

Geometry of n -state Systems, Pure and Mixed

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Abstract. We discuss the geometry of states of quantum systems in an n -dimensional Hilbert space in terms of an explicit parameterization of all such systems. The geometry of the space of pure as well as mixed states for n -state systems is discussed. The parameterization is particularly useful since it allows for the simple construction and isolation of various physically meaningful subspaces of the space of all density matrices. This is used to describe possible geometric phases, their calculation, and analyze entropy and purity (or linear entropy) functions. In particular, we provide conditions under which nontrivial abelian and/or nonabelian geometric phases arise in these subspaces in terms of the given parameterization, an explicit example is given, and multi-dimensional isentropic surfaces are discussed.

M.S. Byrd would like to dedicate this joint work to Professor E.C.G. Sudarshan on his 75th birthday. His insight into this subject contributed to an earlier version of this manuscript and has led to ongoing research in this area which is described in the latter sections.

1. Introduction

Two-state systems are ubiquitous in the physics literature. This is due to several factors, not the least of which is their common properties. All two-state systems share some features due to the two-dimensional Hilbert space which we use to describe them. However, in addition to the more abstract properties, and in part due to those properties, two-state systems share less abstract features which are experimentally observable. For example, the two polarization states of a light beam can undergo a phase change due to the geometry of a fiber through which they are traveling [1] and the two spin states of a spin one-half nucleus can undergo a phase change due to a slowly varying external magnetic field [2]. Each of these phase changes is geometric in nature because the path is reparameterization invariant and is due to the holonomy of the system [3]. They are therefore referred to as geometric phases or Berry phases. Although the physical mechanism for these phases is quite different, as are the systems themselves, they can be described using a kinematical prescription which applies to both two-state systems and looks quite similar in the abstract sense [4].

Two-state systems however, are often not truly comprised of only two states as in the examples above, but are two states of a larger system. For example, they could be two states of an atom or molecule which belong to a set of states which is countably (or even uncountably) infinite. Systems with n states, or n -state systems, also share common features if they have the same value n . For example, three-state systems (see for example [5], [6], [7]) have properties which

are common to each, but which can be quite different from two-state systems. Similarly remarks hold for n -state systems (see for example [7], [8] and [9]).

A natural question to ask is, what properties of n -state systems are similar, and which are different, from their two-state counterparts? In order to answer this question, we will employ the density operator or density matrix. (Here we will often not distinguish between the two.) Many of the common properties of n -state systems are due to the structure of the space of density operators for these systems. This structure can aide in determining many properties of physical systems ranging quantum statistical mechanics and thermodynamics to ordinary quantum mechanics (see [10, 11, 12], [13], [14] and references therein). *This is the objective of this paper, to understand properties of n -state systems which are due to the geometry of the space of states and that are common to all n -state systems.* There are two different, but related, geometries we will consider. One is the geometry of the space of density operators. Second is the geometry associated with the Berry phase.

The particulars of geometric phases for density matrices of three state systems in $SU(3)$ representations were studied in Refs. [15], [16] from a kinematical perspective. There it was shown that nontrivial geometric phases for the pure state density matrices can be associated with subgroups of $SU(3)$. They also gave formulas for the Berry connection one form and curvature two form. Another group theoretical method for deriving these was then pointed out in Ref. [17, 18] along with the necessary differential geometric structures in a particular parameterization (discussed further below).

Here we provide a method for determining, for n -state systems, the mixed state density matrices that will exhibit geometric phases and what type of phases we should expect (abelian *vs.* nonabelian). To do this, we use a generalization of the parameterization and methods in [17, 18] and we restrict to closed evolution of a system which may have previously undergone an evolution which caused it to become mixed. A different approach to the explicit calculation of geometric phases for mixed state density matrices uses a purification technique [19, 20, 21]. More recently, the general geometric phases for open systems have been studied using rather different methods. (See [22, 23] and references therein.)

It is interesting and relevant to note that after an earlier version of this work [24], geometric phases for mixed states were studied in some detail by *Ercolessi et al.* [25] and the specific geometric structures were derived. Moreover, many others followed this work with an emphasis on particular applications, one of the first being the work in Ref. [26].

