Criteria for reachability of quantum states

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Abstract
We address the question of which quantum states can be inter-converted under
the action of a time-dependent Hamiltonian. In particular, we consider the
problem as applied to mixed states, and investigate the difference between pure-
and mixed-state controllabilities introduced in previous work. We provide a
complete characterization of the eigenvalue spectrum for which the state is
controllable under the action of the symplectic group. We also address the
problem of which states can be prepared if the dynamical Lie group is not
sufficiently large to allow the system to be controllable.

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1. Introduction

The subject of control of quantum systems has been a fruitful area of investigation lately.
The growing interest in the subject can be attributed both to theoretical and experimental
breakthroughs that have made control of quantum phenomena an increasingly realistic
objective, as well as the prospect of many exciting new applications such as quantum computers
[1] or quantum chemistry [2], which attracts researchers from various fields.

Among the theoretical problems that have received considerable attention lately is the
issue of controllability of quantum systems. Various aspects such as the controllability of
quantum systems with continuous spectra [3, 4], wavefunction controllability for bilinear
quantum systems [5–7], controllability of distributed systems [8], controllability of molecular
systems [9], controllability of spin systems [10], controllability of quantum evolution in NMR
spectroscopy [11], and controllability of quantum systems on compact Lie groups [12–15]
have been addressed, and related problems such as the dynamical realizability of kinematical
bounds on the optimization of observables [16, 17], and the relation between controllability
and universality of quantum gates [18], as well as the information-theoretic limits of control
[19] have been studied.

In this process, various notions of controllability have been introduced. Recent work on controllability of quantum systems on compact Lie groups has finally shown that the degree of controllability of a quantum system depends on its dynamical Lie group, and that many different notions of controllability are in fact equivalent. In particular, it has been proved that quantum systems evolving on a compact Lie group, such as closed quantum systems with a discrete energy spectrum, are either density matrix/operator controllable, pure-state/wavefunction controllable, or not controllable [20, 21]. For density matrix, operator or completely controllable quantum systems, every kinematically admissible target state or operator can be dynamically realized, and the kinematical bounds on the expectation values (ensemble averages) of observables are always dynamically attainable [17]. Fortunately, many quantum systems have been shown to be completely controllable [13, 14, 21].

Nevertheless, there are quantum systems that are either only pure-state controllable or not controllable at all. For instance, it has been shown that the dynamical Lie group of certain atomic systems with degenerate energy levels is the (unitary) symplectic group, which corresponds to pure-state controllability [21]. Other systems with certain symmetries may be either pure-state controllable or non-controllable depending on the symmetry. For instance, given a system with N equally spaced energy levels and uniform dipole moments for transitions between adjacent levels, the dynamical Lie group is the symplectic group if the dimension of its Hilbert space N is even, but it is the orthogonal group if N is odd [22]. For these systems, the question of dynamical reachability of target states, which is important in many applications, remains. In this paper, we address this problem by studying the action of the dynamical Lie group of pure-state-only and non-controllable quantum systems on the kinematical equivalence classes of states. Explicit criteria for dynamical reachability of states are derived for systems whose dynamical Lie group is the (unitary) symplectic group or the orthogonal group.

2. Quantum states and kinematical/dynamical equivalence classes

We consider a quantum system whose state is represented by a density matrix acting on a Hilbert space $\mathcal{H}$ of dimension N. A density matrix always has a discrete spectrum with non-negative eigenvalues w_n that sum to one, $\sum_n w_n = 1$, and a spectral resolution of the form

$$\rho = \sum_{n=1}^{N} w_n |\Psi_n\rangle\langle\Psi_n| \tag{1}$$

where $|\Psi_n\rangle$ are the eigenstates of ρ. The $|\Psi_n\rangle$ for $1 \leqslant n \leqslant N$ are elements of the Hilbert space $\mathcal{H}$ and can always be chosen so as to form a complete orthonormal set for $\mathcal{H}$. The $\langle\Psi_n|$ are the corresponding dual states defined by

$$\langle\Psi_n \mid \Psi_m\rangle = \delta_{mn} \qquad \forall m, n. \tag{2}$$

Conservation laws such as conservation of energy and probability require the time evolution of any (closed) quantum system to be unitary. Thus, given a Hilbert space vector $|\Psi_0\rangle$, its time evolution is determined by $|\Psi(t)\rangle = U(t)|\Psi_0\rangle$ where $U(t)$ is a unitary operator for all t and $U(0) = I$. Hence, a density matrix ρ_0 must evolve according to

$$\rho(t) = U(t)\rho_0 U(t)^{\dagger} \tag{3}$$

where $U(t)$ is unitary for all times. This constraint of unitary evolution induces kinematical restrictions on the set of target states that are physically admissible from any given initial state.

