Geometric Phases for Three State Systems

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Mark Byrd

Center for Particle Physics
University of Texas at Austin
Austin, Texas 78712-1081

Abstract

The adiabatic geometric phases for general three state systems are discussed. An explicit parameterization for space of states of these systems is given. The abelian and non-abelian connection one-forms or vector potentials that would appear in a three dimensional quantum system with adiabatic characteristics are given explicitly. This is done in terms of the Euler angle parameterization of SU(3) which enables a straight-forward calculation of these quantities and its immediate generalization.

1mbyrd@physics.utexas.edu
1 Introduction

Geometric phases have received a great deal of attention since their description by Berry [1]. The reasons are clear. They are a fundamental property of many quantum mechanical systems. They also have a beautiful description in terms of differential geometry and fiber bundles [2] which is directly related to gauge field theory (see for example [3]). Their physical importance was known long before the excitement about them in the mid 80’s [4], [5], [6]. In spite of all the attention, there have been few worked out examples and the examples that have been worked out, the descriptions haven’t been straightforward. The most well-known example is that of a two state system, namely a magnetic dipole, in a magnetic field. This was the original example given by Berry [1]. Wilczek and Zee originally pointed out that there could exist non-abelian geometric phases [7]. Later people studied fermionic systems with a quadrapole Hamiltonian [8].

Uhlmann later developed machinery, namely a parallel transport [10], for describing the non-abelian geometric phases associated with density matrices. However, this was never applied to three state systems. Arvind et al and Khanna et al studied the geometric phases for three state systems that involve pure state density matrices [11], [12] with a parameterization that was somewhat ad hoc. Mostafazadeh looked at a way of calculating the non-abelian geometric phases for a three state system with a two-fold degeneracy [13] also with ad hoc coordinates. These topics will be brought together here.

In this paper the objective is to use explicit $SU(3)$ representations to extend and/or simplify several aspects of three state systems.

1. The expression for the density matrix for three state systems.
2. The identification of the parameter spaces of these systems.
3. The calculation of the abelian geometric phases for three state systems.
4. The calculation of the non-abelian geometric phases of three state systems with a two-fold degeneracy.

An obvious example of a three state system would be a spin one particle in a magnetic field. If this external magnetic field is “slowly” rotating then we may have the conditions for an adiabatic change in phase. For a proper description of what “slowly” means in this context see [14]. Unless otherwise stated, this paper will be concerned with the adiabatic geometric phases.
\[\begin{align*}
\lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \lambda_2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \lambda_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
\lambda_4 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, & \lambda_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & i \\ i & 0 & 0 \end{pmatrix}, & \lambda_6 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \\
\lambda_7 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & i \\ 0 & i & 0 \end{pmatrix}, & \lambda_8 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.
\end{align*}\]

Table 1: The Gell-Mann Matrices

although with some work this could be extended to non-adiabatic phase changes.

2 The Density Matrix for a System with Three Quantum States

As is demonstrated in the next section the density matrix can be parameterized by the action of an \(SU(3)\) transformation. This will prove convenient for many calculations and is immediately generalizable to a system with an arbitrary number of states. See [15] and below for a discussion.

The density matrix for general pure state three-level systems is given in [11] and [12]. It can be represented in the following way: Let \(\psi\) be a state in a three dimensional complex Hilbert space \(\mathcal{H}^{(3)}\). The density matrix is the matrix \(\rho\) described by (in analogy with two state systems):

\[
\rho = \psi \psi^\dagger = |\psi\rangle\langle\psi| = \frac{1}{3} (1 + \sqrt{3} \vec{n} \cdot \vec{\lambda})
\]

\(\psi \in \mathcal{H}^{(3)}, \quad (\psi, \psi) = 1.\)