In this paper, we provide simple but general geometric arguments which help to analyze the spaces of density operators and their geometric phases. Specifically, in section 2 we give a brief review of density matrices and a parameterization of density operators, *mixed* as well as pure, for an n -state system and discuss the geometry of these spaces. Then, in section 3 we give a brief history and review of geometric phases. We then identify the spaces which could give rise to nontrivial geometric phases by a simple argument involving our explicit parameterization. We also provide an explicit example of a calculation of a non-abelian geometric phase. Finally, in section 4, we briefly discuss the entropy of the space of density matrices and how it is able to be analyzed using the eigenvalue parameterization of the density operator.

2. Density Matrices for n -state Systems

Pure states in Quantum Mechanics are represented by one-dimensional subspaces or rays in Hilbert space, \mathcal{H} . These states can be characterized as orthogonal projections of unit trace

$$\{\text{space of pure states}\} \approx \{\rho \in \text{End}(\mathcal{H}) \mid \rho^\dagger = \rho, \rho^2 = \rho, \text{Tr}\rho = 1\}. \quad (1)$$

Von Neumann and Landau originally introduced the notion of *mixed* states into Quantum Mechanics [27]. To include mixed states into our current discussion, we recall that it is enough

to enlarge (1) by simply relaxing the idempotency condition, $\rho^2 = \rho$ but keeping positive semidefinite condition ($\rho \geq 0$, meaning all eigenvalues are nonnegative), thus

$$\{\text{space of mixed states}\} \approx \{\rho \in \text{End}(\mathcal{H}) \mid \rho^\dagger = \rho, \rho \geq 0, \text{Tr}\rho = 1\}. \quad (2)$$

As mentioned before, two state systems have been studied in great detail. Here we review some of the features that we seek to generalize to systems with n states. Consider first the pure states of a 2-state system. The Hilbert space will be $\mathbb{C}^2 \cong \mathbb{R}^4$. The unit vectors will form $S^3 \subset \mathbb{R}^4$, and the true *physical* states will be obtained by modding out a phase S^1 :

$$S^2 = S^3/S^1 \quad \text{or} \quad \beta : S^1 \rightarrow S^3 \rightarrow S^2 \quad (3)$$

which is the fundamental Hopf (β) fibering. The S^1 is associated with the geometric phase.

In the construction

$$\{\rho \text{ pure}\} \leftrightarrow \text{sphere of radius } \frac{1}{2}, \quad (4)$$

the mixed states can be identified with the *interior* of this two-sphere (fig 1)

$$\{\rho \text{ mixed}\} \leftrightarrow \text{closed ball } D^3 \text{ of radius } \frac{1}{2}, \quad (5)$$

where we have used a radius one for S^3 so a radius one-half for S^2 . The most mixed state is the center of the ball, O , and for any two normalized pure states A and B in the ball,

$$0 \leq \text{overlap}(A, B) \equiv |\langle A|B \rangle|^2 \leq 1$$

is only zero if B is antipodal to A .

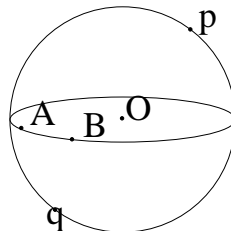


Figure 1. The disk D^3 represents the space of mixed states in a 2-state system. The surface S^2 consists of pure states. The point p and the antipodal point q form an orthogonal pair.

Following a somewhat similar approach, we will proceed to discuss the geometry of the spaces of pure and mixed state density matrices for more general n -state systems.

2.1. Pure State Density Matrices

The space of a pure state density matrix for an n -state system is isomorphic to \mathbb{CP}^{n-1} . This may be seen in two different ways.

First, as above, consider the common example of a pure state for a 2-state system. Use the space $\mathbb{C}^2 \approx \mathbb{R}^4$, restrict to the transformations that preserve the modulus squared, S^3 , and projects out an overall phase to obtain \mathbb{CP}^1 . Similarly, for a 3-state system, one would use the space $\mathbb{C}^3 \approx \mathbb{R}^6$, restricted to the transformations that preserve the modulus squared, S^5 , and project out an overall phase to obtain $\mathbb{CP}^2 \cong S^3/S^1$.

