\mathbf{e}_3$	$\mathbf{e}_7$	$-\mathbf{e}_6$
$\mathbf{e}_3$	$-\mathbf{e}_7$	$-\mathbf{e}_5$	-1	$\mathbf{e}_6$	$\mathbf{e}_2$	$-\mathbf{e}_4$	$\mathbf{e}_1$
$\mathbf{e}_4$	$\mathbf{e}_2$	$-\mathbf{e}_1$	$-\mathbf{e}_6$	-1	$\mathbf{e}_7$	$\mathbf{e}_3$	$-\mathbf{e}_5$
$\mathbf{e}_5$	$-e_6$	$\mathbf{e}_3$	$-\mathbf{e}_2$	$-\mathbf{e}_7$	-1	$\mathbf{e}_1$	$\mathbf{e}_4$
$\mathbf{e}_6$	$\mathbf{e}_5$	$-\mathbf{e}_7$	$\mathbf{e}_4$	$-\mathbf{e}_3$	$-\mathbf{e}_1$	-1	$\mathbf{e}_2$
$\mathbf{e}_7$	$\mathbf{e}_3$	$\mathbf{e}_6$	$-\mathbf{e}_1$	$\mathbf{e}_5$	$-\mathbf{e}_4$	$-\mathbf{e}_2$	-1

of the algebra of quaternions are known as octonions. Octonions [9] are the last of the so-called "consistent arithmetics", the other three being reals, complex numbers and quaternions. While reals and complex numbers are ubiquitous in physics, quaternions have proven useful in discussing classical physics and quantum mechanics. Octonions are somewhat less used in physics. There are seven of them and are denoted by $\mathbf{e}_1 - \mathbf{e}_7$ and their multiplication table is given in table (5.3). These operators can be represented in terms of a Fano plane as well, but owing to the symmetry of all octonions, all lines are now arrowed. Such a diagram is represented in Fig. (5.3).

5.5 Conclusions

In this chapter, we introduced a family of states called X states. Bell states, Werner states and Bell-diagonal states are examples of two-qubit X states. These states were physically motivated in a variety of contexts from spin chains to atomic physics. We analyzed the algebra of a set of operators that were used as a basis to write these states. This algebra was shown to be the su(2)×u(1)×su(2) sub-algebra of su(4). Furthermore, we noted that both the multiplication and commutation tables for this sub-algebra can be represented diagrammatically in terms of seven lines and seven points. This diagram involving seven lines and seven points is a finite projective plane with the smallest number of points (and lines) and is known

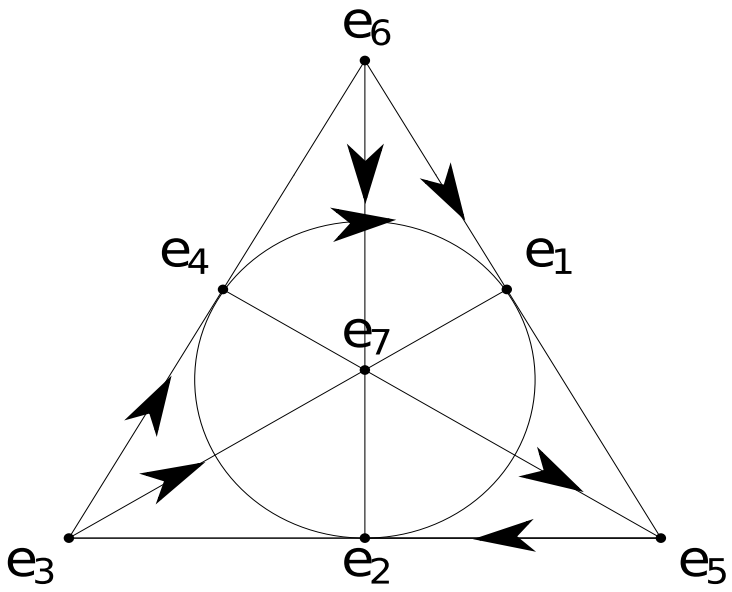

FIGURE 5.3. The multiplication table of octonions represented diagrammatically using seven points and seven lines, with arrows on each line to indicate that when two octonions are considered such that they run along the arrow on a line, their product is the third octonion on the line. When the order of the product runs against the arrow, a minus sign accompanies the product, which is the third octonion on the line. The figure with seven lines and seven points presented is called a Fano plane.

as a Fano plane. Finally, we noted that this connection between algebra and finite geometry is a well known one and presented a related example of presenting the algebra of octonions in terms of the Fano plane as well.

In the next chapter, we will extend these parametric family of X states beyond two qubits to N qubits. We will present both the algebra of these N-qubit X-states and a diagrammatic representation of the operators involved in defining N-qubit X states in terms of simplexes, which are generalizations of triangles.

Chapter 6
X States for N Qubits

"Geometry is not true, it is advantageous."

Henri Poincaré(1854-1912)

6.1 Introduction

[1] In the previous chapter, we introduced X states for two qubits and presented the connection of the algebra of these states to the Fano plane. In this chapter, we will reintroduce two-qubit X states in a new notation that will allow us to generalize these family of states to N qubits. One of the key motivations for studying N-qubit states is to study multipartite entanglement. Entanglement is a key feature of multipartite quantum systems and has been studied as a resource in varied fields such as computing [64], teleportation [13], metrology [23], secret sharing [44] and imaging [87]. Consequently, the characterization and the evolution of multipartite entanglement have generated a lot of interest in recent years.

One question concerns the transformation between any two multipartite states. This question is related to the number of entanglement classes that exist for a given N-qubit state. There is only one class of two-qubit states since it is well known that a Bell state can be probabilistically transformed to any two-qubit state via stochastic local operations and classical communication through which we define equivalence classes [64]. This is not true for a more general multipartite state. For instance, three-qubit pure states can be classified into two classes [32], three-qubit

[1] This chapter is based on [96]

mixed states can be classified into four separate classes [3] and four-qubit states into nine [92]. We will elaborate on this point below.

For two qubits, the Werner state [98] is an example of a one-parameter family that encompasses both separable and entangled states. The Bell-diagonal states are a three-parameter family of states which have maximally mixed marginals [56]. All these are subsets of a seven-parameter family, called X states, that occur in a variety of contexts such as entanglement and its decay under decoherence [102] and in describing other quantum correlations besides entanglement such as discord [6]. They were defined [102] for two-qubit systems as states whose density matrix has non-zero elements only along its diagonal (three real parameters) and anti-diagonal (two complex parameters) in resemblance to the letter X. Recently [70], an algebraic characterization was provided based on the symmetries of the sub-algebra of the states and operators involved as discussed in chapter 5. Extending this algebraic characterization to N-qubit X states, we present several aspects of the algebra of the operators involved and some applications.

These alternative subsets of seven X states describe a wide variety of physics in quantum information while still restricted to about half the number of parameters (7 *vs.* 15) of the general two-qubit system. This restriction helps to calculate entanglement and other correlations analytically [6, 71], allowing for more insight than numerical computations. It can be expected, therefore, that for N qubits, with an exponential increase in the number of parameters, that similar subsets of N-qubit X states with fewer parameters but still embracing most of the phenomena of interest will be worth studying. We develop such a description here.

Before turning to geometric and group theoretic structures of the states and operators involved, note from the elementary viewing as discussed in chapter 5 for $N = 2$ of the density matrix in the form of the letter X, that $2^N - 1$ real parameters

along the diagonal and 2^{N-1} complex values on the anti-diagonal add to a total of $2^{N+1}-1$ real parameters in the X state. In terms of a 2^N-level system in atoms, molecules or quantum optics, degeneracies and selection rules that restrict the couplings also lead to a consideration of such X states.

In the next section, we will rewrite two-qubit X states in a way that will allow is to generalize it to N qubits. We will then present a diagrammatic representation for the algebra that characterizes N-qubit X states and discuss the example of three-qubit X states in explicit detail. We will finally conclude the chapter by talking about detecting different kinds of entanglement with X states.

6.2 Algebraic Characterization of Two-Qubit X States

A two-qubit system is the simplest model to study entanglement. Its 16 operators form a group under multiplication and commutation. A suitable representation involves Pauli matrices and was presented in [69] and in chapter 3. We will use the notation whereby $\sigma_x \otimes \tau_z$ is written as $X_1 Z_2$. With this notation, two-qubit X states can be rewritten as

$$\rho = \frac{1}{2^2} \sum_{i=0}^{2^2-1} (d_i \hat{D}_i + a_i \hat{A}_i). \tag{6.1}$$

Here $\hat{D}_i$ stands for the operator obtained by replacing 0 with I and 1 with Z in the binary rendering of i. The operator $\hat{A}_i$ is obtained by replacing similarly 0 with X and 1 with Y. For example, since the number 2 is represented in binary as 10, we have $\hat{D}_2 = I_1 Z_2 = Z_2$. Similarly, $\hat{A}_2 = X_1 Y_2$. Note that since $\mathrm{Tr}(\rho) = 1$, the coefficient $d_0 = 1$.