Here the dagger denotes the hermitian conjugate, \(\vec{n}\) is a real eight dimensional unit vector, \(\vec{\lambda}\) represents the eight Gell-Mann matrices. The dot product is the ordinary sum over repeated indices \(n^r \lambda_r\). The \((\cdot, \cdot)\) is the inner product on the space \(\mathcal{H}^{(3)}\). The pure state density matrix satisfies:

\[
\rho^\dagger = \rho^2 = \rho \geq 0 \quad \text{Tr}\rho = 1.
\]
This is equivalent to the following conditions on $n$:

$$n^* = n \quad n \cdot n = 1 \quad n \star n = n. \quad (2)$$

The star product is defined by

$$(a \star b)_i = \sqrt{3} d_{ijk} a_j b_k \quad (3)$$

where the $d_{ijk}$ are the components of the completely symmetric tensor appearing in the anticommutation relations

$$\{\lambda_i, \lambda_j\} = \frac{4}{3} \delta_{ij} + 2 d_{ijk} \lambda_k.$$

Explicitly the nonzero $d_{ijk}$ are

$$d_{118} = d_{228} = d_{338} = -d_{888} = \frac{1}{\sqrt{3}} \quad d_{448} = d_{558} = d_{668} = d_{778} = -\frac{1}{2\sqrt{3}}$$

$$d_{146} = d_{157} = -d_{247} = d_{256} = d_{344} = d_{355} = -d_{366} = -d_{377} = \frac{1}{2}.$$

3 Parameter Spaces for Three State Systems

The parameter space of states of the three state systems can easily be seen to be coset spaces of $SU(3)$. The Euler angle parameters are a particularly convenient way in which to see this.

A representation of the coset space $SU(3)/U(2)$ and of the density matrix for the pure states of a three state system may be obtained in terms of the Euler parameters given in [16]. There the group $SU(3)$ is parameterized by

$$D(\alpha, \beta, \gamma, \theta, a, b, c, \phi) = e^{(i\lambda_3 a)} e^{(i\lambda_2 \beta)} e^{(i\lambda_3 \gamma)} e^{(i\lambda_5 \theta)} e^{(i\lambda_3 a)} e^{(i\lambda_2 b)} e^{(i\lambda_3 c)} e^{(i\lambda_8 \phi)}.$$

With this parameterization and the explicit representation of the corresponding adjoint representation in terms of the Euler angle parameters in [17], a parameterization of the density matrix of the three state system may be obtained by the following projection which is analogous to the Hopf map given in [18]:

$$x = \pi(D) = D \left[ \frac{1}{3} (1 - \sqrt{3} \lambda_8) \right] D^{-1}. \quad (4)$$
Here \( x \in SU(3)/U(2) \) and \( D \) represents a point in the space \( SU(3) \). This projection is clearly invariant under the right action of a \( U(2) \) operation defined by \( U \in U(2) \) with

\[
U = e^{(i\lambda_3 a')} e^{(i\lambda_2 b')} e^{(i\lambda_3 c')} e^{(i\lambda_8 \phi')}.
\]

This then defines the projection from \( SU(3) \) to \( SU(3)/U(2) \). Since the second term in equation (4) is simply an adjoint action on \( \lambda_8 \), it can be read directly from the equations given in [17]. There the matrix \( R_{ij} \) that satisfies

\[
D \lambda_i D^{-1} = R_{ij} \lambda_j
\]

was given explicitly.

One may of course note that the projection operator is not unique. Any \( 3 \times 3 \) matrix with a one on its diagonal would be invariant under a \( U(2) \) subgroup and would represent a pure state. It is, however, rather convenient in this parameterization to use this particular matrix:

\[
\frac{1}{3} (1 - \sqrt{3} \lambda_8) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},
\]

so that it is clear that the upper left \( 2 \times 2 \) matrix of zeros will be unaffected by an \( SU(2) \) transformation in that block. This matrix could be substituted for another that has one 1 on a diagonal and zeros elsewhere and still be invariant under (another) \( SU(2) \). The invariance of this with respect to an overall phase gives the \( U(2) \) invariance.