Now one finds an immediate generalization. For an n -state system, one would use the space $\mathbb{C}^n \approx \mathbb{R}^{2n}$, restricted to the transformations that preserve the modulus squared, S^{2n-1} , and

project out an overall phase to obtain \mathbb{CP}^{n-1} . Therefore *the space of pure states for an n -state system is*

$$\mathbb{CP}^{n-1} = \frac{\mathbb{C}^n - \{0\}}{\mathbb{C}^1 - \{0\}} = \frac{S^{2n-1}}{S^1}. \quad (6)$$

The second way to discover this will lead to a parameterization of the density matrices for n -state systems. Consider the density operator for a pure state that is represented by an $n \times n$ matrix of zeros except for a single 1 somewhere on the diagonal, *viz.*,

$$\rho_{\text{pure}} = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & \ddots & & 0 \\ \vdots & & 1 & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}. \quad (7)$$

For convenience we may take the 1 to be in the n^{th} column and n^{th} row.

Now if we wish to transform this into an arbitrary pure state, ρ transforms as $A\rho A^{-1} = A\rho A^\dagger$ under any unitary transformation $A \in U(n)$. On the other hand, any two pure states are always equivalent under a transformation A , *i.e.*, $U(n)$ acts transitively on \mathbb{CP}^{n-1} . From the previous matrix form, it is clear that the little group is $U(n-1) \times U(1)$ hence

$$\frac{U(n)}{U(1) \times U(n-1)} = \frac{SU(n)}{U(n-1)} = \mathbb{CP}^{n-1} = \text{Gr}(1, n), \quad (8)$$

where, the Grassmanian of r -planes in \mathbb{C}^n

$$\text{Gr}(r, n) = \frac{U(n)}{U(r) \times U(n-r)} \quad (9)$$

is well known.

Heuristically, we can go from the form (6) to the form (8) by exhibiting the odd-sphere structure [28]

$$U(n) \cong S^1 \times S^3 \ltimes S^5 \ltimes \cdots \ltimes S^{2n-1}, \quad (10)$$

where the product, (\ltimes) , is a nontrivial (twisted) one. So

$$\frac{U(n)}{U(1) \times U(n-1)} = \text{Gr}(1, n) = \mathbb{CP}^{n-1} = \frac{S^{2n-1}}{S^1}. \quad (11)$$

2.2. Mixed State Density Matrices

Using the pure state operator described above, a parameterization of an n -state density operator matrix can be given. Each pure state can be represented by a matrix which in diagonal form, would consists of zeros everywhere except for a single 1 on the diagonal as indicated by Eq. (7). To achieve a mixture of these states, a convex combination of a complete set, *i.e.* the set of n matrices which has a different nonzero diagonal, is required. This combination may be written as follows:

$$\rho = \left(\sum_i a^i \rho_i \right),$$

where ρ is the mixed state matrix. The ρ_i , $i = 1 \dots n$, are the pure state matrices with the 1 in the i^{th} along the diagonal and satisfy $\text{Tr}(\rho_i \rho_j) = \delta_{ij}$. The a^i satisfy $\sum_i a^i = 1$ and $0 \leq a_i \leq 1$.

The eigenvalues of this matrix, the a^i , can be parameterized by the squared components of an $(n - 1)$ -sphere. For example, for three state systems the eigenvalues can be taken to be

$$a^1 = \cos^2 \phi/2 \sin^2 \theta/2, \quad a^2 = \sin^2 \phi/2 \sin^2 \theta/2, \quad a^3 = \cos^2 \theta/2.$$