The two-qubit density matrix ρ is Hermitian which implies that $\{a_i, d_i\}$ are real. Various choices of the coefficients lead to different states that are of interest. For instance, the Bell density matrix $|\Phi^+\rangle\langle\Phi^+|$ corresponds to $d_3 = a_0 = 1$, $a_3 = -1$

and $d_1 = d_2 = a_1 = a_2 = 0$. The Werner state [98] is given by $|\psi\rangle = \frac{1-p}{4} I_1 I_2 + p|\Phi^+\rangle\langle\Phi^+|$. The choice $a_1 = a_2 = d_1 = d_2 = 0$ corresponds to the general Bell-diagonal state, characterized by the three non-zero coefficients (a_0, a_3, d_3), and has been studied in the context of quantum correlations and decoherence [56].

Two-spin X states arise in various physical systems. In [18], the authors considered entanglement of an atom interacting with a quantized electromagnetic field. In [80], the author studied X states in condensed matter systems for the role of quantum correlations in driving a quantum phase transition. In [102], the authors studied the evolution of entanglement in X states that were subject to spontaneous emission. They showed that X states preserve their form under general forms of decoherence [102] and that some disentangle at finite time. In [71], it was shown that this "sudden death of entanglement" can be hastened, delayed or averted by using local operations.

6.3 Connection to Geometry

We will use the notation from convex geometry whereby the m-face of an N-dimensional polytope refers to an m-dimensional sub-polytope [27]. Also, the N-simplex is an N-dimensional polytope with $N+1$ vertices, an example of which in two dimensions is the triangle. With this notation, we see that the operators of G_2 are associated with three 0-faces (vertices), three 1-faces (edges) and one 2-face (the "face" of the triangle) of a 2-simplex. These definitions will be generalized to understand the diagram related to N-qubit X states in the next section. Motivated by the two-qubit X state, we introduce the N-qubit generalization of X states as

$$\rho = \frac{1}{2^N} \sum_{i=0}^{2^N-1} (d_i \hat{D}_i + a_i \hat{A}_i). \tag{6.2}$$

As before, $\{a_i, d_i\}$ are real and $d_0 = 1$. Note that the commuting elements for the N-qubit X state are given by $\binom{N}{2}$ operators $Z_i Z_j$ where $i \neq j$ and $i, j = 1 \ldots N$,

plus $\binom{N}{4}$ quadruple products $Z_iZ_jZ_kZ_l$, etc., for a total of $2^{N-1}-1$ U(1) operators. The larger set of 2^N operators $\hat{D}_i$ that includes all products of Z_i commute with each other, but not with all the operators $\hat{A}_i$ as do the U(1) elements. The invariance group for N-qubit X states G_N is iteratively constructed from that of the (N-1)-qubit X state by concatenation: $\mathsf{G}_N = \mathsf{G}_{N-1}\times\mathrm{U}(1)\times\mathsf{G}_{N-1}$. For example, G_1 is the SU(2) group of a single qubit X state , the two-qubit X state is given by G_2 =SU(2)×U(1)×SU(2), and the three-qubit X state is given by G_3=SU(2)×U(1)×SU(2)×U(1)×SU(2)×U(1)×SU(2) consisting of 15 operators, three of them, the U(1) elements Z_iZ_j, commuting with every member of the set of fifteen. G_N includes 2^{N-1} SU(2)s in its total of $2^{N+1}-1$ operators. In projective geometry, it corresponds to PG(N,2), generalizing the Fano plane for two qubits. In the related subject called design theory [15], it is called a $2-(2^{N+1}-1,3,1)$ design.

This approach extends to the geometry of the operators involved. First, a general single qubit state is trivially an X state. The three Pauli operators involved in defining this state (besides the unit operator) can be associated with the two endpoints X and Y of a line and the center Z of the line: see bottom line of Fig. 6.4. Such a line is a 1-simplex, whose two 0-faces and one 1-face are associated with the operators involved in defining a single-qubit X state. Next, the triangle involved in defining the two-qubit X state can be thought of as the addition of a 0-face (third vertex). The addition of this 0-face Z_2, and simultaneously multiplying by Y_2 (or alternatively X_2) the end-points of the initial 1-simplex that forms the base of the triangle, brings in two additional 1-faces (vertices) and one 2-face (in-center Z_2Z_1). The density matrix of the X state can now be written as a sum over the seven 4×4 matrices as noted in [70] and chapter 5. Fig. 1 of that reference, now incorporated as the base of the tetrahedron in Fig. 6.4, renders compactly the

states, operators and multiplications between them so that all manipulations and calculations of two-qubit X states reduce to inspection.

6.4 Extension to N-Qubits

In this manner, the operators $\{\hat{D}_i, \hat{A}_i\}$ of an N-qubit X state can be constructed by adding a 0-face to the (N-1)-simplex describing the (N-1)-qubit X state. The number of m-faces of an N-simplex is given by $\binom{N+1}{m+1}$. The sum of all m-faces for $m \leq N$ is $\sum_{m=0}^{N+1} = 2^{N+1} - 1$. These number counts agree with the ones given above of the SU(2) and U(1) operators. Hence, we can associate the states and operators of generalized X states with the m-faces of an N-simplex.

As an example, we consider in detail the three-qubit X states, written explicitly as

$$\rho = \frac{I_1 I_2 I_3}{8} + \frac{1}{8}(d_1 Z_1 + d_2 Z_2 + d_3 Z_1 Z_2 + d_4 Z_3 + d_5 Z_1 Z_3 + d_6 Z_2 Z_3 + d_7 Z_1 Z_2 Z_3)$$
$$+\frac{1}{8}(a_0 X_1 X_2 X_3 + a_1 Y_1 X_2 X_3 + a_2 X_1 Y_2 X_3 + a_3 Y_1 Y_2 X_3 + a_4 X_1 X_2 Y_3 + a_5 Y_1 X_2 Y_3 + a_6 X_1 Y_2 Y_3 + a_7 Y_1 Y_2 Y_3) \quad (6.3)$$

The 15 operators involved may be identified with the four vertices, mid-points of six edges, four face-centers and one body center of a tetrahedron. This diagram is given in the two figures presented.

As in the case of two-qubit X states, different choices of the parameters $\{a_i, b_i\}$ lead to different states that are of physical interest. The choice of $d_4 = 1 = d_5 = d_6 = a_0 = 1$, $a_3 = a_5 = a_6 = -1$ and the other parameters equal to zero corresponds to a GHZ state [38]. Tracing over any subsystem of this density matrix yields a completely mixed state.

There are three commuting elements now, namely $Z_1 Z_2$, $Z_2 Z_3$ and $Z_1 Z_3$, instead of just one for a two-qubit X state. Any two of these are the so-called stabilizers

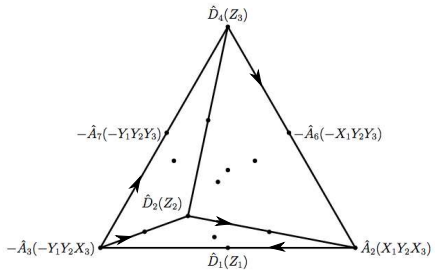

FIGURE 6.1. The tetrahedron or 3-simplex associated with three-qubit X states. In this figure, the 15 operators in Eq. (6.3) are identified with the points of the simplex(vertices, mid-points of edges, face centers and body center of the tetrahedron). For clarity, only a few points are labeled.