Now equation (4) can be rewritten as

\[
x = \left[ \frac{1}{3} (1 - \sqrt{3} R_{8j} \lambda_j) \right] = \left[ \frac{1}{3} (1 + \sqrt{3} n_j \lambda_j) \right]
\]

where we identify the \( R_{8j} \) as the components of a vector that satisfies those properties given in equation (4). This can be viewed as an arbitrary rotation of the vector \( \lambda_8 \) with an adjoint action of the group (equation (5)) and of course it is now clear that \( x \) is identified with \( \rho \).

The vector \( \vec{n} \) has the following components.

\[
n_1 = -R_{81} = -\frac{\sqrt{3}}{2} \cos 2\alpha \sin 2\beta \sin^2 \theta
\]
\[ n_2 = -R_{s2} = \frac{\sqrt{3}}{2} \sin 2\alpha \sin 2\beta \sin^2 \theta \]
\[ n_3 = -R_{s3} = \frac{\sqrt{3}}{2} \cos 2\beta \sin^2 \theta \]
\[ n_4 = -R_{s4} = \frac{\sqrt{3}}{2} \cos(\alpha + \gamma) \cos \beta \sin 2\theta \]
\[ n_5 = -R_{s5} = -\frac{\sqrt{3}}{2} \sin(\alpha + \gamma) \cos \beta \sin 2\theta \]
\[ n_6 = -R_{s6} = -\frac{\sqrt{3}}{2} \cos(\alpha - \gamma) \sin \beta \sin 2\theta \]
\[ n_7 = -R_{s7} = -\frac{\sqrt{3}}{2} \sin(\alpha - \gamma) \sin \beta \sin 2\theta \]
\[ n_8 = -R_{s8} = -1 + \frac{3}{2} \sin^2 \theta \]  \hspace{1cm} (7)

From this, using the equations \( n_i = \psi^\dagger \lambda_i \psi \), it follows that

\[ \psi = e^{i\chi} \begin{pmatrix} e^{i(\alpha+\gamma)} \cos \beta \sin \theta \\ e^{-i(\alpha-\gamma)} \sin \beta \sin \theta \\ \cos \theta \end{pmatrix} \]  \hspace{1cm} (8)

This may be recognized as the third column of the \( SU(3) \) matrix \( D \) above, thus agreeing with the calculation given in [11] and coming full circle in the analysis. In this case the overall phase \( \chi \) may be identified as \(-2\phi/\sqrt{3}\) in the matrix \( D \). In section 3 it will become clear why this works and it will be generalized for the case of non-abelian geometric phases.

Although many of the details have not been worked out for \( SU(n) \) groups, (the Euler angle parameters, the adjoint representation, etc.) the method of identifying the space of the parameters is the same (see [14]). For a system with \( n \) states, one may express a general diagonal density matrix in terms of the squared elements of an \( n-1 \) sphere. Then to take it to a general basis, one acts with the appropriate \( SU(n) \) matrix. The result is always a subset of \( SU(n)/T^{n-1} \), where \( T^{n-1} \) is the maximal \( (n-1) \) torus for the group. If there are degenerate eigenvalues in the matrix, this space is reduced. For example in the case of three states discussed shortly, the parameter space is a subset of \( SU(n)/(SU(2) \times U(1)) \) since there exists a two-fold degeneracy. For an \( m \)-fold degeneracy we reduce the space by \( SU(m) \). In the case of an adiabatic approximation, we will see this is a proper subset, but were we to relax this
condition, the space would be isomorphic to these spaces, not subsets. In this way, one may identify a necessary condition for non-abelian geometric phases, namely the existence of the degeneracy and thus an $SU(m)$ factor in the denominator of the above coset expression.