Definition 1. *Two quantum states represented by density matrices ρ_0 and ρ_1 are kinematically equivalent if there exists a unitary operator U such that $\rho_1 = U\rho_0 U^\dagger$.*

Thus, the constraint of unitary evolution partitions the set of density matrices on $\mathcal{H}$ into (infinitely many) kinematical equivalence classes. It is well known that two density matrices ρ_0 and ρ_1 are kinematically equivalent if and only if they have the same eigenvalues. The kinematical equivalence classes are therefore determined by the eigenvalues of ρ. Furthermore, we introduce the following classification of density matrices according to their eigenvalues, which we shall relate to the degree of controllability of the system.

Definition 2 (Classification of density matrices). *Every density matrix is of one of the following types.*

 (i) *Completely random ensembles: Density matrices whose spectrum consists of a single eigenvalue $w_1 = \frac{1}{N}$ that occurs with multiplicity N.*
 (ii) *Pure-state-like ensembles: Density matrices whose spectrum consists of two distinct eigenvalues, one of which occurs with multiplicity 1 and the other with multiplicity $N - 1$.*
(iii) *General ensembles: Density matrices whose spectrum consists of at least two distinct eigenvalues, at least one of which occurs with multiplicity N_1 where $2 \leqslant N_1 \leqslant N - 2$; or density matrices whose spectrum consists of N distinct eigenvalues ($N \geqslant 2$).*

Note that type (ii) (pure-state-like ensembles) includes density matrices representing pure states such as $\rho = \mathrm{diag}(1, 0, 0, 0)$ but not every density matrix in this class represents a pure state. For instance, $\rho = \mathrm{diag}(0.7, 0.1, 0.1, 0.1)$ is of type (ii) but does *not* represent a pure state.

Given a specific quantum system with a control-dependent Hamiltonian of the form

$$H[f_1(t), \ldots, f_M(t)] = H_0 + \sum_{m=1}^{M} f_m(t) H_m \tag{4}$$

where the $f_m, 1 \leqslant m \leqslant M$, are (independent) bounded measurable control functions, the question arises which states are dynamically reachable from a given initial state. Clearly, the set of potentially dynamically reachable states is restricted to states within the same kinematical equivalence class as the initial state. However, not every kinematically admissible target state is necessarily dynamically reachable. Since the time-evolution operator $U(t)$ has to satisfy the Schrodinger equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} U(t) = H[f_1(t), \ldots, f_M(t)]U(t) \tag{5}$$

where H is the Hamiltonian defined above, only unitary operators of the form

$$U(t) = \exp_+ \left\{ -\frac{\mathrm{i}}{\hbar} H[f_1(t), \ldots, f_M(t)] \right\} \tag{6}$$

where $\exp_+$ denotes the time-ordered exponential, qualify as evolution operators. Using, for instance, the Magnus expansion of the time-ordered exponential, it can be seen that only unitary operators of the form $\exp(x)$, where x is an element in the dynamical Lie algebra $\mathcal{L}$ generated by the skew-Hermitian operators $\mathrm{i}H_0, \ldots, \mathrm{i}H_M$, are dynamically realizable. These operators form the dynamical Lie group S of the system.

Definition 3. *Two kinematically equivalent states ρ_0 and ρ_1 are dynamically equivalent if there exists a unitary operator U in the dynamical Lie group S such that $\rho_1 = U\rho_0 U^\dagger$.*

This dynamical equivalence relation subdivides the kinematical equivalence classes.

In the following, we shall be particularly concerned with the unitary group $U(N)$, the special unitary group $SU(N)$, the (unitary) symplectic group $Sp\left(\frac{N}{2}\right)$ and the (unitary) orthogonal group $SO(N)$. As usual, the unitary group $U(N)$ is the compact Lie group consisting of all regular $N \times N$ matrices U that satisfy $U^\dagger U = UU^\dagger = I$. The special unitary group $SU(N)$ is the subgroup of $U(N)$ consisting of all unitary matrices $U \in U(N)$ whose determinant is +1. For our purposes in this paper, we define the symplectic group and the special orthogonal group as follows.

Definition 4. *The (unitary) symplectic group $Sp(\ell)$ is the subgroup of $SU(2\ell)$ consisting of all unitary operators of dimension 2ℓ that satisfy $U^T J U = J$ for*

$$J = \begin{pmatrix} 0 & I_\ell \\ -I_\ell & 0 \end{pmatrix} \tag{7}$$

where I_ℓ is the identity matrix of dimension ℓ.

Definition 5. *The (unitary) special orthogonal group $SO(N)$ is the subgroup of $SU(N)$ consisting of all unitary operators of dimension N that satisfy $U^T J U = J$ for*

$$J = \begin{pmatrix} 0 & I_\ell \\ I_\ell & 0 \end{pmatrix} \qquad N = 2\ell \qquad J = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & I_\ell \\ 0 & I_\ell & 0 \end{pmatrix} \qquad N = 2\ell + 1. \tag{8}$$

3. Dynamical Lie group action on the kinematical equivalence classes

The set of quantum states that is dynamically accessible from a given initial state ρ_0 depends on the action of the dynamical Lie group S on the kinematical equivalence classes of density operators.

