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Orbits of quantum states and geometry of Bloch vectors for *N*-level systems

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Abstract

Physical constraints such as positivity endow the set of quantum states with a rich geometry if the system dimension is greater than 2. To shed some light on the complicated structure of the set of quantum states, we consider a stratification with strata given by unitary orbit manifolds, which can be identified with flag manifolds. The results are applied to study the geometry of the coherence vector for *n*-level quantum systems. It is shown that the unitary orbits can be naturally identified with spheres in \mathbb{R}^{n^2-1} only for n = 2. In higher dimensions the coherence vector only defines a non-surjective embedding into a closed ball. A detailed analysis of the three-level case is presented. Finally, a refined stratification in terms of symplectic orbits is considered.

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1. Introduction

The Bloch vector [1] provides a representation of the quantum states of a two-level system in terms of real observables, and allows the identification of quantum states with points in a closed ball in 3D Euclidean space, the Bloch ball, which has proved to be extremely useful. In quantum information theory, for instance, the states of a single qubit can be identified with points on the surface of the Bloch ball (if the state is pure) or points inside the ball (if the state is mixed). Unitary operations can be interpreted as rotations of this ball, and dissipative processes as linear or affine contractions of the Bloch ball [1, 2].

Naturally, many efforts have been made to generalize the Bloch ball to higher dimensions by defining a generalized coherence vector similar to the Bloch vector for two-level systems.

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However, while it is easy to define a Bloch [3] or general coherence vector [4, 5] for *N*-level systems, it has become clear that the geometry of quantum states in higher dimensions is far more complex than in the two-level case. Some efforts have been made at determining the set of Bloch vectors corresponding to physical states for higher dimensional systems using the higher trace invariants or Casimir invariants, for instance by Kimura [6], who also demonstrated the complicated and asymmetric structure of the set of Bloch vectors in higher dimensions. Byrd and Khaneja [7] independently provided a similar characterization of the positivity of the density matrix in terms of the coherence vector representation.

In this paper we pursue a different approach to study the structure of quantum states for higher dimensional systems, and the origin of the difference between the two-level case and higher dimensions. In section 2, we define a natural stratification of the set of density matrices in terms of unitary orbits. We show that the unitary orbits can be identified with flag manifolds and determine their dimensions. For two-level systems this stratified set can be identified with a smooth real manifold with boundary, the 3D Bloch ball, with strata given by concentric spheres.

In section 3 we briefly review the definition of the Bloch vector and define a general coherence vector, which can be naturally embedded into a closed ball in \mathbb{R}^{n^2-1} . This embedding is surjective for two-level systems, hence allowing the identification of physical states with points in this closed ball. We show that for higher dimensional systems, however, the embedding is never surjective due to positivity constraints, and the dimensions of the orbit manifolds vary depending on the *multiplicities* of the eigenvalues of the states in each stratum. Furthermore, for two-level systems there exists a total ordering of the strata given by the length of the Bloch vector, or the distance of the unitary orbit from the centre of the Bloch ball—the Bloch vector of pure states has length one, and the shorter the Bloch vector, the more mixed the state is. For higher dimensional systems we show that the length of the system. A detailed analysis of the three-level case concludes section 3.

Finally, in section 4 we briefly consider a refined stratification of the set of density matrices defined by the action of the symplectic group. The symplectic group is of interest because it occurs naturally for quantum systems with certain dynamical symmetries (such as atomic systems with degenerate energy levels) and it is the only proper subgroup of the unitary group that acts transitively on certain unitary orbits [10]. We show that the symplectic orbits of pseudo-pure states agree with the unitary orbits and provide bounds on the dimensions of other symplectic orbits, showing that the symplectic orbits generally have much lower dimension. From a control point of view this means that a 2n-dimensional Hamiltonian control system with dynamical Lie group Sp(n) is pure-state controllable but we cannot control generic ensembles.

2. Density matrices and unitary orbits

Throughout this paper we restrict our attention to quantum systems whose Hilbert space is a finite-dimensional complex vector space \mathbb{C}^n , where *n* is an integer greater than 1, and for simplicity we will often use *V* to denote \mathbb{C}^n with the standard Hermitian inner product $\langle \cdot, \cdot \rangle$. Any physical state of this system can be represented by a density operator, i.e., a positive semi-definite (self-adjoint) linear operator with trace 1. The subset of rank-1 density operators corresponds to pure states of the system, all other density operators to mixed states.

In the following we denote the set of all positive semi-definite operators on V by P(V), the subset of all density matrices by D(V), and the subset of pure states by $D_1(V)$. We also define the class of pseudo-pure states or pure-state-like ensembles as the set of density operators

 $D_{1'}(V)$ whose spectrum consists of exactly two distinct eigenvalues with multiplicities 1 and n-1, respectively. It is well known that D(V) forms a convex subset of the set of Hermitian matrices since given two density matrices $\rho_1, \rho_2 \in D(V)$, the straight line path defined by $\Gamma(t) := (1-t)\rho_1 + t\rho_2$ for $t \in [0, 1]$ is contained in D(V). To see this, note that $\Gamma(t)$ is Hermitian, $\text{Tr}(\Gamma(t)) = 1$ and $\langle \Gamma(t)x \mid x \rangle = (1-t)\langle \rho_1 x \mid x \rangle + t\langle \rho_2 x \mid x \rangle \ge 0$ for all $x \in \mathbb{C}^n$ and $t \in [0, 1]$.

We define the orbit of a quantum state ρ under the action of the dynamical Lie group G to be the set $G \cdot \rho := \{g \cdot \rho \cdot g^{-1} \mid g \in G\}$. The orbits endow the set of quantum states with the structure of a stratified set. In principle, any Lie group G acting on the set of density operators defines a stratification of D(V). However, the orbits under the action of G = U(n) are of particular interest since they determine the most general evolution of the quantum states in a closed system. From a control point of view, the unitary orbit of a state represents the maximal set of states that are reachable from the given state via (open-loop) coherent control, or in the language of quantum computing, by applying a unitary gate to the state.