We can now obtain a parameterization of a general mixed state, one in a generic non-diagonal configuration for an n -state density matrix. Let ρ denote the diagonal density operator where the diagonal elements are the squared components of the $n - 1$ sphere as discussed above and let D denote an $SU(n)$ matrix. Then the mixed state density operator matrix is given by

$$\rho' = D\rho D^{-1}. \quad (12)$$

Note, however, that parameter counting might lead us to believe that we have *too many* parameters since $n - 1$ parameters are required for ρ and $n^2 - 1$ for D , whereas there are only $n^2 - 1$ total parameters for a Hermitian matrix with trace one. This problem is solved, however, by noting that the diagonal density operator commutes with any diagonal operator D (unitary transformation) and is thus invariant under conjugate actions by the Cartan subgroup of $U(n)$; the Cartan subgroup being the exponential of a set of simultaneously diagonalizable elements of the algebra of $SU(n)$, of which there are exactly $n - 1$. This problem was explicitly discussed and solved for two and three state systems in [29]. For n state systems, one can solve this by the same methods. One may parameterize $SU(n)$ using a generalized Euler angle parameterization [30, 31] and construct it such that the elements of the Cartan subgroup are explicitly projected out by the conjugation Eq. (12). To see this, consider an arbitrary, undiagonalized state $\rho' = D\rho D^{-1}$. Now transform to the frame where ρ' is diagonal, $\rho = D^{-1}\rho'D$. This matrix is clearly invariant under unitary transformations d when d is diagonal. Therefore, there is a invariant subgroup, which is comprised of the set of diagonal unitary matrices, for any given density matrix since ρ is invariant under conjugation by all Bd such that d is diagonal and B, d are unitary. B being arbitrary implies that it is invariant under right action by d . This provides the method for identifying the $n - 1$ parameter subgroup under which ρ' is invariant.

In addition to the solution to the “problem” with the “over” parameterization, this parameterization enables one to identify the little group and orbit space of density matrices under conjugation by $SU(n)$. One may then investigate which subspaces may give rise to nontrivial abelian and non abelian geometric phases. This is the subject of the next section.

3. Geometric Phases

Geometric phases in physics have a long and rich history [32], [33]. Pancharatnam studied them in connection with photon polarizations over forty years ago [1]. Later Herzberg and Longuet-Higgins showed that the phases can arise in the Born-Oppenheimer approximation describing polyatomic molecules [34]. Mead and Truhlar showed that motion of nuclei could be described by an effective Hamiltonian with a “gauge potential” to describe the effect of the “fast” motion of the electrons on these nuclei to produce the geometric phase [35]. Some time after this Berry discovered nontrivial phase factors [2] and Simon gave them a geometric description in terms of fiber bundle theory [3] (hence the name, “Berry phase” or “geometric phase”). A classic example is the motion of an electron in the field of a magnetic monopole. Many new interesting topics associated to these phases soon followed. Among these were analyses in group theoretical terms ([36], [37], [38]).

Geometric phases for $SU(3)$ representations have been investigated in [15] and [16] for three-level systems. The Lie subgroups of $SU(3)$ were listed there and it was shown that non-zero dynamical phases can only occur in certain particular subspaces of the form $SU(3)/H$ where H is a (Lie) subgroup of G . Note that the space of density matrices of a pure state in a three state system is also of the form $SU(3)/H$ since it is isomorphic to $SU(3)/U(2) \cong \mathbb{CP}^2$. An explicit set

of coordinates for this manifold were given in [17, 18] in this context. From these observations, we may next comment on the possibility of nontrivial phase factors in different subspaces of the space of all density operators for n -state systems in terms of our particular parameterization.

3.1. Background

A deeper treatment of the geometric phase can be found in [39]. For general references see [32] and [40] in addition to the seminal references given above. Here we sketch the basic concepts needed throughout the section.

Whenever a state in a given quantum mechanical system undergoes a cyclical evolution, any representative vector will acquire a phase independent of representation. It is important to realize the resulting overall phase has *two* contributions. The *dynamical* part depends essentially upon the Hamiltonian, whereas the *geometrical* part depends only upon the closed path of evolution and is reparameterization invariant, hence *geometric*. This geometric phase is just the holonomy of the loop due to the natural connection in the $U(1)$ -bundle associated to the projection $\{\text{vectors}\} \rightarrow \{\text{rays}\}$.