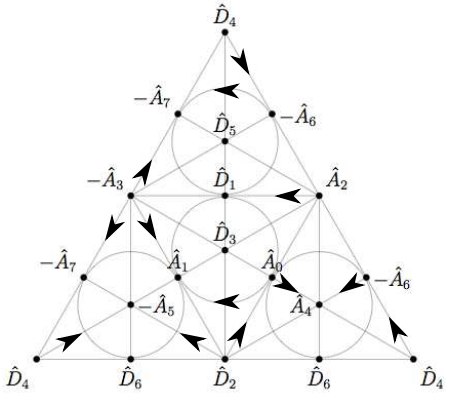

FIGURE 6.2. The tetrahedron or 3-simplex associated with three-qubit X states. The same tetrahedron in Fig. 6.4 is opened out into a planar diagram in (b), resulting in the vertex associated with $\hat{D}_4$ repeated three times. Six lines connecting pairs of face centers and all seven lines through the body center are omitted for clarity. Arrowed lines connecting three operators denote that the product of any two gives the third operator in a cyclic fashion, with a multiplicative $\pm i$. Unarrowed lines denote the product of any two as the third operator, regardless of the order.

of the GHZ state (since the product of any two is the third operator). As with two qubits [70], other choices of commuting operators yield different classes of tripartite X states. Specifically, the choice of Y_1Y_2, Y_2Y_3 and Y_1Y_3 yields an X state all of whose elements are non-zero, a generalization of a similar two-qubit example in [70]. This matrix is explicitly written as

$$\rho = \frac{1}{8}\begin{pmatrix} 1+a_0 & a_1-id_1 & a_2-id_2 & a_3-d_3 & a_4-id_4 & a_5-d_5 & a_6-d_6 & a_7+id_7 \\ a_1+id_1 & 1-a_0 & a_3+d_3 & -a_2-id_2 & a_5+d_5 & -a_4-id_4 & a_7-id_7 & -a_6-d_6 \\ a_2+id_2 & a_3+d_3 & 1-a_0 & -a_1-id_1 & a_6+d_6 & a_7-id_7 & -a_4-id_4 & -a_5-d_5 \\ a_3-d_3 & -a_2+id_2 & -a_1+id_1 & 1+a_0 & a_7+id_7 & -a_6+d_6 & -a_5+d_5 & a_4-id_4 \\ a_4+id_4 & a_5+d_5 & a_6+d_6 & a_7-id_7 & 1-a_0 & -a_1-id_1 & -a_2-id_2 & -a_3-d_3 \\ a_5-d_5 & -a_4+id_4 & a_7+id_7 & -a_6+d_6 & -a_1+id_1 & 1+a_0 & -a_3+d_3 & a_2-id_2 \\ a_6-d_6 & a_7+id_7 & -a_4+id_4 & -a_5+d_5 & -a_2+id_2 & -a_3+d_3 & 1+a_0 & a_1-id_1 \\ a_7-id_7 & -a_6-d_6 & -a_5-d_5 & a_4+id_4 & -a_3-d_3 & a_2+id_2 & a_1+id_1 & 1-a_0 \end{pmatrix}. \tag{6.4}$$

Tracing over any one of the qubits now yields a reduced density matrix whose coherences are non-zero unlike in the previous paragraph. We will return to the importance of this result below.

Consider a GHZ state shared between three parties, Alice, Bob and Charlie. A GHZ state $(|000\rangle + |111\rangle)/\sqrt{2}$ that is subject to a fairly general model of decoherence (such as amplitude damping, phase damping, or spontaneous emission) involves all the operators in Eq. (6.3) and hence evolves as a three-qubit X state. Alternatively, a GHZ state may be defined as $(|+++\rangle + |---\rangle)/\sqrt{2}$, where $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$. While the first definition corresponds to the commuting elements Z_iZ_j, the latter definition corresponds to the commuting elements X_iX_j(a similar result pertains to Y_iY_j). Note that the two definitions of the GHZ state are related by local unitary transformations. If the qubit held by Alice is now traced over, it can be verified that the remaining two-qubit state has no entanglement. But, as the coherences of the two-qubit density matrix are non-zero, there are non-classical correlations that are present between Bob and Charlie that can be quantified by a measure of quantum correlations such as quantum discord [43]. Hence X states characterized by different commuting elements can have drastically

different correlation properties in their marginals. These non-classical correlations may provide speedup for certain tasks [50].

6.5 Witnessing Entanglement in X States

Multipartite entanglement involves exploring entanglement in quantum systems composed of several qudits (D-level systems). The goal in enumerating "types" of multipartite entanglement involving qubit subsystems is to understand classes of states in-equivalent under stochastic local operations and classical communication (SLOCC). While in two-qubit systems, states are either entangled or separable, in three-qubit systems, there can be four distinct classes of entanglement. These four classes can be identified by inspection(for a detailed derivation, see [32]). The first relates to product states in all three qubits. Such states are separable states in all three physical qubits, examples of which are states of the form $|\psi\rangle \otimes |\varphi\rangle \otimes |\chi\rangle$. The second class of states is actually three classes of states that belong in an equivalence class. States that are entangled in two of the three physical qubits belong in this class. States of the type $|\Phi^+\rangle \otimes |0\rangle$ are examples of these so called "biseparable states". The three classes in this biseparable class stated earlier refer to states of the form AB-C, AC-B and BC-A, where AB-C refers to a bipartite entangled state in AB in a product state with respect to C. Having examined separable and biseparable states, the only set of states yet to be classified belong to states not separable with respect to any one qubit. In this set of states, two in-equivalent classes exist. The way to see that is to note that $|W\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$ cannot be written as a sum of two product terms. Hence $|W\rangle$ cannot be converted to $|GHZ\rangle$ by SLOCC alone. Hence there are four classes , namely GHZ, W, biseparable and separable classes of three qubit pure states. Each of these classes can be extended to mixed states as well [2].

Given that multipartite entanglement is characterized by different classes of entanglement, it is desirable to determine whether a given state belongs in a given class of entanglement or not. One simple way of doing this is through the use of "entanglement witnesses" [41]. Given a class of entangled states $\mathcal{C}$, an operator $\mathbf{W}$ is called an entanglement witness if $\forall \rho \notin \mathcal{C}$, $\mathbf{tr}(\mathbf{W}\rho) = 0$ and for at least one $\rho' \in \mathcal{C}$, $\mathbf{tr}(\mathbf{W}\rho') < 0$. Such entanglement witnesses have been constructed for many classes of entanglement. To detect different types of entanglement in three and four qubits, we consider witness operators that detect GHZ-type entanglement, W-type entanglement and the witness corresponding to symmetric Dicke states [41] for $N = 3, 4$ qubits. N-qubit X states characterized by products of Z operators as in Eq.(6.3) are readily seen to possess GHZ-type entanglement for arbitrary N. Consider an X state characterized by products of X operators with $a_0 = a_3 = a_5 = a_6 = d_1 = d_2 = d_4 = d_7 = 0$ and $-a_1 = -a_2 = -a_4 = a_7 = d_3 = d_5 = d_6 = 1$. For this state, $Tr(W_3\rho) = 3/4$ where W_3 is the three-qubit W state. Thus the witness operator $2I/3 - W_3$ detects W-type entanglement in this state. Furthermore, the four-qubit X state characterized by products of X operators with $d_1 = d_2 = d_4 = d_7 = d_8 = d_{11} = d_{13} = d_{14} = a_1 = a_2 = a_4 = a_7 = a_8 = a_{11} = a_{13} = a_{14} = 0$ and $d_3 = d_5 = d_6 = d_9 = d_{10} = d_{12} = d_{15} = a_0 = -a_3 = -a_5 = -a_6 = -a_9 = -a_{10} = -a_{12} = a_{15} = 1$ is a state with $\langle D_{2,4}|\rho|D_{2,4}\rangle = 3/4$. Here $|D_{2,4}\rangle$ is the symmetric Dicke state[2] and $2I/3 - |D_{2,4}\rangle\langle D_{2,4}|$ detects entanglement of the symmetric Dicke type in the given four-qubit X state.

6.6 Conclusions

In summary, we have introduced a family of states called X states for N qubits analogous to those discussed for $N = 2$, and have characterized them by a set of

[2] $|D_{2,4}\rangle = (|0011\rangle + |0101\rangle + |0110\rangle + |1001\rangle + |1010\rangle + |1100\rangle)/\sqrt{6}$. For details see [41].

commuting operators. The algebra of the operators involved defines the family of states and also serves to describe operations on them. We have also presented a scheme for this algebra in terms of N-simplexes. Various entanglement witnesses were shown to detect entanglement in these states.

Chapter 7
Conclusions

"Let this be my last word,
that I trust in your love."-
Rabindranath
Tagore(1861-1941)

Quantum theory has been an active area of investigation for over a century now. Much of this investigation is devoted to understanding various branches such as atomic, molecular and optical systems and the interactions between them. Specific problems in quantum theory have benefited from the perspectives offered by other branches of study. Quantum information theory represents one such perspective wherein the answers sought(and the techniques employed to find these answers) have been influenced by computer science. Algebra and geometry, central to understanding both quantum theory and computer science have also been central to quantum information theory for this reason.

This thesis documents the solutions to specific problems in quantum information theory by employing techniques of algebra and geometry. The first part of the thesis (consisting of chapters 2-4) dealt with a semi-analytic technique to solve operator equations in quantum mechanics. This technique, called unitary integration, separates the non-commuting nature of the operators, a hallmark of quantum mechanics, from the dynamical equations that determine the evolution of systems. By doing this, the geometry of the evolution operator for three-level systems was explored. Specific applications of this solution to geometric phases and other applications in quantum optics and atomic physics were explored. The second part of the thesis (consisting of chapters 5-6) dealt with a class of N-qubit states called

X states. These states are parametrized by $2^{N+1}-1$ parameters and is defined by an equal number of operators. These $2^{N+1}-1$ operators are closed in an algebra. This algebra was explored and was represented geometrically by N-simplexes and connections to other branches of study were presented.