Using this parameterization one gains essentially nothing over the expression of the Bloch sphere for two-state systems. In that case the common parameterization of the Bloch sphere,

$$
\begin{pmatrix}
  a & 0 \\
  0 & 1-a
\end{pmatrix}
$$

is really no different than the one presented here,

$$
\begin{pmatrix}
  \cos^2 \theta & 0 \\
  0 & \sin^2 \theta
\end{pmatrix}
$$

except that positivity is automatic. However in the case of three state systems, we have

$$
\begin{pmatrix}
  \cos^2 \theta & \sin^2 \phi & 0 & 0 \\
  0 & \sin^2 \theta & 0 & \sin^2 \phi \\
  0 & 0 & 0 & \cos^2 \phi
\end{pmatrix}
$$

This is a convenient parameterization since the analogous Bloch sphere would have parameters with a non-rectangular domain. The parameterization given here (see also [13]) then helps with the analysis of three state density matrices and their corresponding entropy [19].

4 Connection, Curvature, and Abelian Geometric Phases

In the spirit and notation of Nakahara [3], we can now derive the connection one form, the curvature and the Geometric Phase of the three state system. The connection one form, sometimes called Berry’s connection, can be written in terms of $\psi$ in the following way. Define the total phase to be

$$
\varphi \equiv i \int \mathcal{A}
$$

$$
\mathcal{A} = \mathcal{A}_\mu dx^\mu = -i \langle \psi | d | \psi \rangle,
$$

(10)
where $d$ is the ordinary exterior derivative. Using equation (7), this becomes

$$\mathcal{A} = d\chi + \sin^2 \theta [\cos^2 \beta (d\alpha + d\gamma) - \sin^2 \beta (d\alpha - d\gamma)].$$

(11)

This agrees with reference [11] if the following identifications are made with those quantities on the left being those of reference [11] and those on the right being ours.

$$\eta \leftrightarrow \chi \quad \theta \leftrightarrow \theta \quad \chi_1 \leftrightarrow \alpha + \gamma \quad \chi_2 \leftrightarrow \alpha - \gamma.$$

The corresponding curvature two form is given by

$$F = d\mathcal{A} = -id\psi^\dagger \wedge d\psi$$

$$= \sin 2\theta \cos^2 \beta d\theta \wedge d(\alpha + \gamma) - \sin^2 \theta \sin 2\beta d\beta \wedge d(\alpha + \gamma)$$

$$- \sin 2\theta \sin^2 \beta d\theta \wedge d(\alpha - \gamma) - \sin^2 \theta \sin 2\beta d\beta \wedge d(\alpha - \gamma).$$

(12)

This then, is the analogue of the “solid angle formula” for the two state systems. In other words, the integral of this curvature two form gives the geometric phase, just as

$$\varphi_g = \frac{1}{2} \Omega$$

in two state systems, where $\Omega$ is the solid angle for the two sphere. The geometric phase is just the integral of the connection one form without the overall phase factor $\chi$, that is,

$$\varphi_g = \int \sin^2 \theta [\cos^2 \beta (d\alpha + d\gamma) - \sin^2 \beta (d\alpha - d\gamma)]$$

$$= \int [\sin^2 \theta \cos 2\beta d\alpha + \sin^2 \theta d\gamma],$$

(13)

which again, agrees with [11].

5 Non-abelian Geometric Phases

In this section a novel way of obtaining geometric phases for 3-state systems is given. This method is a generalization and simplification over the method presented in [13] and a generalization over the method given in the previous section. The way the connection one-forms for the 3-state systems are derived here uses the fact that the state space of the system can be expressed in
terms of the group $SU(3)$. This enables the calculation of the forms without diagonalization of the Hamiltonian. In effect, the Hamiltonian is taken to be in diagonal form initially. It is then “undiagonalized” by an $SU(3)$ action which takes it into a general non-diagonal hermitian matrix. This method has the advantage of being potentially generalizable to other states, not just eigenstates of the Hamiltonian. (Of course, one has to be careful of what the adiabatic assumption means then. This is well described in [14].) It also has the advantage of being generalizable to $SU(n)$. Whereas one does not have a way of finding the eigenvalues of an $n \times n$ matrix, one would be able to use $SU(n)$ matrices and derive the connection forms for an $n$-state system. (Again, see [15].)