Definition 6. *The dynamical Lie group S of a quantum system is said to act transitively on a kinematical equivalence class $\mathcal{C}$ of density matrices if any two states in $\mathcal{C}$ are dynamically equivalent.*

Since the equivalence class of completely random ensembles (type (i) above) consists only of a single state $\rho = \frac{1}{N} I_N$, it follows immediately that *every* group acts transitively on this equivalence class.

Any dynamical Lie group S that does not act transitively on the kinematical equivalence class of pure states, acts transitively only on the trivial kinematical equivalence class of completely random ensembles. Furthermore, from classical results by Montgomery and Samelson [23], it follows that $U(N), SU(N), Sp\left(\frac{1}{2}N\right)$ and $Sp\left(\frac{1}{2}N\right) \times U(1)$ are the *only* dynamical Lie groups (up to isomorphism) that act transitively on the equivalence class of pure states. Therefore, any dynamical Lie group S that is not isomorphic to either $U(N), SU(N), Sp\left(\frac{1}{2}N\right)$ or $Sp\left(\frac{1}{2}N\right) \times U(1)$ acts transitively only on type (i) states, i.e. completely random ensembles. $U(N)$ and $SU(N)$ clearly act transitively on *every* kinematical equivalence class of states, which leaves only $Sp\left(\frac{1}{2}N\right)$ and $Sp\left(\frac{1}{2}N\right) \times U(1)$, whose action on the kinematical equivalence classes of states we shall now address.

We begin by showing that transitive action of $Sp\left(\frac{1}{2}N\right)$ on pure states implies transitive action on all equivalence classes of type (ii). We shall prove this result for the standard representation of $Sp\left(\frac{1}{2}N\right)$ as defined above. To see that this is sufficient, note that lemma 4.2 in [20] shows that whenever the dynamical Lie algebra of a quantum system of the type considered in this paper is *isomorphic* to $sp\left(\frac{1}{2}N\right)$, then it is *conjugate* to $sp\left(\frac{1}{2}N\right)$ via an

element in $U(N)$. Thus, if the dynamical Lie group S of the system is of type $Sp\left(\frac{1}{2}N\right)$ then it is not only isomorphic to the standard representation of $Sp\left(\frac{1}{2}N\right)$, but also there exists a unitary transformation (basis change) B that maps any unitary operator in $U \in S$ to a unitary operator $\tilde{U} = BUB^\dagger$ in the standard representation of $Sp\left(\frac{1}{2}N\right)$, i.e. S is unitarily equivalent to the standard representation of $Sp\left(\frac{1}{2}N\right)$.

Note that theorem 6 in [20] gives a general condition for transitive action of a dynamical Lie group $S \subset U(N)$ on a kinematical equivalence class of states represented by a density matrix ρ: the action is transitive if and only if

$$\dim U(N) - \dim S = \dim \mathcal{C}_\rho - \dim(\mathcal{C}_\rho \cap S) \tag{9}$$

where $\mathcal{C}_\rho$ is the centralizer of ρ and $\mathcal{C}_\rho \cap S$ is the intersection of the centralizer with S. However, since determination of the dimension of $\mathcal{C}_\rho$, and especially $\mathcal{C}_\rho \cap S$, tends to be very difficult in practice (see appendix B for an example) we shall *not* use this result but pursue an alternative approach instead.

Lemma 1. $Sp\left(\frac{1}{2}N\right)$ *acts transitively on all kinematical equivalence classes of density matrices whose eigenvalues satisfy* $w_1 \neq w_2 = w_3 = \cdots = w_N$.

Proof. Any ρ with eigenvalues $w_1 \neq w_2 = w_3 = \cdots = w_N$ can be written as

$$\rho = w_1 |\Psi\rangle\langle\Psi| + w_2 P(|\Psi\rangle^\perp)$$

where $P(|\Psi\rangle^\perp)$ is the projector onto the orthogonal complement of the subspace spanned by $|\Psi\rangle$. Hence, any pair of kinematically equivalent states of this type is of the form

$$\rho_0 = w_1 |\Psi^{(0)}\rangle\langle\Psi^{(0)}| + w_2 P(|\Psi^{(0)}\rangle^\perp)$$
$$\rho_1 = w_1 |\Psi^{(1)}\rangle\langle\Psi^{(1)}| + w_2 P(|\Psi^{(1)}\rangle^\perp).$$