Clearly, there are many interesting and unanswered questions that remain in this field of investigation. For instance, the connection of geometry as explored by unitary integration to entanglement is an open question. A measure of entanglement derived from such a geometric picture would be geometrically and intuitively appealing. Exploration of the geometry of unitary operators belonging to other unitary groups is also an unexplored area of interest. though we have established a class of N qubit states, there are many interesting questions that are yet to be answered. Analytic formulae for multipartite entanglement and quantum discord of multi-qubit systems [94] have to be derived in order to put these parametric family of states to use in quantum information.

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Appendix A
Some Algebras, Sub-Algebras and Groups

Behind it all is surely an idea so simple, so beautiful, that when we grasp it - in a decade, a century, or a millennium - we will all say to each other, how could it have been otherwise? How could we have been so stupid?- John Wheeler(1911-2008)

We enumerate the algebra of su(2), su(3) and su(4) with some sub-algebras. For a detailed introduction to group theory, we refer the readers to [7, 36, 55].

su(2)

The su(2) algebra is defined by the three Pauli matrices σ_i given by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{7.1}$$

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{7.2}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{7.3}$$

These three matrices, along with the unit matrix I are a basis. These matrices are closed with respect to multiplication and commutation.

The algebra can be written compactly as $[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k$ where ε_{ijk} is the completely antisymmetric symbol with three indices. Exponentiation of these matrices generates the SU(2) group. A typical element of the SU(2) group[1] can be

[1] we use the standard notation of using lowercase to denote algebras and uppercase to denote groups

TABLE 7.1. Multiplication table for su(2) algebra

$*$	I	σ_1	σ_2	σ_3
I	I	σ_1	σ_2	σ_3
σ_1	σ_1	I	$i\sigma_3$	$-i\sigma_2$
σ_2	σ_2	$-i\sigma_3$	I	$i\sigma_1$
σ_3	σ_3	$i\sigma_2$	$-i\sigma_1$	I

TABLE 7.2. Commutation table for su(2) algebra

$[,]$	I	σ_1	σ_2	σ_3
I	0	0	0	0
σ_1	0	0	$2i\sigma_3$	$-2i\sigma_2$
σ_2	0	$-2i\sigma_3$	0	$2i\sigma_1$
σ_3	0	$2i\sigma_2$	$-2i\sigma_1$	0

written as $U = e^{-i\theta_1\sigma_1}e^{-i\theta_2\sigma_2}e^{-i\theta_3\sigma_3}e^{-i\theta_0 I}$. Note that $U^\dagger U = I$. Any one of the Pauli matrices and the unit matrix forms a sub-algebra of the su(2) algebra. For instance, I, σ_3 is a u(1) sub-algebra of su(2) and hence $e^{-i\theta\sigma_3}$ is a U(1) subgroup of SU(2).

su(3)

We use the standard Gell-Mann basis for three-level systems. They are given by

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

$$\lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}; \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}.$$

$$\lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}; \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \tag{7.4}$$

These matrices are Hermitian and obey $\mathsf{Tr}(\lambda_i\lambda_j) = 2\delta_{ij}$. Like su(2) algebra, the commutation relations between different Gell-Mann matrices is given by $[\lambda_i, \lambda_j] = 2if_{ijk}\lambda_k$. Here f_{ijk} is completely antisymmetric with $f_{123} = 1$, $f_{147} = f_{165} = f_{246} = f_{257} = f_{345} = f_{376} = 1/2$, and $f_{458} = f_{678} = \sqrt{3}/2$.

su(4)

su(4) algebra is represented in terms of the tensor product of two Pauli matrix sets. The sixteen matrices are given by $I = I \otimes I$, $\vec{\sigma} = \vec{\sigma} \otimes I$, $\vec{\tau} = I \otimes \vec{\tau}$ and $\vec{\sigma} \otimes \vec{\tau}$. These sixteen operators are closed with respect to both multiplication and commutation. The explicit matrix representations of operators proportional to the sixteen matrices defined above are given in Eq. (7.5). Their multiplication table is presented in table 7.5 and the commutation table of the sixteen operators is presented in table 7.6.

Various sub-algebras can be identified from the tables presented upon inspection. Trivially, the matrices $\vec{\sigma}$ and $\vec{\tau}$ form a su(2)⊗su(2) sub-algebra of su(4). The operators $\{\sigma_1\tau_1, \sigma_2\tau_2, \sigma_3\tau_3, \sigma_1\tau_2, \sigma_2\tau_1, \sigma_3, \tau_3\}$ are closed under a su(2)⊗u(1)⊗su(2) sub-algebra. Note that there are many other sets of seven operators corresponding to the operators that commute with any given operator that are also examples of the same sub-algebra. Similarly, the operators $\{O_9 + O_{11}, O_{10} + 2O_{12}, O_3 + 2O_4, O_5 + 2O_7, O_6 + 2O_8, 2O_{13} + 2O_{14}, 2O_{16} - 2O_{15}, (2O_2 - O_3 + 2O_4)/\sqrt{3}\}$ are closed under a su(3) subalgebra of su(4). Finally, one can verify that the ten operators $\{O_2, O_3, O_5, O_6, O_{11}, O_{12}, O_{13}, O_{14}, O_{15}, O_{16}\}$ are closed under the so(5) sub-algebra of su(4). Since so(n-1) ∈ so(n), we can also readily identify various so(4), so(3) and so(2) sub-algebras of su(4).

A general SU(4) operator can hence be written as $U = \Pi_{i=1}^{16} e^{i\theta_i O_i}$. All of the matrices identified above as belonging to different sub-algebras immediately can be ex-

ponentiated to yield various subgroups. Thus the subgroups SU(2)×U(1)×SU(2), SU(3), SO(5) etc can be written down by exponentiating various matrices identified as sub-algebras before.

The Algebra g_3

The group G_N was defined in chapter 6 iteratively as $\mathsf{G}_N = \mathsf{G}_{N-1} \times U(1) \times \mathsf{G}_{N-1}$. The algebra g_N involves a set of $2^{N+1} - 1$ operators. For $N = 3$, g_3 is defined as g_3 =su(2)×u(1)×su(2)×u(1)×su(2)×u(1)×su(2). The $2^4 - 1 = 15$ operators are explicitly given by $\hat{D}_0 = I$, $\hat{D}_1 = Z_1$, $\hat{D}_2 = Z_2$, $\hat{D}_3 = Z_2Z_1$, $\hat{D}_4 = Z_3$, $\hat{D}_5 = Z_3Z_1$, $\hat{D}_6 = Z_3Z_2$, $\hat{D}_7 = Z_3Z_2Z_1$, $\hat{A}_0 = X_3X_2X_1$, $\hat{A}_1 = X_3X_2Y_1$, $\hat{A}_2 = X_3Y_2X_1$, $\hat{A}_3 = X_3Y_2Y_1$, $\hat{A}_4 = Y_3X_2X_1$, $\hat{A}_5 = Y_3X_2Y_1$, $\hat{A}_6 = Y_3Y_2X_1$ and $\hat{A}_7 = Y_3Y_2Y_1$. Their multiplication table is presented in table 7.7 and their commutation table is presented in table 7.8.