In the original derivation by Berry, the motion was adiabatic, and the connection was shown to arise from the effect of the “slow” variables on the “fast” variables. Since the Lie algebra of the holonomy is generated by the curvature of the connection (the theorem of Ambrose and Singer, see [41]), the geometric phase is a gauge invariant concept.

The removal of the adiabatic approximation was carried out in [39]. They also consider *non-cyclic* evolution with the tacit understanding that the open path could be closed, *e.g.*, by tracing geodesics from a common point through the initial and final points. The path is then closed, and the geodesic segments do not alter the holonomy. This naturally leads to a treatment of the effective dynamics of the particular system as a gauge theory, where the symmetries involved depend upon many different aspects of that particular system; the external parameters used, the adiabatic approximation, etc.

For a generic path, the holonomy group is $U(1)$ for individual states. In the case of degenerate eigenvalues, the holonomy group is enlarged to $U(n)$, $n > 1$ provided the evolution of the system does not remove this degeneracy [42]. In that case the states carry a degeneracy index which labels the representation of the gauge group.

The approach we take below is not to try to produce an overall symmetry group for the theory, but to consider only the little group of a particular mixed state density matrix. This will provide a gauge group for all matrices in the $SU(n)$ orbit of this state. We will then investigate the possible geometric phases within such orbits. Of course this gauge group will, in general, *not* be abelian. The terms *abelian* and *non-abelian geometric phases* then simply refer to the commutativity of the gauge group involved.

3.2. Geometric Phases for Mixed States

We have said that geometric phases depend on the dynamical path of a particular system. The easiest way to determine the possible geometric phases for a system is to consider the eigenvalues associated with the effective dynamics of that system. For n -state systems we note that for different sets of eigenvalues of the system, there exists the possibility of nontrivial abelian and non-abelian geometric phases depending on the particular set of eigenvalues. This, and the geometry of the spaces of the density matrices, are exhibited in our particular parameterization rather nicely.

First consider the nontrivial example of a three state system. When each of the three eigenvalues of the mixed state density operator are nonzero and are different, the space of transformations of ρ is $SU(3)/(U(1) \times U(1))$, *i.e.*, the little group or stability group is $(U(1) \times U(1))$. This is a flag manifold $Fl(3) \cong U(3)/U(1)^3 \cong \mathbb{CP}^2 \ltimes \mathbb{CP}^1$. One can see that we may have non trivial geometric phases only of the abelian type. When the matrix ρ

contains 3 nonzero eigenvalues with 2 identical and one different, the transformation space is $SU(3)/(SU(2) \times U(1))$ and we may possibly observe geometric phases of the nonabelian type which is also the case when all eigenvalues are identical. Of course these spaces exhibit only the possibility of observing geometric phases. Our ability to actually observe them depends on the effective dynamics of the particular system and on the path in parameter space.

For the generic case of n -state systems there is an immediate generalization of the argument for 3-state systems. If we have an n -state density operator with all eigenvalues different and nonzero, then the space of transformations is $Fl(n) \cong U(n)/U(1)^n \cong SU(n)/(U(1) \times \cdots \times U(1))$, where there are $n - 1$ of these $U(1)$ factors. If two of the eigenvalues are degenerate, there is one factor of $SU(2)$ replacing one of the $U(1)$ s. If three are degenerate, there is a factor of $SU(3)$, etc. This extends the ideas of [15] and [16] from the case of pure 3-state systems to the case of pure and mixed n -state systems. This goes further and offers a scheme for the parameterization of these with $SU(n)$ groups and uses the direct connection between these groups and the transformation spaces of the density operators.

One can now see that the space of mixed state density matrices is locally isomorphic to the following spaces. When all of the eigenvalues are different the space is $(SU(n)/T^{n-1}) \times D^{n-1}$, (see also [43] for another proof) where the component D^{n-1} is the $(n - 1)$ dimensional disc. This comes from the parameterization of the diagonal elements in terms of the $(n - 1)$ -sphere and is topologically a disc but is geometrically an $(n - 1)$ dimensional rectangle or rectangular solid. When there are two degenerate eigenvalues the space is $[SU(n)/(SU(2) \times T^{n-2})] \times D^{n-2}$ and so on. Here we have used the fact that $T^1 \cong U(1)$.