The aim is to find the adiabatic non-abelian geometric phase associated to the two-fold degeneracy of energy eigenvalues of the general Hamiltonian for a 3-state system. These are the simplest non-abelian geometric phases.

Let $H(t) = H(\vec{R}(t))$ be the time dependent Hamiltonian of the system and let $E_n(t)$ be its eigenvalues. Then if the Hamiltonian is periodic in time with period $T$, i.e., the curve $C : [0, T] \rightarrow M$ is closed. Here $M$ is the manifold parameterized by the coordinates $\vec{R}$. For the adiabatic approximation, $n$ labels the eigenstates, $|\psi\rangle$, of the Hamiltonian and does not change. This means there is a unitary matrix $U(n)$ relating $|\psi(T)\rangle$ and $|\psi(0)\rangle$ which is given by

$$e^{-\frac{i}{\hbar}\int_0^T E_n(t) dx \left[ e^{i \oint A_n} \right]}.$$ 

Here $\mathcal{P}$ is the path-ordering operator and $A_n$ is a Lie algebra valued (connection) one-form whose matrix elements are locally given by:

$$A_n^{ab} = i \langle n, a, \vec{R} | d | n, b, \vec{R} \rangle. \quad (14)$$

It is important to note that the Hamiltonian is a $3 \times 3$ Hermitian matrix which can be viewed as an element of the algebra of $SU(3)$, i.e.,

$$H(\vec{R}) = b \sum_{i=0}^{8} R^i \lambda_i,$$

where $R^i$ are real parameters, the $\lambda_i$ are $\lambda_0 = 1_{3 \times 3}$ and the Gell-Mann matrices of Table (1). Here the constant $b$ is taken to be one. The adiabaticity assumption may then be expressed as $T \gg 1$. 
The Hamiltonian, $H$, can be expressed in terms of the diagonalized Hamiltonian, $H_D$.

$$H(\vec{R}) = U(\vec{R}) H_D U^{-1}(\vec{R}) ,$$

where $U(\vec{R}) \in SU(3)$ and

$$H_D = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_1 & 0 \\ 0 & 0 & E_3 \end{pmatrix} .$$

In this form it is obvious that $M \subset \mathbb{C}P^2$ and what is more, it is clear from (6) that only the angles $\alpha, \beta, \gamma$ and $\theta$ will remain since $\lambda_1, \lambda_2, \lambda_3$ and $\lambda_8$ commute with $H_D$. Explicitly, the Hamiltonian in undiagonalized form, $H$, is given by

$$
\begin{align*}
H_{11} &= E_1 (\cos^2 \beta \cos^2 \theta + \sin^2 \beta) + E_3 \cos^2 \beta \sin^2 \theta \\
H_{12} &= (E_1 - E_3) e^{-2i\alpha} \cos \beta \sin \beta \sin^2 \theta \\
H_{13} &= (E_3 - E_1) e^{-i(\alpha + \gamma)} \cos \beta \sin \theta \cos \theta \\
H_{21} &= (E_1 - E_3) e^{2i\alpha} \cos \beta \sin \beta \sin^2 \theta \\
H_{22} &= E_1 (\sin^2 \beta \cos^2 \theta + \cos^2 \beta) + E_3 \sin^2 \beta \sin^2 \theta \\
H_{23} &= (E_1 - E_3) e^{i(\alpha - \gamma)} \sin \beta \sin \theta \cos \theta \\
H_{31} &= (E_3 - E_1) e^{i(\alpha + \gamma)} \cos \beta \sin \theta \cos \theta \\
H_{32} &= (E_1 - E_3) e^{-i(\alpha - \gamma)} \sin \beta \sin \theta \cos \theta \\
H_{33} &= E_1 \cos^2 \theta + E_3 \sin^2 \theta
\end{align*}
$$

It can easily be shown that these angles parameterize $\mathbb{C}P^2$. In this way one can easily identify the patches needed for certain circumstances. This is analogous to the calculation here.