TABLE 7.3. Multiplication table for su(3) algebra

$*$	I	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8
I	I	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8
λ_1	λ_1	$\frac{2I}{3}+\frac{\lambda_8}{\sqrt{3}}$	$i\lambda_3$	$-i\lambda_2$	$\frac{\lambda_6}{2}+\frac{i\lambda_7}{2}$	$\frac{\lambda_7}{2}-\frac{i\lambda_6}{2}$	$\frac{\lambda_4}{2}+\frac{i\lambda_5}{2}$	$\frac{\lambda_5}{2}-\frac{i\lambda_4}{2}$	$\frac{\lambda_1}{\sqrt{3}}$
λ_2	λ_2	$-i\lambda_3$	$\frac{2I}{3}+\frac{\lambda_8}{\sqrt{3}}$	$i\lambda_1$	$-\frac{\lambda_7}{2}+\frac{i\lambda_6}{2}$	$\frac{\lambda_6}{2}+\frac{i\lambda_7}{2}$	$\frac{\lambda_5}{2}-\frac{i\lambda_4}{2}$	$-\frac{\lambda_4}{2}-\frac{i\lambda_5}{2}$	$\frac{\lambda_2}{\sqrt{3}}$
λ_3	λ_3	$i\lambda_2$	$-i\lambda_1$	$\frac{2I}{3}+\frac{\lambda_8}{\sqrt{3}}$	$\frac{\lambda_4}{2}+\frac{i\lambda_5}{2}$	$\frac{\lambda_5}{2}-\frac{i\lambda_4}{2}$	$-\frac{\lambda_6}{2}-\frac{i\lambda_7}{2}$	$-\frac{\lambda_7}{2}+\frac{i\lambda_6}{2}$	$\frac{\lambda_3}{\sqrt{3}}$
λ_4	λ_4	$\frac{\lambda_6}{2}-\frac{i\lambda_7}{2}$	$-\frac{\lambda_7}{2}-\frac{i\lambda_6}{2}$	$\frac{\lambda_4}{2}-\frac{i\lambda_5}{2}$	$\frac{2\lambda_0}{3}+\frac{\lambda_3}{2}-\frac{\lambda_8}{2\sqrt{3}}$	$\frac{i\lambda_3}{2}+\frac{1}{2}i\sqrt{3}\lambda_8$	$\frac{\lambda_1}{2}+\frac{i\lambda_2}{2}$	$-\frac{\lambda_2}{2}+\frac{i\lambda_1}{2}$	$-\frac{\lambda_4}{2\sqrt{3}}-\frac{1}{2}i\sqrt{3}\lambda_5$
λ_5	λ_5	$\frac{\lambda_7}{2}+\frac{i\lambda_6}{2}$	$\frac{\lambda_6}{2}-\frac{i\lambda_7}{2}$	$\frac{\lambda_5}{2}+\frac{i\lambda_4}{2}$	$-\frac{i\lambda_3}{2}-\frac{1}{2}i\sqrt{3}\lambda_8$	$\frac{2I}{3}+\frac{\lambda_3}{2}-\frac{\lambda_8}{2\sqrt{3}}$	$\frac{\lambda_2}{2}-\frac{i\lambda_1}{2}$	$\frac{\lambda_1}{2}+\frac{i\lambda_2}{2}$	$-\frac{\lambda_5}{2\sqrt{3}}+\frac{1}{2}i\sqrt{3}\lambda_4$
λ_6	λ_6	$\frac{\lambda_4}{2}-\frac{i\lambda_5}{2}$	$\frac{\lambda_5}{2}+\frac{i\lambda_4}{2}$	$-\frac{\lambda_6}{2}+\frac{i\lambda_7}{2}$	$\frac{\lambda_1}{2}-\frac{i\lambda_2}{2}$	$\frac{\lambda_2}{2}+\frac{i\lambda_1}{2}$	$\frac{2I}{3}-\frac{\lambda_3}{2}-\frac{\lambda_8}{2\sqrt{3}}$	$\frac{1}{2}i\sqrt{3}\lambda_8-\frac{i\lambda_3}{2}$	$-\frac{\lambda_6}{2\sqrt{3}}-\frac{1}{2}i\sqrt{3}\lambda_7$
λ_7	λ_7	$\frac{\lambda_5}{2}+\frac{i\lambda_4}{2}$	$-\frac{\lambda_4}{2}+\frac{i\lambda_5}{2}$	$-\frac{\lambda_7}{2}-\frac{i\lambda_6}{2}$	$-\frac{\lambda_2}{2}-\frac{i\lambda_1}{2}$	$\frac{\lambda_1}{2}-\frac{i\lambda_2}{2}$	$\frac{i\lambda_3}{2}-\frac{1}{2}i\sqrt{3}\lambda_8$	$\frac{2I}{3}-\frac{\lambda_3}{2}-\frac{\lambda_8}{2\sqrt{3}}$	$-\frac{\lambda_7}{2\sqrt{3}}+\frac{1}{2}i\sqrt{3}\lambda_6$
λ_8	λ_8	$\frac{\lambda_1}{\sqrt{3}}$	$\frac{\lambda_2}{\sqrt{3}}$	$\frac{\lambda_3}{\sqrt{3}}$	$-\frac{\lambda_4}{2\sqrt{3}}+\frac{1}{2}i\sqrt{3}\lambda_5$	$-\frac{\lambda_5}{2\sqrt{3}}-\frac{1}{2}i\sqrt{3}\lambda_4$	$-\frac{\lambda_6}{2\sqrt{3}}+\frac{1}{2}i\sqrt{3}\lambda_7$	$-\frac{\lambda_7}{2\sqrt{3}}-\frac{1}{2}i\sqrt{3}\lambda_6$	$\frac{2I}{3}-\frac{\lambda_8}{\sqrt{3}}$

TABLE 7.4. Commutation table for su(3) algebra

$[,]$	I	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8
I	0	0	0	0	0	0	0	0	0
λ_1	0	0	$2i\lambda_3$	$-2i\lambda_2$	$i\lambda_7$	$-i\lambda_6$	$i\lambda_5$	$-i\lambda_4$	0
λ_2	0	$-2i\lambda_3$	0	$2i\lambda_1$	$i\lambda_6$	$i\lambda_7$	$-i\lambda_4$	$-i\lambda_5$	0
λ_3	0	$2i\lambda_2$	$-2i\lambda_1$	0	$i\lambda_5$	$-i\lambda_4$	$-i\lambda_7$	$i\lambda_6$	0
λ_4	0	$-i\lambda_7$	$-i\lambda_6$	$-i\lambda_5$	0	$i\lambda_3 + i\sqrt{3}\lambda_8$	$i\lambda_2$	$i\lambda_1$	$-i\sqrt{3}\lambda_5$
λ_5	0	$i\lambda_6$	$-i\lambda_7$	$i\lambda_4$	$-i\lambda_3 - i\sqrt{3}\lambda_8$	0	$-i\lambda_1$	$i\lambda_2$	$i\sqrt{3}\lambda_4$
λ_6	0	$-i\lambda_5$	$i\lambda_4$	$i\lambda_7$	$-i\lambda_2$	$i\lambda_1$	0	$i\sqrt{3}\lambda_8 - i\lambda_3$	$-i\sqrt{3}\lambda_7$
λ_7	0	$i\lambda_4$	$i\lambda_5$	$-i\lambda_6$	$-i\lambda_1$	$-i\lambda_2$	$i\lambda_3 - i\sqrt{3}\lambda_8$	0	$i\sqrt{3}\lambda_6$
λ_8	0	0	0	0	$i\sqrt{3}\lambda_5$	$-i\sqrt{3}\lambda_4$	$i\sqrt{3}\lambda_7$	$-i\sqrt{3}\lambda_6$	0

$$O_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; O_2 = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}; O_3 = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}; O_4 = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}$$

$$O_5 = \begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}; O_6 = \begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{pmatrix}; O_7 = \begin{pmatrix} 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & -\frac{1}{4} \\ \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 \end{pmatrix}; O_8 = \begin{pmatrix} 0 & 0 & -\frac{i}{4} & 0 \\ 0 & 0 & 0 & \frac{i}{4} \\ \frac{i}{4} & 0 & 0 & 0 \\ 0 & -\frac{i}{4} & 0 & 0 \end{pmatrix}$$

$$O_9 = \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \end{pmatrix}; O_{10} = \begin{pmatrix} 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 \end{pmatrix}; O_{11} = \begin{pmatrix} 0 & \frac{1}{4} & 0 & 0 \\ \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{4} \\ 0 & 0 & -\frac{1}{4} & 0 \end{pmatrix}; O_{12} = \begin{pmatrix} 0 & -\frac{i}{4} & 0 & 0 \\ \frac{i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{4} \\ 0 & 0 & -\frac{i}{4} & 0 \end{pmatrix}$$

$$O_{13} = \begin{pmatrix} 0 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ \frac{1}{4} & 0 & 0 & 0 \end{pmatrix}; O_{14} = \begin{pmatrix} 0 & 0 & 0 & -\frac{1}{4} \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ -\frac{1}{4} & 0 & 0 & 0 \end{pmatrix}; O_{15} = \begin{pmatrix} 0 & 0 & 0 & -\frac{i}{4} \\ 0 & 0 & \frac{i}{4} & 0 \\ 0 & -\frac{i}{4} & 0 & 0 \\ \frac{i}{4} & 0 & 0 & 0 \end{pmatrix}; O_{16} = \begin{pmatrix} 0 & 0 & 0 & -\frac{i}{4} \\ 0 & 0 & -\frac{i}{4} & 0 \\ 0 & \frac{i}{4} & 0 & 0 \\ \frac{i}{4} & 0 & 0 & 0 \end{pmatrix} \quad (7.5)$$