For the case of three state systems we may list 3 possibilities: all three eigenvalues are different, two are the same and one is different, and all are the same. Respectively the spaces of their density matrices are locally $(SU(3)/T^2) \times D^2$, $[SU(3)/(SU(2) \times T^1)] \times D^2$ and a single point.

It is worth noting also that one may arrange the eigenvalues of a diagonalized density matrix such that the identical eigenvalues appear next to each other along the diagonal. This means that when the matrix is in nondiagonal form, the group transformations can be expressed in a block diagonal form. These transformations are always allowed since they correspond to a simple change of basis. In this way we may observe the symmetry breaking associated to the differences in eigenvalue degeneracies. For instance, if three eigenvalues of a three state system are equal, one can be “distorted,” or changed slightly (by an outside influence such as an external magnetic field on a three state molecule). Then if the population of one of the states is changed, we have broken the symmetry group from $SU(3)$ to $SU(2) \times U(1)$.

Before we leave this topic, one final note is in order. We have discussed the possibility of identifying geometric phases within a system if degeneracies are present. This is not useful unless we are able to experimentally identify degeneracies. Such degeneracies may be identified directly, or by using state tomography data and the relations given in [44], which are able to identify degeneracies using the coherence vector parameterization of the density matrix.

3.3. An Explicit Example: Non-abelian Geometric Phases

In this section an example of geometric phases for 3-state systems is given. This method is a generalization and simplification of the method presented in [37] and provides an explicit example of the utility of the previous discussion. Specifically, we will find the adiabatic non-abelian geometric phase associated with a two-fold degeneracy of energy eigenvalues of the general Hamiltonian for a 3-state system. The phases acquired will come from the subgroup $SU(2) \times U(1)$. The two-dimensional subspace gives rise to the possibility of a non-abelian geometric phase which would mix the two degenerate energy eigenvalues.

The way the connection one-forms for the 3-state systems are derived here using the state space of the system is expressed in terms of the group $SU(3)$. Our method has the advantage

of being 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 [45].) It also has the advantage of being generalizable to $SU(n)$ given the aforementioned generalized Euler angles. 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. In addition, the methods of [25] and [44] enable, in principle, the experimental identification of degeneracies and therefore the orbit space structure.

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.*, then the curve $C:[0, T] \rightarrow M$ is closed; 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

$$e^{-\frac{i}{\hbar} \int_0^T E_n(t) dt} \mathcal{P} \left[e^{i \oint_C A_n} \right],$$

where \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:

$$A_n^{ab} = i \langle n, a, \vec{R} | d | n, b, \vec{R} \rangle. \quad (13)$$

It is important to note that the Hamiltonian is a 3×3 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, $\lambda_0 = \mathbb{1}_{3 \times 3}$ and the λ_i are the Gell-Mann matrices. 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 $M \subset \mathbb{CP}^2$ and what is more, it is clear from ([17, 18]) that only the angles α, β, γ and θ will remain since $\lambda_1, \lambda_2, \lambda_3$ and λ_8 commute with H_D . Explicitly, the Hamiltonian in undiagonalized form, H , is given by

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

It can easily be shown that these angles parameterize \mathbb{CP}^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 (13). 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 (12) with D a variable matrix in $SU(n)$. 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.

4. Entropy

By now, the von Neumann *entropy* [27] S is well known in quantum information theory as providing a measure of our uncertainty about a quantum system described by a density operator ρ in analogy with the Shannon entropy [14]. The definition of the von Neumann entropy is

$$S(\rho) = -\text{Tr}(\rho \ln \rho)$$

Intuitively, it gives us a way to identify parts of the space of density operators as having different “purities.” Yet there is another measure of the purity also referred to as the linear entropy given by

$$L(\rho) = \frac{1}{2}(1 - \text{Tr}(\rho^2)).$$

Each is clearly zero if and only if $\text{Tr}(\rho^2) = 1$, that is, when ρ is in a pure state.