Before we attempt to classify the orbits, we recall the following standard result from linear algebra:

Proposition 1. Let ρ_1 and ρ_2 be two density matrices. The following are equivalent:

(i) ρ_1 and ρ_2 are unitarily equivalent, i.e., $\rho_2 = U\rho_1 U^{\dagger}$ for some unitary matrix U. (ii) ρ_1 and ρ_2 have the same spectrum, i.e., the same eigenvalues including multiplicity. (iii) $\operatorname{Tr}(\rho_1^r) = \operatorname{Tr}(\rho_2^r)$ for all r = 1, 2, ..., n.

This result shows immediately that the orbit of a density matrix under U(n) is uniquely determined by its spectrum, i.e., two density matrices belong to the same unitary orbit if and only if they have the same eigenvalues λ_i with the same multiplicities n_i . Each orbit \mathcal{O} can therefore be represented by a canonical diagonal density matrix of the form

$$\rho = \operatorname{diag}(\lambda_1 I_{n_1}, \dots, \lambda_r I_{n_r}) \tag{1}$$

where the eigenvalues shall be ordered such that $\lambda_i > \lambda_j$ for i < j to ensure a unique representation. Since the λ_i can be arbitrary real numbers in [0, 1] provided they satisfy $\sum_{i=1}^{r} n_i \lambda_i = 1$, we see immediately that there are infinitely many distinct orbits corresponding to the (uncountably) infinitely many possible choices for the λ_i . Thus, we can say that the unitary group U(n) partitions the set of density matrices D(V) into an uncountably infinite family of (distinct) orbits or strata.

We can define a (partial) ordering on this stratification via majorization. Let ρ_1 , ρ_2 be two density operators with eigenvalues $a_m^{(i)}$, i = 1, 2, counted with multiplicity and ordered in a non-increasing sequence. $\rho_1 \prec \rho_2$ if

$$\sum_{m=1}^{k} a_m^{(1)} \leqslant \sum_{m=1}^{k} a_m^{(2)} \qquad k = 1, \dots, n-1$$

$$\sum_{m=1}^{n} a_m^{(1)} = \sum_{m=1}^{n} a_m^{(2)}.$$
(2)

For instance, $\rho_1 = \frac{1}{5} \text{diag}(1, 1, 3) \prec \rho_2 = \frac{1}{5} \text{diag}(2, 2, 1)$ since $1 \leq 2, 1 + 1 \leq 2 + 2$ and 1 + 1 + 3 = 2 + 2 + 1. Majorization has been shown to be a useful way to compare the degree of disorder of physical systems [8] and naturally defines a partial ordering on the unitary orbits (strata) via $\mathcal{O}_1 \prec \mathcal{O}_2$ if $\mathcal{O}_i = \mathcal{O}[\rho_i]$ and $\rho_1 \prec \rho_2$. However, note that only some orbits can be compared that way. Consider $\rho_1 = \frac{1}{8} \text{diag}(5, 2, 1)$ and $\rho_2 = \frac{1}{8} \text{diag}(4, 4, 0)$. We have 5 > 4 but 5 + 2 < 4 + 4. Hence, neither orbit majorizes the other.

To determine the nature of the strata given by the orbits, we define the *isotropy subgroup* or stabilizer at ρ as the subgroup G_{ρ} of elements in G that leave ρ invariant, i.e., for which we have $g \cdot \rho \cdot g^{-1} = \rho$. We shall show that the orbit of an element $\rho \in D(V)$ under the unitary group U(n) can be identified with a certain type of manifold called a flag manifold. For the purpose of proving this result we observe that U(n) is a compact Lie group and hence a compact topological group⁵ and the space of density matrices is a Hausdorff space⁶, and we have the following result (see [9], for instance):

Proposition 2. If G is a compact topological group acting on a Hausdorff space X and G_x is the isotropy group at x then the map $\phi : G/G_x \mapsto G \cdot x$ is a homeomorphism.

Theorem 1. Let U(n) act on D(V) by conjugation and ρ be a quantum state with $r \ge 1$ distinct eigenvalues λ_i with (geometric) multiplicity n_i . Then the orbit of ρ is homeomorphic to the flag manifold

$$U(n)/[U(n_1) \times U(n_2) \times \cdots \times U(n_r)]$$

of real dimension $n^2 - \sum_{i=1}^r n_i^2$.

Proof. Let E_i be the eigenspaces of ρ with dim $E_i = n_i$. Since ρ is unitarily equivalent to the diagonal matrix diag $(\lambda_1 I_{n_1}, \ldots, \lambda_r I_{n_r})$, we have an orthogonal direct sum decomposition of $V = \mathbb{C}^n$ of the form $V = E_1 \oplus \cdots \oplus E_r$. $g \in U(n)$ stabilizes ρ if and only if g preserves the eigenspaces E_i , i.e., the restriction of g to each eigenspace must be an isometry, i.e., g preserves the eigenspaces E_i . Hence, the orbit of ρ is homeomorphic to the flag manifold $U(n)/[U(n_1) \times U(n_2) \times \cdots \times U(n_r)]$ by proposition 2.

Corollary 1. If $\rho \in D_{1'}(V)$ (pseudo-pure state) then the orbit of ρ is homeomorphic to $U(n)/[U(1) \times U(n-1)]$, which is homeomorphic to the complex projective space \mathbb{CP}^{n-1} .

To illustrate the result, we explicitly compute the orbits under the action of U(n) for n = 2 and n = 3.

Example 1. Let ρ be a 2 × 2 density matrix. ρ is unitarily equivalent to diag(r, 1 - r) with $0 \leq r \leq 1$. If r = 1 - r then $\rho = I_2/2$ and the orbit of ρ is homeomorphic to U(2)/U(2), i.e., a single point. Otherwise, its orbit is homeomorphic to $U(2)/[U(1) \times U(1)] \simeq \mathbb{CP}^1$.