TABLE 7.5. Multiplication table for su(4) algebra

$*$	O_1	O_2	O_3	O_4	O_5	O_6	O_7	O_8	O_9	O_{10}	O_{11}	O_{12}	O_{13}	O_{14}	O_{15}	O_{16}
O_1	O_1	O_2	O_3	O_4	O_5	O_6	O_7	O_8	O_9	O_{10}	O_{11}	O_{12}	O_{13}	O_{14}	O_{15}	O_{16}
O_2	O_2	$\frac{O_1}{4}$	O_4	$\frac{O_3}{4}$	$\frac{iO_6}{2}$	$-\frac{iO_5}{2}$	$\frac{iO_8}{2}$	$-\frac{iO_7}{2}$	O_{11}	O_{12}	$\frac{O_9}{4}$	$\frac{O_{10}}{4}$	$\frac{iO_{16}}{2}$	$-\frac{iO_{15}}{2}$	$\frac{iO_{14}}{2}$	$-\frac{iO_{13}}{2}$
O_3	O_3	O_4	$\frac{O_1}{4}$	$\frac{O_2}{4}$	O_7	O_8	$\frac{O_5}{4}$	$\frac{O_6}{4}$	$\frac{iO_{10}}{2}$	$-\frac{iO_9}{2}$	$\frac{iO_{12}}{2}$	$-\frac{iO_{11}}{2}$	$\frac{iO_{15}}{2}$	$-\frac{iO_{16}}{2}$	$-\frac{iO_{13}}{2}$	$\frac{iO_{14}}{2}$
O_4	O_4	$\frac{O_3}{4}$	$\frac{O_2}{4}$	$\frac{O_1}{16}$	$\frac{iO_8}{2}$	$-\frac{iO_7}{2}$	$\frac{iO_6}{8}$	$-\frac{iO_5}{8}$	$\frac{iO_{12}}{2}$	$-\frac{iO_{11}}{2}$	$\frac{iO_{10}}{8}$	$-\frac{iO_9}{8}$	$-\frac{O_{14}}{4}$	$-\frac{O_{13}}{4}$	$\frac{O_{16}}{4}$	$\frac{O_{15}}{4}$
O_5	O_5	$-\frac{iO_6}{2}$	O_7	$-\frac{iO_8}{2}$	$\frac{O_1}{4}$	$\frac{iO_2}{2}$	$\frac{O_3}{4}$	$\frac{iO_4}{2}$	O_{13}	O_{15}	$-\frac{iO_{16}}{2}$	$-\frac{iO_{14}}{2}$	$\frac{O_9}{4}$	$\frac{iO_{12}}{2}$	$\frac{O_{10}}{4}$	$\frac{iO_{11}}{2}$
O_6	O_6	$\frac{iO_5}{2}$	O_8	$\frac{iO_7}{2}$	$-\frac{iO_2}{2}$	$\frac{O_1}{4}$	$-\frac{iO_4}{2}$	$\frac{O_3}{4}$	O_{16}	O_{14}	$\frac{iO_{13}}{2}$	$\frac{iO_{15}}{2}$	$-\frac{iO_{11}}{2}$	$\frac{O_{10}}{4}$	$-\frac{iO_{12}}{2}$	$\frac{O_9}{4}$
O_7	O_7	$-\frac{iO_8}{2}$	$\frac{O_5}{4}$	$-\frac{iO_6}{8}$	$\frac{O_3}{4}$	$\frac{iO_4}{2}$	$\frac{O_1}{16}$	$\frac{iO_2}{8}$	$\frac{iO_{15}}{2}$	$-\frac{iO_{13}}{2}$	$\frac{O_{14}}{4}$	$-\frac{O_{16}}{4}$	$\frac{iO_{10}}{8}$	$\frac{O_{11}}{4}$	$-\frac{iO_9}{8}$	$-\frac{O_{12}}{4}$
O_8	O_8	$\frac{iO_7}{2}$	$\frac{O_6}{4}$	$\frac{iO_5}{8}$	$-\frac{iO_4}{2}$	$\frac{O_3}{4}$	$-\frac{iO_2}{8}$	$\frac{O_1}{16}$	$\frac{iO_{14}}{2}$	$-\frac{iO_{16}}{2}$	$-\frac{O_{15}}{4}$	$\frac{O_{13}}{4}$	$\frac{O_{12}}{4}$	$-\frac{iO_9}{8}$	$-\frac{O_{11}}{4}$	$\frac{iO_{10}}{8}$
O_9	O_9	O_{11}	$-\frac{iO_{10}}{2}$	$-\frac{iO_{12}}{2}$	O_{13}	O_{16}	$-\frac{iO_{15}}{2}$	$-\frac{iO_{14}}{2}$	$\frac{O_1}{4}$	$\frac{iO_3}{2}$	$\frac{O_2}{4}$	$\frac{iO_4}{2}$	$\frac{O_5}{4}$	$\frac{iO_8}{2}$	$\frac{iO_7}{2}$	$\frac{O_6}{4}$
O_{10}	O_{10}	O_{12}	$\frac{iO_9}{2}$	$\frac{iO_{11}}{2}$	O_{15}	O_{14}	$\frac{iO_{13}}{2}$	$\frac{iO_{16}}{2}$	$-\frac{iO_3}{2}$	$\frac{O_1}{4}$	$-\frac{iO_4}{2}$	$\frac{O_2}{4}$	$-\frac{iO_7}{2}$	$\frac{O_6}{4}$	$\frac{O_5}{4}$	$-\frac{iO_8}{2}$
O_{11}	O_{11}	$\frac{O_9}{4}$	$-\frac{iO_{12}}{2}$	$-\frac{iO_{10}}{8}$	$\frac{iO_{16}}{2}$	$-\frac{iO_{13}}{2}$	$\frac{O_{14}}{4}$	$-\frac{O_{15}}{4}$	$\frac{O_2}{4}$	$\frac{iO_4}{2}$	$\frac{O_1}{16}$	$\frac{iO_3}{8}$	$\frac{iO_6}{8}$	$\frac{O_7}{4}$	$-\frac{O_8}{4}$	$-\frac{iO_5}{8}$
O_{12}	O_{12}	$\frac{O_{10}}{4}$	$\frac{iO_{11}}{2}$	$\frac{iO_9}{8}$	$\frac{iO_{14}}{2}$	$-\frac{iO_{15}}{2}$	$-\frac{O_{16}}{4}$	$\frac{O_{13}}{4}$	$-\frac{iO_4}{2}$	$\frac{O_2}{4}$	$-\frac{iO_3}{8}$	$\frac{O_1}{16}$	$\frac{O_8}{4}$	$-\frac{iO_5}{8}$	$\frac{iO_6}{8}$	$-\frac{O_7}{4}$
O_{13}	O_{13}	$-\frac{iO_{16}}{2}$	$-\frac{iO_{15}}{2}$	$-\frac{O_{14}}{4}$	$\frac{O_9}{4}$	$\frac{iO_{11}}{2}$	$-\frac{iO_{10}}{8}$	$\frac{O_{12}}{4}$	$\frac{O_5}{4}$	$\frac{iO_7}{2}$	$-\frac{iO_6}{8}$	$\frac{O_8}{4}$	$\frac{O_1}{16}$	$-\frac{O_4}{4}$	$\frac{iO_3}{8}$	$\frac{iO_2}{8}$
O_{14}	O_{14}	$\frac{iO_{15}}{2}$	$\frac{iO_{16}}{2}$	$-\frac{O_{13}}{4}$	$-\frac{iO_{12}}{2}$	$\frac{O_{10}}{4}$	$\frac{O_{11}}{4}$	$\frac{iO_9}{8}$	$-\frac{iO_8}{2}$	$\frac{O_6}{4}$	$\frac{O_7}{4}$	$\frac{iO_5}{8}$	$-\frac{O_4}{4}$	$\frac{O_1}{16}$	$-\frac{iO_2}{8}$	$-\frac{iO_3}{8}$
O_{15}	O_{15}	$-\frac{iO_{14}}{2}$	$\frac{iO_{13}}{2}$	$\frac{O_{16}}{4}$	$\frac{O_{10}}{4}$	$\frac{iO_{12}}{2}$	$\frac{iO_9}{8}$	$-\frac{O_{11}}{4}$	$-\frac{iO_7}{2}$	$\frac{O_5}{4}$	$-\frac{O_8}{4}$	$-\frac{iO_6}{8}$	$-\frac{iO_3}{8}$	$\frac{iO_2}{8}$	$\frac{O_1}{16}$	$\frac{O_4}{4}$
O_{16}	O_{16}	$\frac{iO_{13}}{2}$	$-\frac{iO_{14}}{2}$	$\frac{O_{15}}{4}$	$-\frac{iO_{11}}{2}$	$\frac{O_9}{4}$	$-\frac{O_{12}}{4}$	$-\frac{iO_{10}}{8}$	$\frac{O_6}{4}$	$\frac{iO_8}{2}$	$\frac{iO_5}{8}$	$-\frac{O_7}{4}$	$-\frac{iO_2}{8}$	$\frac{iO_3}{8}$	$\frac{O_4}{4}$	$\frac{O_1}{16}$