For $n = 2$ our parameterization is quite useful. Write

$$\rho \approx \begin{pmatrix} \cos^2 \theta/2 & 0 \\ 0 & \sin^2 \theta/2 \end{pmatrix} \quad 0 \leq \theta \leq \pi/2$$

where \approx means up to unitary equivalence. Hence

$$S[\rho(\theta)] = -(\cos^2 \theta/2) \ln(\cos^2 \theta/2) - (\sin^2 \theta/2) \ln(\sin^2 \theta/2).$$

As θ varies from 0 to $\pi/2$, the entropy varies from 0 to its maximum $= \ln 2$, and the state varies from a pure one to the maximally mixed one. Of course, it is enough to compute the entropy for a diagonalized density matrix, since $\text{Tr} M = \text{Tr} A M A^{-1}$ for any two operators A , M .

If a diagonal representative of a 3-state system is

$$\rho \cong \begin{pmatrix} \cos^2 \phi/2 \sin^2 \theta/2 & 0 & 0 \\ 0 & \sin^2 \phi/2 \sin^2 \theta/2 & 0 \\ 0 & 0 & \cos^2 \theta/2 \end{pmatrix} \quad 0 \leq \theta, \phi \leq \pi \quad (14)$$

the von Neumann entropy is

$$S(\rho) = -\text{Tr}(\rho \ln \rho) = \begin{cases} 0 & \text{for pure states,} \\ 0 \leq S \leq \ln 3 & \text{for generic states,} \\ \ln 3 & \text{for the most "mixed" state.} \end{cases}$$

The generalization to an n -state system is obvious, with similar limits

$$S(\rho) = -\text{Tr}(\rho \ln \rho) = \begin{cases} 0 & \text{for pure states,} \\ 0 \leq S \leq \ln n & \text{for generic states,} \\ \ln n & \text{for the most "mixed" state.} \end{cases}$$

4.1. Isentropic Curves

For two-state systems the purity is well described in terms of either the linear entropy or the von Neumann entropy in the sense that both are monotonic in the one parameter. However, these two functions are quite different for systems with more than two states. We will discuss three state systems in some detail to provide an example. Our parameterization and the low dimensional example enables us to graph these functions.

We first note that two-state systems with the same the von Neumann entropy or the same linear entropy are related by a unitary transformation. The surfaces of constant entropy are pairs of points (except for the maximally mixed state where the two points coincide) as can be seen from Fig. 2 and the relation $\sin^2 \theta = 1 - \cos^2 \theta$ ensures that equivalent entropy values are related by a unitary transformation.

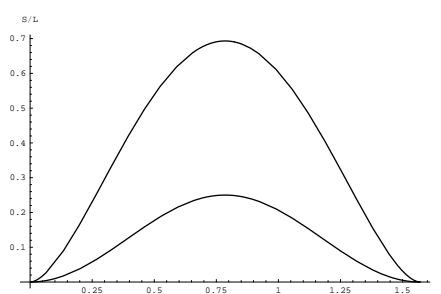


Figure 2. Graph of the von Neumann entropy and the linear entropy versus the single parameter which parameterizes the eigenvalues of the density operator. The upper curve is the von Neumann entropy and the lower curve is the linear entropy. Here $0 \leq \theta \leq \pi/2$.

By contrast, the entropy of a three-state system has surfaces of constant entropy which are one-dimensional curves. These integral curves show that different sets of eigenvalues have the same entropy. However, since eigenvalues are not changed by unitary transformations, there exist density operators with the same entropy which are not equivalent under unitary transformations. This is most easily seen by viewing a contour plot as shown for the von Neumann entropy in Fig. 3. Clearly the isentropic hypersurfaces of an n -state system are $n - 2$ dimensional.