Since \mathbb{CP}^1 is diffeomorphic to the sphere S^2 , this shows that any U(2) orbit of a two-level system is homeomorphic to S^2 , except the trivial orbit of the completely random ensemble $I_2/2$ which consists of a single point.

Furthermore, note that the requirement of positivity of ρ reduces to $0 \le r \le 1$ and hence $r^2 \le r$, or equivalently, $\text{Tr}(\rho^2) = r^2 + (1 - r)^2 = 1 - 2r + 2r^2 \le 1 - 2r + 2r = 1$. We shall see that this implies that the set of all 2×2 density matrices (the union of all orbits) is homeomorphic to a closed ball in \mathbb{R}^3 .

Thus, we have a neat mathematical justification for the Bloch ball description of a twolevel system, which will be discussed in detail later.

 $^{^{5}}$ A topological group is a topological space *X* endowed with a group structure that allows us to 'multiply' elements of the space and compute inverses such that both operations are continuous with respect to the topology. The unitary group, for instance, is a multiplicative group since multiplication of two unitary matrices gives a unitary matrix, every unitary matrix has an inverse given by the Hermitian conjugate, and the identity provides a neutral element. Furthermore, as a subset of the complex matrices the unitary group is naturally endowed with a topology that allows us to separate two unitary matrices by open sets, and matrix multiplication and Hermitian conjugation are continuous with respect to this topology.

 $^{^{6}}$ A Hausdorff space basically is a space endowed with a topology that allows us to separate points by disjoint open sets.

 Manifold
 Dim.

	Maiilioid	Dim.
n = 3		
$\rho = \operatorname{diag}(a, a, a)$	point	0
$\rho = \operatorname{diag}(a, b, b)$	$U(3)/[S^1 \times U(2)]$	4
$\rho = \operatorname{diag}(a, b, c)$	$U(3)/[S^1 \times S^1 \times S^1]$	6
n = 4		
$\rho = \operatorname{diag}(a, a, a, a)$	point	0
$\rho = \operatorname{diag}(a, b, b, b)$	$U(4)/[S^1 \times U(3)]$	6
$\rho = \operatorname{diag}(a, a, b, b)$	$U(4)/[U(2) \times U(2)]$	8
$\rho = \operatorname{diag}(a, b, c, c)$	$U(4)/[S^1 \times S^1 \times U(2)]$	10
$\rho = \operatorname{diag}(a, b, c, d)$	$U(4)/[S^1 \times S^1 \times S^1 \times S^1]$	12

All parameters a, b, c, ... are in [0, 1] such that $Tr(\rho) = 1$ and different letters represent different values.

Example 2. Let ρ be a 3 × 3 density matrix. If ρ has only one eigenvalue with multiplicity 3 then $\rho = I_3/3$ and its orbit is homeomorphic to U(3)/U(3), which is a single point as before.

If ρ has two distinct eigenvalues then it is a pseudo-pure state unitarily equivalent to $\rho = \text{diag}(1 - 2a, a, a)$ where $0 \leq a \leq 1$ and $a \neq 1/3$. Its isotropy subgroup is therefore $U(1) \times U(2)$, and its orbit is homeomorphic to $U(3)/[U(1) \times U(2)]$ and has dimension 9 - 1 - 4 = 4.

If ρ is a generic ensemble with three distinct eigenvalues a, b, c, then its canonical form is $\rho = \text{diag}(a, b, c)$ and its isotropy subgroup is $U(1) \times U(1) \times U(1)$. Hence, its orbit is homeomorphic to $U(3)/[U(1) \times U(1) \times U(1)]$ and has real dimension 9 - 3 = 6.

The results of the previous example are summarized in table 1. The table also provides a complete classification of the orbits for n = 4.

The previous two examples clearly show the difference between two-level systems and higher dimensional systems (n > 2). While all orbit manifolds (except the trivial orbit of the completely random ensemble) for two-level systems are homeomorphic to a sphere, no such homeomorphism is possible in the latter case, i.e., the orbit manifolds for higher dimensional systems can *never* be *identified* with spheres in a higher dimensional Euclidean space. That is, although we can always *embed* the quantum states of the system in a compact subset (closed ball) of a real vector space of sufficiently high dimension, there is no one-to-one correspondence between spheres in this ball and orbits of quantum states, *except for* n = 2, which explains the difficulties one encounters when trying to generalize intuitive reasoning valid for the Bloch ball for n = 2 to Bloch vectors in higher dimensions.

3. Coherence vector and embeddings of quantum states

3.1. Definition of Bloch or coherence vector

For a two-level system any density operator can be expanded as

$$\rho = \frac{1}{2}(I_2 + x\sigma_x + y\sigma_y + z\sigma_z)$$

where I_2 is the 2D identity matrix, and $\sigma_x = |1\rangle\langle 2| - |2\rangle\langle 1|, \sigma_y = i(|1\rangle\langle 2| + |2\rangle\langle 1|)$ and $\sigma_z = i(|1\rangle\langle 1| - |2\rangle\langle 2|)$ are the usual (unnormalized) 2D Pauli matrices. The coordinates x, y and z are real since the Pauli matrices are Hermitian and $* = \text{Tr}(\rho\sigma_*)$ for * = x, y, z. Hence, the state of any two-level system can be characterized completely by the real vector $\mathbf{s} = (\mathbf{x}, \mathbf{y}, \mathbf{z})$, called the Bloch vector.