TABLE 7.6. Commutation Table for su(4) matrices

$[,]$	O_1	O_2	O_3	O_4	O_5	O_6	O_7	O_8	O_9	O_{10}	O_{11}	O_{12}	O_{13}	O_{14}	O_{15}	O_{16}
O_1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
O_2	0	0	0	0	iO_6	$-iO_5$	iO_8	$-iO_7$	0	0	0	0	iO_{16}	$-iO_{15}$	iO_{14}	$-iO_{13}$
O_3	0	0	0	0	0	0	0	0	iO_{10}	$-iO_9$	iO_{12}	$-iO_{11}$	iO_{15}	$-iO_{16}$	$-iO_{13}$	iO_{14}
O_4	0	0	0	0	iO_8	$-iO_7$	$\frac{iO_6}{4}$	$-\frac{iO_5}{4}$	iO_{12}	$-iO_{11}$	$\frac{iO_{10}}{4}$	$-\frac{iO_9}{4}$	0	0	0	0
O_5	0	$-iO_6$	0	$-iO_8$	0	iO_2	0	iO_4	0	0	$-iO_{16}$	$-iO_{14}$	0	iO_{12}	0	iO_{11}
O_6	0	iO_5	0	iO_7	$-iO_2$	0	$-iO_4$	0	0	0	iO_{13}	iO_{15}	$-iO_{11}$	0	$-iO_{12}$	0
O_7	0	$-iO_8$	0	$-\frac{iO_6}{4}$	0	iO_4	0	$\frac{iO_2}{4}$	iO_{15}	$-iO_{13}$	0	0	$\frac{iO_{10}}{4}$	0	$-\frac{iO_9}{4}$	0
O_8	0	iO_7	0	$\frac{iO_5}{4}$	$-iO_4$	0	$-\frac{iO_2}{4}$	0	iO_{14}	$-iO_{16}$	0	0	0	$-\frac{iO_9}{4}$	0	$\frac{iO_{10}}{4}$
O_9	0	0	$-iO_{10}$	$-iO_{12}$	0	0	$-iO_{15}$	$-iO_{14}$	0	iO_3	0	iO_4	0	iO_8	iO_7	0
O_{10}	0	0	iO_9	iO_{11}	0	0	iO_{13}	iO_{16}	$-iO_3$	0	$-iO_4$	0	$-iO_7$	0	0	$-iO_8$
O_{11}	0	0	$-iO_{12}$	$-\frac{iO_{10}}{4}$	iO_{16}	$-iO_{13}$	0	0	0	iO_4	0	$\frac{iO_3}{4}$	$\frac{iO_6}{4}$	0	0	$-\frac{iO_5}{4}$
O_{12}	0	0	iO_{11}	$\frac{iO_9}{4}$	iO_{14}	$-iO_{15}$	0	0	$-iO_4$	0	$-\frac{iO_3}{4}$	0	0	$-\frac{iO_5}{4}$	$\frac{iO_6}{4}$	0
O_{13}	0	$-iO_{16}$	$-iO_{15}$	0	0	iO_{11}	$-\frac{iO_{10}}{4}$	0	0	iO_7	$-\frac{iO_6}{4}$	0	0	0	$\frac{iO_3}{4}$	$\frac{iO_2}{4}$
O_{14}	0	iO_{15}	iO_{16}	0	$-iO_{12}$	0	0	$\frac{iO_9}{4}$	$-iO_8$	0	0	$\frac{iO_5}{4}$	0	0	$-\frac{iO_2}{4}$	$-\frac{iO_3}{4}$
O_{15}	0	$-iO_{14}$	iO_{13}	0	0	iO_{12}	$\frac{iO_9}{4}$	0	$-iO_7$	0	0	$-\frac{iO_6}{4}$	$-\frac{iO_3}{4}$	$\frac{iO_2}{4}$	0	0
O_{16}	0	iO_{13}	$-iO_{14}$	0	$-iO_{11}$	0	0	$-\frac{iO_{10}}{4}$	0	iO_8	$\frac{iO_5}{4}$	0	$-\frac{iO_2}{4}$	$\frac{iO_3}{4}$	0	0

TABLE 7.7. Multiplication table for $\mathfrak{g}_3$

$*$	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	$\hat{D}_3$	$\hat{D}_4$	$\hat{D}_5$	$\hat{D}_6$	$\hat{D}_7$	$\hat{A}_0$	$\hat{A}_1$	$\hat{A}_2$	$\hat{A}_3$	$\hat{A}_4$	$\hat{A}_5$	$\hat{A}_6$	$\hat{A}_7$
$\hat{D}_0$	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	$\hat{D}_3$	$\hat{D}_4$	$\hat{D}_5$	$\hat{D}_6$	$\hat{D}_7$	$\hat{A}_0$	$\hat{A}_1$	$\hat{A}_2$	$\hat{A}_3$	$\hat{A}_4$	$\hat{A}_5$	$\hat{A}_6$	$\hat{A}_7$
$\hat{D}_1$	$\hat{D}_1$	$\hat{D}_0$	$\hat{D}_3$	$\hat{D}_2$	$\hat{D}_5$	$\hat{D}_4$	$\hat{D}_7$	$\hat{D}_6$	$i\hat{A}_1$	$-i\hat{A}_0$	$i\hat{A}_3$	$-i\hat{A}_2$	$i\hat{A}_5$	$-i\hat{A}_4$	$i\hat{A}_7$	$-i\hat{A}_6$
$\hat{D}_2$	$\hat{D}_2$	$\hat{D}_3$	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_6$	$\hat{D}_7$	$\hat{D}_4$	$\hat{D}_5$	$i\hat{A}_2$	$i\hat{A}_3$	$-i\hat{A}_0$	$-i\hat{A}_1$	$i\hat{A}_6$	$i\hat{A}_7$	$-i\hat{A}_4$	$-i\hat{A}_5$
$\hat{D}_3$	$\hat{D}_3$	$\hat{D}_2$	$\hat{D}_1$	$\hat{D}_0$	$\hat{D}_7$	$\hat{D}_6$	$\hat{D}_5$	$\hat{D}_4$	$-\hat{A}_3$	$\hat{A}_2$	$\hat{A}_1$	$-\hat{A}_0$	$-\hat{A}_7$	$\hat{A}_6$	$\hat{A}_5$	$-\hat{A}_4$
$\hat{D}_4$	$\hat{D}_4$	$\hat{D}_5$	$\hat{D}_6$	$\hat{D}_7$	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	$\hat{D}_3$	$i\hat{A}_4$	$i\hat{A}_5$	$i\hat{A}_6$	$i\hat{A}_7$	$-i\hat{A}_0$	$-i\hat{A}_1$	$-i\hat{A}_2$	$-i\hat{A}_3$
$\hat{D}_5$	$\hat{D}_5$	$\hat{D}_4$	$\hat{D}_7$	$\hat{D}_6$	$\hat{D}_1$	$\hat{D}_0$	$\hat{D}_3$	$\hat{D}_2$	$-\hat{A}_5$	$\hat{A}_4$	$-\hat{A}_7$	$\hat{A}_6$	$\hat{A}_1$	$-\hat{A}_0$	$\hat{A}_3$	$-\hat{A}_2$
$\hat{D}_6$	$\hat{D}_6$	$\hat{D}_7$	$\hat{D}_4$	$\hat{D}_5$	$\hat{D}_2$	$\hat{D}_3$	$\hat{D}_0$	$\hat{D}_1$	$-\hat{A}_6$	$-\hat{A}_7$	$\hat{A}_4$	$\hat{A}_5$	$\hat{A}_2$	$\hat{A}_3$	$-\hat{A}_0$	$-\hat{A}_1$
$\hat{D}_7$	$\hat{D}_7$	$\hat{D}_6$	$\hat{D}_5$	$\hat{D}_4$	$\hat{D}_3$	$\hat{D}_2$	$\hat{D}_1$	$\hat{D}_0$	$-i\hat{A}_7$	$i\hat{A}_6$	$i\hat{A}_5$	$-i\hat{A}_4$	$i\hat{A}_3$	$-i\hat{A}_2$	$-i\hat{A}_1$	$i\hat{A}_0$
$\hat{A}_0$	$\hat{A}_0$	$-i\hat{A}_1$	$-i\hat{A}_2$	$-\hat{A}_3$	$-i\hat{A}_4$	$-\hat{A}_5$	$-\hat{A}_6$	$i\hat{A}_7$	$\hat{D}_0$	$i\hat{D}_1$	$i\hat{D}_2$	$-\hat{D}_3$	$i\hat{D}_4$	$-\hat{D}_5$	$-\hat{D}_6$	$-i\hat{D}_7$
$\hat{A}_1$	$\hat{A}_1$	$i\hat{A}_0$	$-i\hat{A}_3$	$\hat{A}_2$	$-i\hat{A}_5$	$\hat{A}_4$	$-\hat{A}_7$	$-i\hat{A}_6$	$-i\hat{D}_1$	$\hat{D}_0$	$\hat{D}_3$	$i\hat{D}_2$	$\hat{D}_5$	$i\hat{D}_4$	$i\hat{D}_7$	$-\hat{D}_6$
$\hat{A}_2$	$\hat{A}_2$	$-i\hat{A}_3$	$i\hat{A}_0$	$\hat{A}_1$	$-i\hat{A}_6$	$-\hat{A}_7$	$\hat{A}_4$	$-i\hat{A}_5$	$-i\hat{D}_2$	$\hat{D}_3$	$\hat{D}_0$	$i\hat{D}_1$	$\hat{D}_6$	$i\hat{D}_7$	$i\hat{D}_4$	$-\hat{D}_5$
$\hat{A}_3$	$\hat{A}_3$	$i\hat{A}_2$	$i\hat{A}_1$	$-\hat{A}_0$	$-i\hat{A}_7$	$\hat{A}_6$	$\hat{A}_5$	$i\hat{A}_4$	$-\hat{D}_3$	$-i\hat{D}_2$	$-i\hat{D}_1$	$\hat{D}_0$	$-i\hat{D}_7$	$\hat{D}_6$	$\hat{D}_5$	$i\hat{D}_4$
$\hat{A}_4$	$\hat{A}_4$	$-i\hat{A}_5$	$-i\hat{A}_6$	$-\hat{A}_7$	$i\hat{A}_0$	$\hat{A}_1$	$\hat{A}_2$	$-i\hat{A}_3$	$-i\hat{D}_4$	$\hat{D}_5$	$\hat{D}_6$	$i\hat{D}_7$	$\hat{D}_0$	$i\hat{D}_1$	$i\hat{D}_2$	$-\hat{D}_3$
$\hat{A}_5$	$\hat{A}_5$	$i\hat{A}_4$	$-i\hat{A}_7$	$\hat{A}_6$	$i\hat{A}_1$	$-\hat{A}_0$	$\hat{A}_3$	$i\hat{A}_2$	$-\hat{D}_5$	$-i\hat{D}_4$	$-i\hat{D}_7$	$\hat{D}_6$	$-i\hat{D}_1$	$\hat{D}_0$	$\hat{D}_3$	$i\hat{D}_2$
$\hat{A}_6$	$\hat{A}_6$	$-i\hat{A}_7$	$i\hat{A}_4$	$\hat{A}_5$	$i\hat{A}_2$	$\hat{A}_3$	$-\hat{A}_0$	$i\hat{A}_1$	$-\hat{D}_6$	$-i\hat{D}_7$	$-i\hat{D}_4$	$\hat{D}_5$	$-i\hat{D}_2$	$\hat{D}_3$	$\hat{D}_0$	$i\hat{D}_1$
$\hat{A}_7$	$\hat{A}_7$	$i\hat{A}_6$	$i\hat{A}_5$	$-\hat{A}_4$	$i\hat{A}_3$	$-\hat{A}_2$	$-\hat{A}_1$	$-i\hat{A}_0$	$i\hat{D}_7$	$-\hat{D}_6$	$-\hat{D}_5$	$-i\hat{D}_4$	$-\hat{D}_3$	$-i\hat{D}_2$	$-i\hat{D}_1$	$\hat{D}_0$