Since $Sp\left(\frac{1}{2}N\right)$ acts transitively on the equivalence class of pure states, there exists a unitary operator $U \in Sp\left(\frac{1}{2}N\right)$ such that $U|\Psi^{(0)}\rangle = |\Psi^{(1)}\rangle$. Furthermore, U automatically maps the orthogonal complement of $|\Psi^{(0)}\rangle$ onto the orthogonal complement of $|\Psi^{(1)}\rangle$ since it is unitary and thus we have

$$U\rho^{(0)}U^\dagger = w_1 |\Psi^{(1)}\rangle\langle\Psi^{(1)}| + w_2 P(|\Psi^{(1)}\rangle^\perp) = \rho^{(1)}.$$

Hence, $Sp\left(\frac{1}{2}N\right)$ acts transitively on all equivalence classes of density matrices whose eigenvalues satisfy $w_1 \neq w_2 = w_3 = \cdots = w_N$. $\square$

However, the action of $Sp\left(\frac{1}{2}N\right)$ on the class of pure states is not two-point transitive as the following example shows.

Example 1. Let $N = 2\ell$ and $\vec{a}$ and $\vec{b}$ be two unit vectors in $\mathbb{C}^N$. Since $N = 2\ell$, we can partition the vectors as follows:

$$\vec{a} = \begin{pmatrix} \vec{a}_1 \\ \vec{a}_2 \end{pmatrix} \qquad \vec{b} = \begin{pmatrix} \vec{b}_1 \\ \vec{b}_2 \end{pmatrix}$$

where $\vec{a}_j, \vec{b}_j$ for $j = 1, 2$ are vectors in $\mathbb{C}^\ell$. Since $Sp(\ell)$ acts transitively on the unit sphere in $\mathbb{C}^N$ it follows that there exists a $U \in Sp(\ell)$ such that $U\vec{a} = \vec{b}$. However, since any unitary operator in $Sp(\ell)$ satisfies $U^T J U = J$ with J as in (7), we have $U = J^\dagger U^* J$ and thus $J^\dagger U^* J \vec{a} = \vec{b}$ or equivalently $U J \vec{a}^* = J \vec{b}^*$. Noting that

$$J\vec{a}^* = \begin{pmatrix} -\vec{a}_2^* \\ \vec{a}_1^* \end{pmatrix} \qquad J\vec{b}^* = \begin{pmatrix} -\vec{b}_2^* \\ \vec{b}_1^* \end{pmatrix}$$

it thus follows that U maps $\vec{c} \equiv J\vec{a}^*$ onto $\vec{d} \equiv J\vec{b}^*$. Therefore, given two (orthogonal) unit vectors of the form $\vec{a}$ and $\vec{c}$, it is not possible to find a unitary transformation in $Sp(\ell)$ that maps these two vectors onto two arbitrary (orthogonal) unit vectors. Rather, once we have chosen the image of $\vec{a}$, the image of $\vec{c}$ is fixed.

This lack of two-point transitivity has serious implications for the action of $Sp(\frac{1}{2}N)$, in particular it implies non-transitive action on all kinematical equivalence classes of type (iii).

Lemma 2. $Sp(\frac{1}{2}N)$ *does not act transitively on kinematical equivalence classes of density matrices with at least three distinct eigenvalues, two of which having multiplicity 1.*

Proof. Any two kinematically equivalent density matrices can be written as

$$\rho_0 = \sum_{n=1}^{N} w_n |\Psi_n\rangle\langle\Psi_n| \qquad \rho_1 = \sum_{n=1}^{N} w_n |\Phi_n\rangle\langle\Phi_n|.$$

Since there are at least three distinct eigenvalues and two of them have multiplicity 1, we may assume $w_1 \neq w_n$ for all $n \neq 1$ and $w_2 \neq w_n$ for all $n \neq 2$. Thus, $|\Psi_n\rangle$ and $|\Phi_n\rangle$ for $n = 1, 2$ are unique up to phase factors and any U such that $\rho_1 = U\rho_0 U^\dagger$ must map $|\Psi_n\rangle$ onto $|\Phi_n\rangle$ (modulo phase factors) for $n = 1, 2$, i.e.

$$U|\Psi_1\rangle = e^{i\phi_1}|\Phi_1\rangle \qquad U|\Psi_2\rangle = e^{i\phi_2}|\Phi_2\rangle.$$

However, suppose $|\Psi_1\rangle \doteq \vec{a}$, $|\Psi_2\rangle \doteq \vec{c}$ and $|\Phi_1\rangle \doteq \vec{b}$ but $|\Phi_2\rangle \neq e^{i\phi}\vec{d}$, where $\vec{a}, \vec{b}, \vec{c}$ and $\vec{d}$ are as defined in example 1. This example then shows that it is impossible to find a $U \in Sp(\frac{1}{2}N)$ that simultaneously maps $|\Psi_1\rangle$ onto $|\Phi_1\rangle$ and $|\Psi_2\rangle$ onto $|\Phi_2\rangle$. Therefore, there does not exist a unitary operator in $Sp(\frac{1}{2}N)$ such that $\rho_1 = U\rho_0 U^\dagger$. $\qquad\square$

Lemma 3. $Sp(\frac{1}{2}N)$ *does not act transitively on equivalence classes of density matrices that have at least one nonzero eigenvalue that occurs with multiplicity greater than 1 but less than* $N - 1$.