For an *n*-level system we can proceed in a similar fashion. Let

$$\sigma_{r,s}^{x} = |r\rangle\langle s| - |s\rangle\langle r| \qquad \sigma_{r,s}^{y} = i(|r\rangle\langle s| + |s\rangle\langle r|)$$

$$\sigma_{r}^{z} = i\sqrt{2/(r+r^{2})} \left(\sum_{k=1}^{r} |k\rangle\langle k| - r|r+1\rangle\langle r+1|\right) \qquad (3)$$

for $1 \le r \le n-1$ and $r < s \le n$ be the generalized Pauli matrices in dimension *n*. The set $\{\tilde{\sigma}_k\}_{k=1}^{n^2-1} = \{\sigma_{r,s}^x, \sigma_{r,s}^y, \sigma_r^z \mid 1 \le r < n, r < s \le n\}$ forms a basis for the space of $n \times n$ traceless Hermitian matrices satisfying the *orthogonality* condition

$$\langle \tilde{\sigma}_k \mid \tilde{\sigma}_\ell \rangle = \operatorname{Tr}(\tilde{\sigma}_k \tilde{\sigma}_\ell) = 2\delta_{k,\ell}.$$
(4)

Every density matrix can be expanded with respect to this basis

$$\rho = \frac{1}{n}I_n + \frac{1}{2}\sum_{k=1}^{n^2 - 1}\tilde{s}_k\tilde{\sigma}_k$$
(5)

where $\tilde{s}_k = \text{Tr}(\rho \tilde{\sigma}_k)$ for $k = 1, ..., n^2 - 1$. The resulting real vector $\tilde{\mathbf{s}} = (\tilde{s}_k)_{k=1}^{n^2-1}$ is the Bloch vector of the *n*-dimensional system.

Although the Bloch vector defined above is useful, it is generally more elegant, and often more convenient, to work with an *orthonormal* basis. To this end, we define the normalized Pauli matrices $\{\sigma_k\}_{k=1}^{n^2-1} = \left\{\frac{1}{\sqrt{2}}\tilde{\sigma}_k\right\}_{k=1}^{n^2-1}$, which satisfy the *orthonormality* condition

$$\langle \sigma_k \mid \sigma_\ell \rangle = \operatorname{Tr}(\sigma_k \sigma_\ell) = \delta_{k,\ell}.$$
 (6)

Furthermore, $\{\sigma_k \mid k = 1, ..., n^2 - 1\}$ together with $\sigma_0 = I_n / \sqrt{n}$ forms an orthonormal basis for all Hermitian $n \times n$ matrices, and we can expand any density matrix in terms of this ON basis

$$\rho = \sum_{k=0}^{n^2 - 1} s_k \sigma_k \tag{7}$$

where $s_k = \text{Tr}(\rho \sigma_k)$ for $k = 0, ..., n^2 - 1$. Since $1 = \text{Tr}(\rho) = \sqrt{n}s_0$, we have $s_0 = 1/\sqrt{n}$ for all density matrices. Hence, ρ is completely determined by the real $n^2 - 1$ vector $\mathbf{s} = (\mathbf{s}_1, ..., \mathbf{s}_{n^2-1})$. This vector is often called the general coherence vector. Equations (5) and (7) are equivalent, and we easily see that $\tilde{\mathbf{s}} = 2\mathbf{s}$, i.e., the standard Bloch vector differs from the coherence vector only by a factor of 2.

Note that our definition of the coherence vector with respect to the generalized Pauli matrices is not the only one possible. One can define a coherence vector with respect to other bases as has been considered by various authors in the literature. Although this will change the coherence vector representation of the states, it does not affect the structure of the set of density matrices in general.

It is easy to verify that the mapping that takes ρ to the real coherence vector **s**, or equivalently the Bloch vector $\tilde{s} = 2\mathbf{s}$, defines an embedding of the density matrices into a closed ball in \mathbb{R}^{n^2-1} for all n > 1. However, the two-level case is special in that the embedding defined is surjective. We shall now discuss the nature of the resulting differences between the n = 2 and n > 2 case, and provide a detailed analysis of the three-level case.

3.2. Bloch ball picture for n = 2

For two-level systems the embedding defined above is not only one-to-one but also surjective, and hence provides a homeomorphism between orbits of density matrices under U(n) and

the closed ball of radius 1 (Bloch vector as defined above) or radius 1/2 (coherence vector as defined above) in \mathbb{R}^3 . Unitary transformations of a density matrix can be interpreted as real rotations of the ball. Example 1 shows that the action of the unitary group on the set of quantum states partitions it into an uncountably infinite number of distinct orbit manifolds, homeomorphic to concentric, two-dimensional spheres in the Bloch ball, with the exception of the trivial orbit of the completely random ensemble, which is mapped to the single point at the centre of the ball.

It is also easy to see that the distance of an orbit from the centre of the ball is determined by $\text{Tr}(\rho^2)$ via $\tilde{r} = 2\text{Tr}(\rho^2) - 1$ (Bloch vector) or $r = \text{Tr}(\rho^2) - 1/2$ (coherence vector). Pure states ($\text{Tr}(\rho^2) = 1$) have maximal distance from the centre of the ball and hence form its boundary. Furthermore, the disorder of an orbit is completely determined by its distance $r(\mathcal{O})$ from the centre, i.e., $\mathcal{O}_1 \prec \mathcal{O}_2$ if $r(\mathcal{O}_1) < r(\mathcal{O}_2)$.

From the point of view of controllability of quantum systems, it is also worth noting that all orbits (with the exception of the completely random ensemble) have the same dimension and geometry. Hence, any group that acts transitively on the class of pure states, for instance, will also act transitively on all classes of mixed states and vice versa. Of course, the only such groups are U(2) or SU(2). Hence, pure-state and mixed-state controllability are equivalent notions for two-level systems.

3.3. Bloch ball picture for n > 2

For n > 2 the situation is quite different due to the fact that the embedding into a closed ball in \mathbb{R}^{n^2-1} defined by $\rho \mapsto \mathbf{s}$ is not surjective. It is easy to see that the distance of each unitary orbit from the centre in \mathbb{R}^{n^2-1} remains completely determined by $\text{Tr}(\rho^2)$:

$$\|\mathbf{s}\|^{2} = \sum_{k=1}^{n^{2}-1} \mathbf{s}_{k}^{2} = \operatorname{Tr}(\rho^{2}) - \frac{1}{n}.$$
(8)

However, a glance at the dimensions of the orbits in table 1 shows immediately that each orbit is only a submanifold of a sphere of a fixed distance from the origin. For instance, as we have shown in the previous section, the orbit of pure states for n = 3 corresponds to a fourdimensional submanifold of the seven-dimensional boundary sphere with radius $\sqrt{1-1/3}$ in \mathbb{R}^8 . Since there is only a single orbit of pure states, the remainder of the points on the boundary sphere do not correspond to physical states.