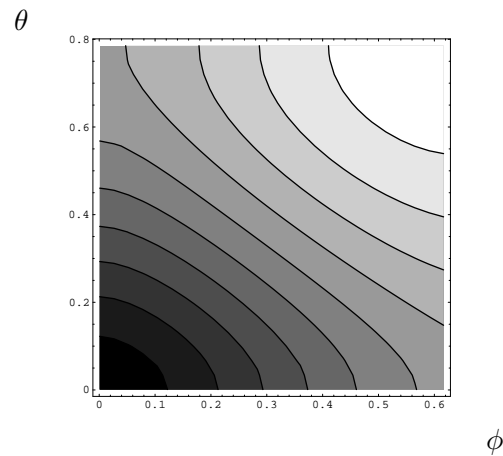


Figure 3. Graph of the von Neumann entropy as a contour plot with the two parameters (angles) which parameterize the eigenvalues of the density operator as the axes shown. The lines on the graph are integral curves of S with larger values in lighter shades of gray.

4.2. Linear Entropy vs. von Neumann Entropy

Now we can clearly show the different functional dependences of the linear entropy and the von Neumann entropy by superposing two graphs, one the contour plot of the linear entropy and the other the contour plot of the von Neumann entropy (Fig. 4). Whereas there is no possibility of changing one without changing the other for a two state system, a three state system is quite different. The graph Fig. 4 clearly shows that, for a three state system, one may change the von Neumann entropy while keeping the linear entropy constant, or vice versa. The plot also identifies regions of the parameter space which show the greatest difference between the two.

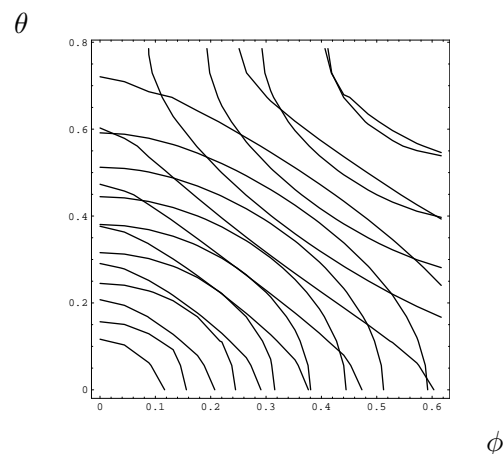


Figure 4. Graph of the von Neumann entropy and the linear entropy as contour plots. (The angles are the same two parameters as in Fig. 3.) The lines on the graph are integral curves of S and L .

This graphical representation of the von Neumann entropy leads to several questions. For example, could we use this to optimize information gain versus the information loss for certain measurements? If we want to answer this question, we would require the “subentropy” [46] which provides a lower bound on the information which can be extracted from a quantum

system. Another open question is, how might one optimize the difference between the von Neumann entropy and the subentropy and what are the implications for quantum information processing? This is the subject of future work.

5. Conclusions and Comments

We have shown that the mixed state density matrices for n -state systems can be parameterized in terms of squared components of an $(n - 1)$ -sphere and unitary matrices. This lets one immediately identify the little groups and therefore orbits of the space of density matrices for particular sets of eigenvalues. The little groups can be seen as structure that describes possible geometric phases for the system. Thus when a system described by an n -state density matrix undergoes a change in the physical parameter space (the orbit space), the system may exhibit a geometric phase with a “gauge group” that corresponds to the little group of the space. Given the parameterization presented here, the identification of the little group is transparent.

This parameterization of the density matrices gives an *explicit* parameterization of the pure and mixed state density matrices that is amenable to calculations. In particular, one may parameterize the unitary matrices for $SU(n)$ in terms of generalized Euler angles. Generalized Euler angles were constructed explicitly for $SU(3)$ in [17, 18] and recently extended to $SU(n)$ [30, 31]. Using the explicit parameterization, the geometric phases can be calculated for the case of n -state systems using the methods of [17, 18] and [47] which are based on the kinematical approach of Refs. [15, 16].

Parameterizing the eigenvalues in terms of the squared components of the $(n - 1)$ -sphere, enables the graphical representation of the entropy for n -state systems which, in turn, enables the identification of isentropic curves. In the case of three states, these integral curves of the von Neumann entropy indicate that the orbits of the adjoint representation of $SU(3)$ must have two labels. This immediately generalizes to n -dimensional systems which have $n - 2$ dimensional isentropic hypersurfaces. We believe the work here provides simple geometric constructions and arguments which can be used very generally for a variety of applications.

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