Proof. Suppose w_1 has multiplicity N_1 where $2 \leqslant N_1 \leqslant N - 2$. If $Sp(\frac{1}{2}N)$ acts transitively on the selected equivalence class of states then we must be able to map the N_1-dimensional eigenspace $E^{(0)}(w_1)$ for ρ_0 onto the corresponding eigenspace $E^{(1)}(w_1)$ for ρ_1 by a unitary operator in $Sp(\frac{1}{2}N)$ for any ρ_0 and ρ_1 in the same equivalence class. However, it is easy to see that this is not always possible. Suppose $E^{(0)}(w_1)$ contains a pair of vectors of the form $\vec{a}, \vec{c}$ as defined above and $E^{(1)}(w_1)$ contains a vector $\vec{b}$ but the related vector $\vec{d}$ is in the orthogonal complement of $E^{(1)}(w_1)$. Then it is impossible to map $E^{(0)}(w_1)$ onto $E^{(1)}(w_1)$ by a $U \in Sp(\frac{1}{2}N)$. Since the orthogonal complement of $E^{(1)}(w_1)$ has at least dimension 2, we can always choose $E^{(1)}(w_1)$ such that $\vec{d} \in E^{(1)}(w_1)^\perp$. Hence, $Sp(\frac{1}{2}N)$ does not act transitively on the selected equivalence class of states. $\qquad\square$

Given any two mixed states ρ_0 and ρ_1 related by $\rho_1 = U\rho_0 U^\dagger$ for some $U \in Sp(\frac{1}{2}N) \times U(1)$, we can find a $\tilde{U} \in Sp(\frac{1}{2}N)$ such that $\rho_1 = \tilde{U}\rho_0\tilde{U}^\dagger$. For instance, if $\det U = e^{i\alpha}$, setting $\tilde{U} = e^{-i\alpha/N} U$ produces an operator with $\det(\tilde{U}) = 1$ that obviously satisfies

$$\tilde{U}\rho_0\tilde{U}^\dagger = U\rho_0 U^\dagger = \rho_1.$$

Thus, $Sp(\frac{1}{2}N) \times U(1)$ acts transitively on a kinematical equivalence class $\mathcal{C}$ of density matrices if and only if $Sp(\frac{1}{2}N)$ does. Combining this observation with the previous lemmas yields the following theorem.

Theorem 1.

- $U(N)$ and $SU(N)$ *act transitively on all kinematical equivalence classes.*
- $Sp\left(\frac{1}{2}N\right)$ *and* $Sp\left(\frac{1}{2}N\right) \times U(1)$ *act transitively on all kinematical equivalence classes of density matrices of type (i) or (ii) and only those.*
- *Any other dynamical Lie group acts transitively only on the trivial kinematical equivalence class of completely random ensembles.*

4. Criteria for reachability of target states

Having established that the action of the dynamical Lie groups $Sp\left(\frac{1}{2}N\right)$ and $Sp\left(\frac{1}{2}N\right) \times U(1)$ is *not* transitive on any kinematical equivalence class of density matrices of type (iii), and that all other dynamical Lie groups except $U(N)$ and $SU(N)$ act transitively only on the trivial kinematical equivalence class of completely random ensembles, the question of identifying states that are kinematically but not dynamically equivalent arises.

Since dynamical Lie groups can be very complicated, it would be unrealistic to expect that simple criteria for dynamical equivalence of states can be derived for arbitrary dynamical Lie groups. However, for certain types of dynamical Lie groups of special interest, such as $Sp\left(\frac{1}{2}N\right)$ [or $Sp\left(\frac{1}{2}N\right) \times U(1)$] and $SO(N)$ [or $SO(N) \times U(1)$], this is possible, as will be shown in the following.