For mixed states the situation is more complicated since each sphere of fixed radius r from the origin now generally contains an uncountably infinite number of distinct orbits, all satisfying $\text{Tr}(\rho_m) = 1$ and $\text{Tr}(\rho_m^2) = r^2$ but differing in higher trace invariants, e.g., $\text{Tr}(\rho_m^k) \neq \text{Tr}(\rho_{m'}^k)$ for some $2 < k \leq n$. The dimensions of the orbits contained within each sphere vary depending on the type of ensemble but each sphere (except for the boundary) generally contains a set of positive measure of orbits corresponding to physical states, and often a positive-measure set of points that do not belong to physical orbits. Moreover, the degree of disorder of an orbit can no longer be properly characterized by its distance from the centre of the ball. Orbits contained in the same sphere can often not be compared with respect to our partial ordering and may have different von-Neumann entropy. Furthermore, orbits at different distances from the origin may have the same von-Neumann entropy.

3.4. Analysis of the n = 3 case

To illustrate the general statements above, let us consider the n = 3 case and the set of orbits determined by the family of states $\rho = \text{diag}(a, b, c)$ with b, c given by

$$b = \frac{1}{2}(1 - a + K)$$
 $c = \frac{1}{2}(1 - a - K)$ $K = \sqrt{-1 + 2a - 3a^2 + 2c_2}$

Note that we have $\text{Tr}(\rho) = a + b + c = 1$ and $\text{Tr}(\rho^2) = c_2$ for all *a*. However, for ρ to represent a physical state *a*, *b*, *c* must be real and have values in [0, 1]. These constraints imply that the argument of *K* must be non-negative and $K \leq 1 - a$, or equivalently $K^2 \leq (1 - a)^2$. This yields the inequalities

$$3a^2 - 2a + 1 \leqslant 2c_2 \tag{9}$$

$$2a^2 - 2a + 1 \geqslant c_2 \tag{10}$$

which must be simultaneously satisfied. To ensure that there is a one-to-one correspondence between parameter values (a, c_2) and orbits, we further require $a \ge b \ge c$. Since a+b+c = 1 it implies $a \ge 1/3$. The constraint $b \ge c$ is automatically satisfied because *K* is real and ≥ 0 , whereas the constraint $a \ge b$ implies

$$6a^2 - 4a + 1 \geqslant c_2. \tag{11}$$

Inequality (9) is satisfied for

$$a \in \left[\frac{1-K_1}{3}, \frac{1+K_1}{3}\right]$$

for $K_1 = \sqrt{6c_2 - 2}$. Inequality (11) is satisfied for

$$a \in \left[0, \frac{1 - K_1/6}{3}\right] \cup \left[\frac{1 + K_1/6}{3}, 1\right]$$

For $c_2 \leq 1/2$, inequality (10) is satisfied for $a \in [0, 1]$, and for $c_2 > 1/2$ it is satisfied for

$$a \in \left[0, \frac{1-K_2}{2}\right] \cup \left[\frac{1+K_2}{2}, 1\right]$$

for $K_2 = \sqrt{2c_2 - 1}$. Combining these inequalities and noting that $a \ge 1/3$ leads to

$$c_2 \leq \frac{1}{2}$$
: $a \in \left[\frac{1}{3}(1+K_1/6), \frac{1}{3}(1+K_1)\right]$ (12)

$$c_2 > \frac{1}{2}$$
: $a \in \left[\frac{1}{2}(1+K_2), \frac{1}{3}(1+K_1)\right].$ (13)

Figure 1 illustrates the situation. The solid curve corresponds to $3a^2 - 2a + 1 = 2c_2$, the dash-dot line to $6a^2 - 4a + 1 = c_2$ and the dashed line to $2a^2 - 2a + 1 = c_2$. The points (a, c_2) on the solid line correspond to orbits of pseudo-pure states $\rho = \text{diag}(a, \frac{1}{2}(1-a), \frac{1}{2}(1-a))$, and the points on dash-dot line correspond to orbits of pseudo-pure states of the form $\rho = \text{diag}(a, a, 1 - 2a)$. The points below the solid curve correspond to non-Hermitian matrices. The points (a, c_2) above the dashed line correspond to non-positive Hermitian matrices. The points between these two curves represent physical states. However, only points in the shaded region between the curves satisfy all inequalities and represent unique orbits.

The figure also shows that for any $c_2 \in (1/3, 1)$, there exists a positive-measure set (interval) of *a*-values that correspond to distinct physical orbits, embedded in a sphere of fixed radius $r = \sqrt{c_2 - 1/3}$ from the origin. This shows that the number of distinct orbits contained within each sphere of radius $0 < r < \sqrt{2/3}$ is uncountably infinite. A unique orbit of fixed distance from the centre of the ball exists only for the special cases $c_2 = 1/3$ and $c_2 = 1$, the former corresponding to the trivial (i.e., zero-dimensional) orbit of the completely random ensemble a = b = c = 1/3 that forms the centre of the ball, and the latter to the four-dimensional orbit of pure states contained within the boundary sphere of the ball. Most of these orbits are generic and hence have dimension 6. However, each sphere also contains



Figure 1. Diagram indicating parameter values corresponding to physical orbits.

at least one (two if $c_2 \le 1/2$) pseudo-pure orbits of dimension 4, corresponding to the points (a, c_2) on the boundary curves $2c_2 = 3a^2 - 2 + 1$ and $c_2 = 6a^2 - 4 + 1$, respectively.