As is well known, the matrix that diagonalizes $H$ is composed of its eigenvectors. Therefore, given that $H = UH_DU^{-1}$, $H_D = U^{-1}HU$, so we have our $|\psi\rangle$s, the eigenvectors of $H$, they are

$$
\begin{pmatrix} e^{-i(\alpha + \gamma)} \cos \beta \cos \theta \\
-e^{i(\alpha - \gamma)} \sin \beta \cos \theta \\
-\sin \theta \end{pmatrix}, \begin{pmatrix} e^{-i(\alpha + \gamma)} \sin \beta \\
e^{i(\alpha + \gamma)} \cos \beta \\
0 \end{pmatrix}, \begin{pmatrix} e^{-i(\alpha + \gamma)} \cos \beta \sin \theta \\
-e^{i(\alpha - \gamma)} \sin \beta \sin \theta \\
\cos \theta \end{pmatrix} .
$$

One can check that these are already orthonormal due to the fact that $U \in SU(3)$.
Now all that needs to be done is calculate the connection forms given by (14). These are given by

\[ A_1 = \cos 2\beta \cos^2 \theta \, d\alpha + \cos^2 \theta \, d\gamma, \]

and

\[ A_2 = \begin{pmatrix}
-\cos 2\beta \, d\alpha - d\gamma & e^{-2i\gamma}[\sin 2\beta \sin \theta \, d\alpha - i \sin \theta \, d\beta] \\
e^{2i\gamma}[\sin 2\beta \sin \theta \, d\alpha + i \sin \theta \, d\beta] & \cos 2\beta \sin^2 \theta \, d\alpha + \sin^2 \theta \, d\gamma
\end{pmatrix}.\]

This is a expression in terms of SU(3) Euler angle coordinates. We can generalize this by using the expression (3). This allows us to express the density matrix for an \( n \)-state system in terms of the Euler angle coordinates and the components of the \( n - 1 \) sphere along the diagonal and an overall scale factor. Thus the eigenvalues need not be those of the Hamiltonian but of any observable. Then a similar analysis holds for states that are not eigenvectors of the Hamiltonian but eigenvectors of another observable with the caution that, as stated before, one must be careful of what one means by an adiabatic approximation.

### 6 Conclusions/Comments

The diagonalized density matrices can be parameterized by the squared elements of the sphere (an \( n - 1 \) sphere for a system of \( n \) states) combined with an SU(\( n \)) action. This novel parameterization helps to identify the parameter spaces of these systems. The spaces are isomorphic to subspaces of SU(\( n \))/T\( n \) for all eigenvalues unique, to subspaces of SU(\( n \))/(SU(2) \times T^{n-1}) for one two-fold degeneracy, SU(\( n \))/(SU(3) \times T^{n-2}) for one three-fold degeneracy, etc. This is because the density matrix and Hamiltonian are both in the algebra of the group and can represented as \( UAU^{-1} \), where \( U \in SU(n) \) and \( A \) is the non-diagonal density matrix or Hamiltonian. When this is the Hamiltonian, we immediately know the eigenvectors because they are the rows of the matrix that diagonalizes the Hamiltonian. This enables the evaluation (in principle) of the geometric phases for the \( n \)-state systems. Here we have shown this explicitly for the case of three quantum states.

In this analysis the Euler angle parameterization has been extremely useful and although its generalization to SU(\( n \)) is possible, the decomposition into components of the spheres and SU(\( n \)) actions is independent of the parameterization.
In applications to multi-pole Hamiltonians were discussed. I would like to add that there are phenomenological nuclear physics models that use $SU(3)$. These multi-pole Hamiltonians are expressible in terms of the differential operators in [16], and [17]. The author expects to perform a further analysis of the relations to those and other multi-pole Hamiltonians in the near future.

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