4.1. Systems with dynamical Lie group $Sp\left(\frac{1}{2}N\right)$ or $Sp\left(\frac{1}{2}N\right) \times U(1)$

To address the problem of finding criteria for dynamical equivalence of states for systems whose dynamical Lie group S is isomorphic (unitarily equivalent) to $Sp\left(\frac{1}{2}N\right)$, we recall that any unitary operator $U \in Sp(\ell)$ satisfies $U^T J U = J$ for J as defined in (7). Thus, any dynamical evolution operator U for a system of dimension $N = 2\ell$ with dynamical Lie group of type $Sp(\ell)$ must satisfy

$$U^T \tilde{J} U = \tilde{J} \tag{10}$$

for a matrix $\tilde{J}$, which is unitarily equivalent to (7).[3] Therefore, we must have

$$U = \tilde{J}^\dagger U^* \tilde{J} \qquad U^\dagger = \tilde{J}^\dagger U^T \tilde{J}.$$

Two kinematically equivalent states ρ_0 and ρ_1 are thus dynamically equivalent if and only if there exists a unitary operator U such that

$$\rho_1 = U \rho_0 U^\dagger \quad \text{and} \quad \rho_1 = \tilde{J}^\dagger U^* \tilde{J} \rho_0 \tilde{J}^\dagger \tilde{U}^T \tilde{J}$$

or equivalently,

$$\rho_1 = U \rho_0 U^\dagger \quad \text{and} \quad \underbrace{(\tilde{J} \rho_1 \tilde{J}^\dagger)^*}_{\tilde{\rho}_1} = U \underbrace{(\tilde{J} \rho_0 \tilde{J}^\dagger)^*}_{\tilde{\rho}_0} U^\dagger. \tag{11}$$

Example 2. Let $N = 4$ and $S = Sp(2)$ with $\tilde{J} = J$ as in (7).

(i) Then $\rho_0 = \mathrm{diag}(a, a, b, b)$ $\left(0 \leqslant a, b \leqslant \frac{1}{2}, a + b = \frac{1}{2}\right)$ and $\rho_1 = \mathrm{diag}(a, b, b, a)$ are dynamically equivalent since there exists a unitary operator U such that $\rho_1 = U \rho_0 U^\dagger$ and any such U clearly maps $\tilde{\rho}_0 = \mathrm{diag}(b, b, a, a)$ to $\tilde{\rho}_1 = \mathrm{diag}(b, a, a, b)$.

(ii) ρ_0 and $\rho_2 = \mathrm{diag}(a, b, a, b)$, on the other hand, are not dynamically equivalent (unless $b = a$) since $\tilde{\rho}_2 = \rho_2$ but $\tilde{\rho}_0 \neq \rho_0$ and there cannot be a unitary operator such that $\rho_1 = U \rho_0 U^\dagger = U \tilde{\rho}_0 U^\dagger$ if $\rho_0 \neq \tilde{\rho}_0$.

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[3] See appendix A for details about how to determine $\tilde{J}$.

This shows that $S = Sp(2)$ divides any kinematical equivalence class of states with two distinct eigenvalues of multiplicity $\ell = 2$ into at least two disjoint subsets of dynamically equivalent states.

Sometimes the condition $U^T \tilde{J} U = \tilde{J}$ can also be used directly to show that two states are not dynamically equivalent.

Example 3. Consider again $N = 4$ and $S = Sp(2)$ with $\tilde{J} = J$ as in (7) as well as the initial state $\rho_0 = \mathrm{diag}(a, b, c, d)$ where $0 \leqslant a, b, c, d \leqslant 1$, $a + b + c + d = 1$ and a, b, c, d are mutually different. We can conclude that the state $\rho_1 = \mathrm{diag}(b, a, c, d)$ is not dynamically equivalent to ρ_0 since we would require a unitary operator of the form

$$
U = \begin{pmatrix}
0 & e^{i\phi_1} & 0 & 0 \\
e^{i\phi_2} & 0 & 0 & 0 \\
0 & 0 & e^{i\phi_3} & 0 \\
0 & 0 & 0 & e^{i\phi_4}
\end{pmatrix}
$$

which does not satisfy $U^T J U = J$.

Another way of showing that two (kinematically equivalent) density matrices are not dynamically equivalent is to prove that (11) cannot have a solution by showing that the related linear system

$$
\rho_1 U - U \rho_0 = 0 \qquad \tilde{\rho}_1 U - U \tilde{\rho}_0 = 0 \tag{12}
$$

does not have a solution. To verify this, we note that the linear system above can be rewritten in the form $\mathcal{A} \vec{U} = 0$ where $\mathcal{A}$ is a matrix with $2N^2$ rows and N^2 columns and $\vec{U}$ is a column vector of length N^2. If the null space of $\mathcal{A}$ is empty then there is no $\vec{U}$ such that $\mathcal{A} \vec{U} = 0$ and hence there is no $N \times N$ matrix U that satisfies (12). However, note that if the linear system above *does* have a solution, this does not imply that the states in question are dynamically equivalent since the solution to the linear equation is in general not unitary.