Furthermore, for $c_2 \leq 1/2$ all values of (a, c_2) that correspond to Hermitian matrices actually correspond to positive Hermitian operators, i.e., physical states. Hence, the union of all orbits with $c_2 \leq 1/2$ fills a ball of radius $1/\sqrt{6}$. For $c_2 \geq 1/2$, however, the positivity constraint kicks in and eliminates more and more *a*-values as c_2 approaches 1. This means that the physical orbits inside the ball get sparser as c_2 increases. However, for each $c_2 < 1$ the orbits always occupy a positive measure set of the sphere S^7 they are embedded in since for each $c_2 < 1$ there is a 1D set of positive measure of *a* values representing disjoint physical orbits of dimension 6. Hence, the union of these orbits (not counting the one or two pseudopure orbits) occupies a set of positive measure inside each seven-dimensional sphere S^7 . For $c_2 = 1$ the positivity constraint eliminates all *a*-values but a = 1 and hence the boundary sphere contains only the single four-dimensional orbit of proper pure states.

As regards the ordering of orbits, we have $\mathcal{O}[a, c_2] \prec \mathcal{O}[a, c'_2]$ if $c_2 < c'_2$ since $K(a, c_2) < K(a, c'_2)$ for $c_2 < c'_2$ and *a* fixed. In general, however, we cannot compare orbits that have the same distance from the origin since $a + b = \frac{1}{2}(1 + a + K)$ is monotonically *decreasing* over the valid range of *a* for $c_2 > 1/2$, and non-monotonic for $c \leq 1/2$, i.e., a < a' typically implies a + b > a' + b'. See figure 2 for a plot of $a + b = \frac{1}{2}(1 + a + K)$ as a function of *a* for various values of c_2 . Figure 3, for comparison, shows a plot of the von-Neumann entropy of the orbits $S[\mathcal{O}] = -[a \log(a) + b \log(b) + c \log(c)]$ as a function of the largest eigenvalue *a* for various values of c_2 . Note that for $c_2 \ge 1/2$ fixed, the von-Neumann entropy increases as a function of *a*, and for c < 1/2 it is non-monotonic as a function of *a*. Also note that for sufficiently large values of *S*, there are many orbits of varying distance from the centre with the same von-Neumann entropy *S* although for *fixed a* the orbits with the largest distance from the centre have the smallest entropy, which is in accord with our partial ordering of the orbits.

4. Actions of the symplectic group

In the previous sections we have shown that the action of the unitary group on the set of quantum states endows it with the structure of a stratified set and studied the properties of the strata defined by the unitary orbit manifolds. This stratification of the set of density matrices



Figure 2. a + b = (1 + a + K)/2 as a function of *a* for various values of c_2 .



Figure 3. von-Neumann entropy of orbits as a function of a for various values of c_2 .

was justified on physical grounds since the dynamics of a (closed) quantum system is usually determined by the action of the unitary group.

Some physical systems, however, exhibit symmetries that restrict the dynamics to a proper subgroup of the unitary group. For instance, the dynamics of an atomic system comprising two *n*-fold degenerate energy levels subject to coherent control fields of various polarizations is governed by the symplectic group Sp(n) due to dynamical symmetries [10]. Physical systems that exhibit symplectic symmetry are also of special interest in quantum control since they are pure-state controllable but lack mixed-state controllability [10]. This means, for instance, that we can steer the system from any pure initial state to any other pure state; however, if the system is initially in a mixed state, then it may not be possible to steer it to another mixed state even if this state is unitarily equivalent to the initial state, since the set of unitary operations at our disposal is limited and there may not be a sympletic unitary transformation that achieves the desired aim [11].

The action of the symplectic group also induces a stratification of the set of density matrices. Since the sympletic group Sp(n) is a subgroup of the unitary group U(2n), it naturally follows that the sympletic orbits are smaller than the unitary orbits. Hence, there will be more sympletic orbits. We can also think of the action of the symplectic group as partitioning the unitary orbits into symplectic suborbits. The stratification induced by the symplectic group is therefore a refinement of the stratification induced by U(2n). The remainder of this section is devoted to exploring the relation between the symplectic and unitary orbits/stratification.

Mathematically, the symplectic group Sp(n) is the subgroup of unitary transformations $A \in U(2n)$ that satisfy $A^T J A = J$ for

$$I = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \tag{14}$$

where I_n is the identity matrix in dimension n. Note that, technically, any group G that satisfies $\{S^T J S = J \mid \forall S \in G\}$ for a matrix J unitarily equivalent to the J in (14) is a representation of Sp(n) but we shall assume the standard representation with J as in (14) here. The condition $S^T J S = J$ then implies that any $2n \times 2n$ complex matrix $S \in Sp(n)$ must be of the form

$$S = \begin{pmatrix} A & B \\ -B^* & A^* \end{pmatrix}$$
(15)

where A and B are $n \times n$ complex matrices and A^* denotes the complex conjugate of the A.

We now show that Sp(n) acts transitively on the unitary orbits of some states, but for the majority of states the symplectic orbits have lower dimension than the unitary orbits. The following results are an extension of earlier results showing that Sp(n) acts transitively only on pure-state-like and completely random ensembles [11].

Proposition 3. If ρ is the completely random ensemble $I_{2n}/2n$ or a pseudo-pure state then its orbit under Sp(n) is the same as the orbit under U(2n), i.e., Sp(n) acts transitively on this orbit.

Proof. The orbit of any pseudo-pure state $\rho \in D_{1'}(V)$ under U(2n) is homeomorphic to \mathbb{CP}^{2n-1} by corollary 1. The assertion that Sp(n) acts transitively on the unitary orbits of pseudo-pure states hence follows directly from the well-known fact that Sp(n) acts transitively on \mathbb{CP}^{2n-1} via the isomorphism $\phi : \mathbb{H}^n \xrightarrow{\cong} \mathbb{C}^{2n}$ discussed in appendix A. Since the orbit of $\rho = I_{2n}/2n$ under U(2n) consists of a single point, the assertion that Sp(n) acts transitively on this orbit is trivial.