TABLE 7.8. Commutation table for g_3

$[,]$	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	$\hat{D}_3$	$\hat{D}_4$	$\hat{D}_5$	$\hat{D}_6$	$\hat{D}_7$	$\hat{A}_0$	$\hat{A}_1$	$\hat{A}_2$	$\hat{A}_3$	$\hat{A}_4$	$\hat{A}_5$	$\hat{A}_6$	$\hat{A}_7$
$\hat{D}_0$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\hat{D}_1$	0	0	0	0	0	0	0	0	$2i\hat{A}_1$	$-2i\hat{A}_0$	$2i\hat{A}_3$	$-2i\hat{A}_2$	$2i\hat{A}_5$	$-2i\hat{A}_4$	$2i\hat{A}_7$	$-2i\hat{A}_6$
$\hat{D}_2$	0	0	0	0	0	0	0	0	$2i\hat{A}_2$	$2i\hat{A}_3$	$-2i\hat{A}_0$	$-2i\hat{A}_1$	$2i\hat{A}_6$	$2i\hat{A}_7$	$-2i\hat{A}_4$	$-2i\hat{A}_5$
$\hat{D}_3$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\hat{D}_4$	0	0	0	0	0	0	0	0	$2i\hat{A}_4$	$2i\hat{A}_5$	$2i\hat{A}_6$	$2i\hat{A}_7$	$-2i\hat{A}_0$	$-2i\hat{A}_1$	$-2i\hat{A}_2$	$-2i\hat{A}_3$
$\hat{D}_5$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\hat{D}_6$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\hat{D}_7$	0	0	0	0	0	0	0	0	$-2i\hat{A}_7$	$2i\hat{A}_6$	$2i\hat{A}_5$	$-2i\hat{A}_4$	$2i\hat{A}_3$	$-2i\hat{A}_2$	$-2i\hat{A}_1$	$2i\hat{A}_0$
$\hat{A}_0$	0	$-2i\hat{A}_1$	$-2i\hat{A}_2$	0	$-2i\hat{A}_4$	0	0	$2i\hat{A}_7$	0	$2i\hat{D}_1$	$2i\hat{D}_2$	0	$2i\hat{D}_4$	0	0	$-2i\hat{D}_7$
$\hat{A}_1$	0	$2i\hat{A}_0$	$-2i\hat{A}_3$	0	$-2i\hat{A}_5$	0	0	$-2i\hat{A}_6$	$-2i\hat{D}_1$	0	0	$2i\hat{D}_2$	0	$2i\hat{D}_4$	$2i\hat{D}_7$	0
$\hat{A}_2$	0	$-2i\hat{A}_3$	$2i\hat{A}_0$	0	$-2i\hat{A}_6$	0	0	$-2i\hat{A}_5$	$-2i\hat{D}_2$	0	0	$2i\hat{D}_1$	0	$2i\hat{D}_7$	$2i\hat{D}_4$	0
$\hat{A}_3$	0	$2i\hat{A}_2$	$2i\hat{A}_1$	0	$-2i\hat{A}_7$	0	0	$2i\hat{A}_4$	0	$-2i\hat{D}_2$	$-2i\hat{D}_1$	0	$-2i\hat{D}_7$	0	0	$2i\hat{D}_4$
$\hat{A}_4$	0	$-2i\hat{A}_5$	$-2i\hat{A}_6$	0	$2i\hat{A}_0$	0	0	$-2i\hat{A}_3$	$-2i\hat{D}_4$	0	0	$2i\hat{D}_7$	0	$2i\hat{D}_1$	$2i\hat{D}_2$	0
$\hat{A}_5$	0	$2i\hat{A}_4$	$-2i\hat{A}_7$	0	$2i\hat{A}_1$	0	0	$2i\hat{A}_2$	0	$-2i\hat{D}_4$	$-2i\hat{D}_7$	0	$-2i\hat{D}_1$	0	0	$2i\hat{D}_2$
$\hat{A}_6$	0	$-2i\hat{A}_7$	$2i\hat{A}_4$	0	$2i\hat{A}_2$	0	0	$2i\hat{A}_1$	0	$-2i\hat{D}_7$	$-2i\hat{D}_4$	0	$-2i\hat{D}_2$	0	0	$2i\hat{D}_1$
$\hat{A}_7$	0	$2i\hat{A}_6$	$2i\hat{A}_5$	0	$2i\hat{A}_3$	0	0	$-2i\hat{A}_0$	$2i\hat{D}_7$	0	0	$-2i\hat{D}_4$	0	$-2i\hat{D}_2$	$-2i\hat{D}_1$	0

Appendix B
Copyright Information

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Appendix C
Symbols and Abbreviations

$\dot{x}$	$\frac{dx}{dt}$
$\mathcal{R}$	Real part of
$\mathcal{I}$	Imaginary part of
BCH	Baker-Campbell-Hausdorff
$su(N)$	Special unitary Lie algebra in N dimensions
$SU(N)$	Special unitary Lie group in N dimensions
$H.c.$	Hermitian conjugate
LOCC	Local operations and classical communication

Vita

Sai Vinjanampathy was born in Chennai (Madras), Tamilnadu, India. He attended Kendriya Vidyalaya where he pursued all of his schooling. He finished his undergraduate studies at Madras University May 2002. He earned a master of science degree in physics from the Indian Institute of Technology, Madras in 2004. In 2005, he came to Louisiana State University to pursue graduate studies in physics and astronomy.