4.2. Systems with dynamical Lie group $SO(N)$ or $SO(N) \times U(1)$

From the previous discussion, we know that $SO(N)$ does not act transitively on any kinematical equivalence class other than the trivial one. However, we can establish criteria for dynamical equivalence of states similar to those for $Sp(\frac{1}{2}N)$ by noting that any unitary operator $U \in SO(N)$ must satisfy $U^T J U = J$ for J as in (8). Therefore, two kinematically equivalent states ρ_0 and ρ_1 are dynamically equivalent under the action of a dynamical Lie group S which is unitarily equivalent to $SO(N)$, if there exists a unitary operator U such that

$$
\rho_1 = U \rho_0 U^\dagger \quad \text{and} \quad \underbrace{(\tilde{J} \rho_1 \tilde{J}^\dagger)^*}_{\tilde{\rho}_1} = U \underbrace{(\tilde{J} \rho_0 \tilde{J}^\dagger)^*}_{\tilde{\rho}_0} U^\dagger \tag{13}
$$

with $\tilde{J}$ unitarily equivalent to (8), and determined as described in appendix A.

Example 4. Consider a system with $N = 5$ and Hamiltonian $H = H_0 + f(t) H_1$, where

$$
H_0 = \begin{pmatrix}
-2 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 2
\end{pmatrix} \qquad
H_1 = \begin{pmatrix}
0 & 1 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 1 & 0
\end{pmatrix}.
$$

It can be verified using the algorithm described in [14] that the Lie algebra of this system has dimension 10, which is equal to the dimension of $so(5)$. Using the technique described in appendix A, we find that both of the generators iH_0 and iH_1 of the Lie algebra satisfy $x^T \tilde{J} + \tilde{J}x = 0$ for

$$\tilde{J} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

which is unitarily equivalent to the standard J for $so(5)$. We can thus conclude that its dynamical Lie algebra is $so(5)$ and its dynamical Lie group is $SO(5)$. Furthermore, note that the two pure states

$$\rho_0 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad \rho_1 = \begin{pmatrix} 0.5 & 0 & 0 & 0 & 0.5 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 & 0.5 \end{pmatrix}$$

are not dynamically equivalent since $(\tilde{J}\rho_1\tilde{J}^\dagger)^* = \rho_1$ but $(\tilde{J}\rho_0\tilde{J}^\dagger)^* \neq \rho_0$ and it is thus impossible to find a unitary transformation such that $U\rho_0 U^\dagger = \rho_1 = U(\tilde{J}\rho_0\tilde{J}^\dagger)^* U^\dagger$.

5. Conclusion

The question of dynamical equivalence of kinematically equivalent quantum states has been addressed by studying the action of the dynamical Lie group of the system on the kinematical equivalence classes. For systems whose dynamical Lie group is unitarily equivalent to either $Sp(\frac{1}{2}N)$ or $SO(N)$, explicit criteria for dynamical reachability/equivalence of states have been given, and their application illustrated with several examples.

Furthermore, we have provided a classification of density matrices according to their eigenvalues, which divides mixed quantum states into three main types: (i) completely random ensembles, (ii) pure-state-like ensembles and (iii) general ensembles. We have also proved that the dynamical Lie group $Sp(\frac{1}{2}N)$ acts transitively on all equivalence classes of quantum states of type (i) and (ii), but *only* those.

Although it is known that a pure-state controllable system whose dynamical Lie group S is isomorphic to $Sp(\frac{1}{2}N)$ is *not* density matrix controllable in general [20], this result shows that there are more than just a few examples of kinematically equivalent density matrices that are not dynamically reachable from one another in this case. In fact, the action of S is *not* transitive on *almost all* kinematical equivalence classes. This is in marked contrast to the action of S for a density matrix controllable system, which is transitive on *all* kinematical equivalence classes, as well as the action of S for a non-controllable system, which is transitive only on the trivial kinematical equivalence class of completely random ensembles.

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Appendix A. Finding J for dynamical Lie groups of type $Sp\left(\frac{1}{2}N\right)$ or $SO(N)$

For the results of the previous sections to be truly useful, we must also address the question of how to determine the $\tilde{J}$ matrix of a given system. To this end, note that the elements of the dynamical Lie algebra L associated with the dynamical groups $Sp\left(\frac{1}{2}N\right)$ and $SO(N)$ must satisfy a relation similar to the one satisfied by the elements of the group, namely any $x \in L$ must satisfy

$$x^T \tilde{J} + \tilde{J}x = 0 \tag{A.1}$$

where $\tilde{J}$ is the same as for the related group. Thus, given a system with total Hamiltonian (4), this implies in particular that the generators iH_m of the dynamical Lie algebra must satisfy (A.1).