Proposition 4. Let $\rho = \text{diag}(\lambda_1, \ldots, \lambda_{2n})$ where $0 \leq \lambda_i \leq 1$ are the eigenvalues of ρ counted with multiplicity, satisfying $\sum_{i=1}^{2n} \lambda_i = 1$. Then the orbit of ρ is a homogeneous manifold of real dimension at most $2n^2$.

Proof. Since ρ is diagonal the isotropy subgroup G_{ρ} contains the maximal torus T^n of Sp(n), namely all matrices of the form diag $(z_1, \ldots, z_n, z_1, \ldots, z_n)$ with $z_i \in U(1) \simeq S^1$. Since G_{ρ} is a closed subgroup of the Lie group Sp(n), proposition 2 implies that the orbit is a homogeneous manifold of real dimension no more than dim_{\mathbb{R}} $(Sp(n)/T^n) = n(2n+1) - n = 2n^2$.

For certain special cases we can improve this bound on the orbit dimensions.

Table 2. Dimensions of the orbits of various types of ensembles classified by their spectrum under the unitary group U(2n) and the symplectic group Sp(n) for n = 2 and n = 3. The orbits under the symplectic group are in general much smaller than the orbits under the unitary group, except in the case of pure-state-like (and completely random) ensembles, for which the sympletic orbits have the same dimension as the unitary orbit. Note that in all cases it is assumed that different letters a, b, \ldots represent different values in [0, 1].

N = 4	U(4)	<i>Sp</i> (2)
$\rho = \operatorname{diag}(a, a, a, a)$	0	0
$\rho = \operatorname{diag}(a, b, b, b)$	6	6
$\rho = \operatorname{diag}(a, a, b, b)$	8	6
$\rho = \operatorname{diag}(a, b, c, c)$	10	$\leqslant 8$
$\rho = \operatorname{diag}(a, b, c, d)$	12	$\leqslant 8$
N = 6	U(6)	Sp(3)
$\rho = \operatorname{diag}(a, a, a, a, a, a)$	0	0
$\rho = \operatorname{diag}(a, b, b, b, b, b)$	10	10
$\rho = \operatorname{diag}(a, a, b, b, b, b)$	16	$\leq 21 - 10 = 11$
$\rho = \operatorname{diag}(a, b, c, c, c, c)$	18	$\leq 21 - 10 = 11$
$\rho = \operatorname{diag}(a, b, b, c, c, c)$	22	$\leq 2 \times 3^2 = 18$
$\rho = \operatorname{diag}(a, b, c, d, d, d)$	24	≤18
$\rho = \operatorname{diag}(a, a, b, b, c, c)$	24	≤18
$\rho = \operatorname{diag}(a, a, a, b, b, b)$	18	$\leqslant 3^2 + 3 = 12$
$\rho = \operatorname{diag}(a, b, c, c, d, d)$	26	≤18
$\rho = \operatorname{diag}(a, b, c, d, e, e)$	28	≤18
$\rho = \text{diag}(a, b, c, d, e, f)$	30	≤18

Proposition 5. If $\rho = \text{diag}(\sigma_n, \sigma_n)$ where σ_n is a diagonal $n \times n$ density matrix but not a multiple of I_n then the sympletic orbit of ρ is a homogeneous manifold of real dimension at most $2n^2 - 1$. If $\rho = \text{diag}(aI_n, bI_n)$ with $0 \leq a, b \leq 1$ and $a \neq b$ then the orbit of ρ under Sp(n) is a homogeneous manifold of real dimension $n^2 + n$.

Proof. In the former case, observe that the isotropy subgroup at ρ contains not only the maximal torus T^n , but also all matrices of the form $\{zJ \mid z \in S^1\}$. Since the matrix J is not symplectic-equivalent to any element of the maximal torus T^n , the first statement follows immediately from the previous proposition.

In the second case, note that any element Q that belongs to the isotropy subgroup at ρ must satisfy $Q\rho Q^{\dagger} = \rho$. Since Q must also be in Sp(n), it must be of the form (15) for some $A, B \in \text{endo}_{\mathbb{C}}(\mathbb{C}^n)$. This implies the matrices A and B must satisfy the relations $aAA^{\dagger} + bBB^{\dagger} = aI_n$ and $aBB^{\dagger} + bAA^{\dagger} = bI_n$ and hence $ab(a^2 - b^2)BB^{\dagger} = 0$. As 0 < a, b, < 1 and $a \neq b$ by assumption, we must have B = 0 and $A \in U(n)$. Thus, the isotropy subgroup at ρ is $\binom{A & 0}{0 & A^*}$ with $A \in U(n)$. From theorem 1, the orbit of ρ is a homogeneous manifold of real dimension $n(2n+1) - n^2 = n^2 + n$.

Proposition 6. If $\rho = \text{diag}(D_{2n-2\ell}, \alpha I_{2\ell})$, where $D_{2n-2\ell}$ is a diagonal $(2n - 2\ell) \times (2n - 2\ell)$ complex matrix, $I_{2\ell}$ is the identity $2\ell \times 2\ell$ complex matrix, and $\alpha \in [0, 1]$, then the orbit of ρ is a homogeneous manifold of real dimension at most $n(2n + 1) - \ell(2\ell + 1)$.

Proof. We note the isotropy subgroup at ρ contains the group $\binom{l_{2n-2\ell}}{\varrho_{2\ell}} | Q \in Sp(\ell) \}$, which is isomorphic to the subgroup $Sp(\ell)$. Hence, the orbit of ρ is a homogeneous manifold of real dimension at most $n(2n + 1) - \ell(2\ell + 1)$ as desired.