Equation (A.1) can be written as a system of linear equations of the form

$$\mathcal{L}_m \vec{J} = 0 \qquad 0 \leqslant m \leqslant M$$

where $\mathcal{L}_m$ is a square matrix of dimension N^2 determined by the generators iH_m and $\vec{J}$ is a column vector of length N^2. The solutions $\vec{J}$ of the above matrix equation can be found by computing the null space of the operator

$$\begin{pmatrix} \tilde{\mathcal{L}}_0 \\ \vdots \\ \tilde{\mathcal{L}}_M \end{pmatrix}.$$

If the dynamical Lie group is of type $Sp\left(\frac{1}{2}N\right)$ or $SO(N)$ then the null space contains a single element $\vec{J}$, which can be rearranged into a square matrix whose eigenvalues agree with those of the standard J for the group defined above. That is, concretely,

- if $N = 2\ell$ and $\tilde{J}$ has two distinct eigenvalues $+i$ and $-i$, both of which occur with multiplicity ℓ then the dynamical Lie group is $Sp(\ell)$;
- if $N = 2\ell$ and $\tilde{J}$ has two distinct eigenvalues $+1$ and -1, both of which occur with multiplicity ℓ then the dynamical Lie group is $SO(2\ell)$;
- if $N = 2\ell + 1$ and $\tilde{J}$ has two distinct eigenvalues $+1$ and -1, occurring with multiplicities $\ell + 1$ and ℓ, respectively, then the dynamical Lie group is $SO(2\ell + 1)$.

Hence, the algorithm not only determines $\tilde{J}$ but it also allows us to decide whether the dynamical Lie group is of type $Sp\left(\frac{1}{2}N\right)$ or $SO(N)$.

Note that the dynamical Lie group S can only be $Sp\left(\frac{1}{2}N\right)$ or $SO(N)$ if all the partial Hamiltonians H_m of the system have zero trace. However, if any of the partial Hamiltonians H_m have nonzero trace then the dynamical Lie group of the system can still be $Sp\left(\frac{1}{2}N\right) \times U(1)$ or $SO(N) \times U(1)$. To deal with this situation, we note that $S \simeq Sp\left(\frac{1}{2}N\right) \times U(1)$ or $S \simeq SO(N) \times U(1)$ is possible only if the generators

$$x_m = iH_m - \frac{i}{N}\mathrm{Tr}(H_m)I_N \qquad 0 \leqslant m \leqslant M \tag{A.2}$$

of the related trace-zero Lie algebra L' satisfy (A.1) for $0 \leqslant m \leqslant M$ and we can thus proceed as above to determine $\tilde{J}$.

Appendix B. Comparison of theorem 1 with theorem 6 in [20]

To demonstrate the difficulty in using theorem 6 in [20] to verify whether the dynamical Lie group S of a system acts transitively on an equivalence class of density operators, we shall consider a simple example.

Assume that the dynamical Lie group of the system is $Sp(2) \subset U(4)$. According to theorem 1 above, $Sp(2)$ does *not* act transitively on the kinematical equivalence class represented by $\rho = \text{diag}(a, a, b, b)$ with $0 \leqslant a, b \leqslant \frac{1}{2}$ and $a + b = \frac{1}{2}$ since ρ is of type (iii).

To show that the action is not transitive using theorem 6 in [20], we note first that $\dim U(4) = 16$ and $\dim Sp(2) = 10$. Thus, the left-hand side in (9) is $\dim U(4) - \dim Sp(2) = 6$.

To compute the right-hand side, we need to determine the centralizer $\mathcal{C}_\rho$ of ρ. Noting that

$$\rho = \begin{pmatrix} a I_2 & 0 \\ 0 & b I_2 \end{pmatrix}$$

where I_2 is the identity matrix in dimension 2, we see that ρ commutes with every unitary matrix of the form

$$U_C = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}$$

where A_1 and A_2 are arbitrary unitary matrices in $U(2)$. Thus, the centralizer of ρ is $U(2) \times U(2)$ and its dimension is $4 + 4 = 8$.

To compute the intersection of $\mathcal{C}_\rho$ with $S = Sp(2)$, we recall that any matrix in $Sp(2)$ must preserve J as defined in (7). Concretely, this means $U_C^T J U_C = J$, i.e.

$$U_C^T J U_C = \begin{pmatrix} 0 & A_1^T A_2 \\ -A_2^T A_1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & I_2 \\ -I_2 & 0 \end{pmatrix}.$$

Thus, we must have $A_1^T A_2 = I_2$. Noting that A_1 and A_2 are unitary, this is only possible if $A_1 = A_2^*$, i.e. if A_1 is the complex conjugate of A_2, since $(A_2^*)^T A_2 = A_2^\dagger A_2 = I$. Hence, the intersection of the centralizer $\mathcal{C}_\rho$ with $S = Sp(2)$ is $U(2)$, which has dimension 4. Hence, $\dim \mathcal{C}_\rho - \dim(\mathcal{C}_\rho \cap Sp(2)) = 8 - 4 = 4 \neq 6$, i.e. the left- and right-hand sides in (9) are *not* equal. Thus we have shown using theorem 6 that the action of $Sp(2)$ on the kinematical equivalence class of ρ is not transitive.

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