In table 2 we compare the dimensions of the orbits of various types of ensembles under U(2n) with those of the orbits under Sp(n) for n = 2 and n = 3. The classification of the

orbits is based on the spectrum of ρ . Note that the spectrum of ρ uniquely determines the unitary orbit (or equivalence class) ρ belongs to. However, two density matrices with the same spectrum may belong to different symplectic orbits. For instance, $\rho_0 = \text{diag}(a, b, a, b)$ and $\rho_1 = \text{diag}(a, a, b, b)$ are unitarily equivalent but belong to different orbits under the symplectic group as defined above. See example 1 in [11].

5. Conclusion

We have shown that the action of a Lie group on the set of quantum states endows it with the structure of a stratified set with strata given by the orbit manifolds. In particular, we studied the stratification of the set of states induced by the action of the unitary group, which is especially useful since the unitary orbits are of interest in quantum control and computing, where they determine the maximal set of quantum states that are reachable from a given set via a coherent control or by applying a unitary gate. Furthermore, there are many properties of quantum states such as von-Neumann or Renyi entropy that depend only on the unitary stratification. We have shown that the unitary orbits can be identified with flag manifolds whose type and dimension depend only on the *multiplicity* of the eigenvalues of the states belonging to the orbit. We have also determined the dimensions of the orbit manifolds and shown that we can define a partial ordering related to the degree of disorder in the system on this stratification via majorization.

To better understand the geometry and structure of the set of quantum states, we studied the embedding of the quantum states and their associated orbit manifolds of an *n*-level system into real Euclidean space provided by the coherence vector. We showed that the coherence vector we defined always maps the quantum states into a closed ball in \mathbb{R}^{n^2-1} in such a manner that the orbit manifolds are mapped to submanifolds of spheres of fixed radius from the centre. For n = 2 this embedding is surjective, hence justifying the identification of the set of quantum states with the closed ball in \mathbb{R}^3 , and the identification of the orbits with concentric spheres inside this ball. By comparing the dimensions of the orbits we also showed that this embedding is *no* longer surjective for n > 2 and the orbit manifolds in this case are proper submanifolds of spheres in \mathbb{R}^{n^2-1} of lower dimension. The manifold of pure states is always a submanifold of the boundary sphere, which contains no other orbits, while all other spheres of fixed distance from the centre generally contain infinitely many disjoint orbits of varying dimensions, and depending on the distance of the sphere from the centre, a positive measure set of points which do not correspond to quantum states at all. A detailed analysis for the three-level case was provided.

Finally, we studied systems whose natural evolution is restricted to a subgroup of the unitary group such as the symplectic group due to dynamical symmetries. We showed that we can define a refined stratification based on the smaller orbits of this subgroup. In the case of the symplectic group we have shown that the orbits of all pseudo-pure states agree with the unitary orbits, while the symplectic orbits of all other (mixed) states have lower dimension than the unitary orbits. From the point of view of control this means that we can control pure and pseudo pure states for such systems but not generic ensembles.

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Appendix. The symplectic group

The symplectic group Sp(n) is usually defined as the Lie group of automorphisms on \mathbb{H}^n , where \mathbb{H} is the skew-field of quaternions, that preserve the canonical symplectic inner product

$$\langle q \mid q'
angle = \sum_{i=1}^n ar{q}_i q'_i$$

where **q** and **q**' are *n*-vectors whose entries q_i are quaternions and conjugation $\bar{\mathbf{q}}$ is over \mathbb{H} .

The (skew-field) of quaternions \mathbb{H} can be regarded as a vector space over \mathbb{R} with the standard basis $\{1, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ subject to the multiplicative relations: $\mathbf{e}_i^2 = -1$ for $1 \le i \le 3$ and $\mathbf{e}_i \mathbf{e}_j = -\mathbf{e}_j \mathbf{e}_i = \mathbf{e}_k$ for any even permutation (i, j, k) of the set (1, 2, 3). Since the field of complex numbers \mathbb{C} is isomorphic to $\mathbb{R} \cdot \mathbf{1} \oplus \mathbb{R} \cdot \mathbf{e}_1$ and every quaternion q can be written as

$$q = q_0 + q_1 \mathbf{e}_1 + \mathbf{q}_2 \mathbf{e}_2 + \mathbf{q}_3 \mathbf{e}_3 = (\mathbf{q}_0 + \mathbf{q}_1 \mathbf{e}_1) + \mathbf{e}_2(\mathbf{q}_2 - \mathbf{q}_3 \mathbf{e}_1)$$

we may also regard \mathbb{H} as a vector space over \mathbb{C} with basis $\{\mathbf{1}, \mathbf{e_2}\}$. We therefore obtain an isomorphism $\phi : \mathbb{H}^n \to \mathbb{C}^{2n}$ of complex vector spaces via $\phi(q_1, \ldots, q_n) = (z_1, \ldots, z_{2n})$ where $q_i = z_i + z_{n+i}\mathbf{e_2}$. Consequently,

$$\langle q \mid q' \rangle = \sum_{i=1}^n \bar{q}_i q'_i = \left(\sum_{i=1}^{2n} z_i^* z'_i\right) + e_2 \left(\sum_{i=1}^n (z_i z'_{n+i} - z_{n+i} z'_i)\right).$$

The isomorphism ϕ allows us to identify an isometry A of \mathbb{H}^n , with a complex automorphism of \mathbb{C}^{2n} that preserves both the canonical Hermitian inner product and the canonical skew-symmetric bilinear form on \mathbb{C}^{2n} defined by

$$S(\mathbf{z}, \mathbf{z}') = \sum_{i=1}^{n} (z_i \mathbf{z}'_{n+i} - \mathbf{z}_{n+i} \mathbf{z}'_i)$$

where $z = (z_1, ..., z_{2n})$ and $z' = (z'_1, ..., z'_{2n})$.

Since A preserves the canonical Hermitian inner product on \mathbb{C}^{2n} , $A \in U(2n)$. Since A leaves invariant the canonical skew-symmetric bilinear form $S(\cdot, \cdot)$, it is equivalent to having $A^T J A = J$.

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