Non-reachable target states for pure-state controllable and non-controllable quantum systems

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Outline of the talk

- Representation of pure and mixed quantum states
- Kinematical equivalence classes of density matrices
- Dynamical Lie group action on kinematical equivalence classes
- Criteria for dynamical reachability of states
- Examples of non-reachable states for systems with
  - dynamical Lie group $Sp(\frac{N}{2})$ (pure-state controllable)
  - dynamical Lie group $SO(N)$ (not controllable)

States of a Quantum System

- Von Neumann: The state of any quantum system can be represented by a density operator $\hat{\rho}$ acting on a Hilbert space $\mathcal{H}$.

- Density operator: positive operator with trace one $\Rightarrow$ pure point spectrum with eigenvalues w_n satisfying $0 \leq w_n \leq 1$, $\sum_n w_n = 1$.

- Spectral resolution: $\hat{\rho} = \sum_n w_n |\Psi_n\rangle\langle\Psi_n|$ where $|\Psi_n\rangle$ are the eigenstates and $\langle\Psi_n|$ their duals.

- If the rank of $\hat{\rho}$ is one then $\hat{\rho}$ represents a pure state, otherwise a mixed state.

- A pure state $\hat{\rho} = |\Psi\rangle\langle\Psi|$ can also be represented by the wavefunction $|\Psi\rangle$.

Pure & Mixed-State Examples

Density operators representing pure states:

$$\hat{\rho}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \; \hat{\rho}_2 = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

Note that $\hat{\rho}_2 = |\Psi\rangle\langle\Psi|$ for $|\Psi\rangle = (1,0,0,1)^T/\sqrt{2}$.

Density operators representing mixed states:

$$\hat{\rho}_3 = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \; \hat{\rho}_4 = \begin{pmatrix} \frac{2}{5} & 0 & 0 & 0 \\ 0 & \frac{3}{10} & 0 & 0 \\ 0 & 0 & \frac{1}{5} & 0 \\ 0 & 0 & 0 & \frac{1}{10} \end{pmatrix}, \; \hat{\rho}_5 = \begin{pmatrix} \frac{1}{4} & 0 & 0 & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{4} & 0 \\ 0 & \frac{1}{4} & \frac{1}{4} & 0 \\ \frac{1}{4} & 0 & 0 & \frac{1}{4} \end{pmatrix}.$$

Evolution of Quantum States

- Non-dissipative system: evolution operator $\hat{U}(t, t_0)$ satisfies SE

$$i\hbar \frac{d}{dt}\hat{U}(t, t_0) = \hat{H}[\mathbf{f}(t)]\hat{U}(t, t_0)$$

  where $\hat{H}[\mathbf{f}(t)]$ is the total Hamiltonian of the system.

- External control: $\hat{H}$ depends on control fields [to be determined]

$$\mathbf{f}(t) = (f_1(t), \ldots, f_M(t))$$

- Conservation of energy & probability: unitary evolution for all times

$\Rightarrow$ $\hat{U}(t, t_0)$ restricted to unitary group $U(N)$

$\Rightarrow$ $\hat{\rho}_0$ and $\hat{\rho}_1$ kinematically equivalent iff $\hat{\rho}_1 = \hat{U}\hat{\rho}_0\hat{U}^\dagger$ for some unitary $\hat{U}$

$\Leftrightarrow$ $\hat{\rho}_0$ and $\hat{\rho}_1$ kinematically equivalent iff they have the same eigenvalues

Dynamical Lie Groups & Reachable Sets

- Kinematical constraint: dynamical Lie group must be subgroup of $U(N)$

  $\Rightarrow$ Partitioning of density operators into kinematical equivalence classes [KEC]
  $\Rightarrow$ dynamically reachable states must be subsets of KEC

- Dynamical Lie group S: determines sets of dynamically equivalent states

  $\Rightarrow$ $\hat{\rho}_0$, $\hat{\rho}_1$ dynamically equivalent iff $\hat{\rho}_1 = \hat{U}\hat{\rho}_0\hat{U}^\dagger$ for $\hat{U} \in S$
  $\Rightarrow$ set of dynamically reachable states = KEC iff S transitive on KEC

- Transitive Action:

  – $U(N)$, $SU(N)$ transitive on all kinematical equivalence classes

  – Only $U(N)$, $SU(N)$, and if N even, $Sp(\frac{N}{2})$, $Sp(\frac{N}{2}) \times U(1)$ transitive on the KEC of pure states [Montgomery & Samulson (1943)]

  – Any other dynamical Lie group transitive only on the trivial KEC of completely random ensembles $[\hat{\rho} = \frac{1}{N}\hat{I}_N]$

Dynamical Equivalence of States for $S \simeq Sp(\frac{N}{2})$

- $Sp(\frac{N}{2})$ transitive on completely random ensembles and KEC of density operators $\hat{\rho}$ with two distinct eigenvalues, one of which occuring with multiplicity $N-1$.
- Otherwise: kinematically equivalent, dynamically non-reachable states exist
- Criteria for dynamical equivalence of states: For any $S \simeq Sp(\frac{N}{2})$ there exists $\hat{J}$ such that any $\hat{U} \in S$ satisfies $\hat{U}^T \hat{J} \hat{U} = \hat{J}$

  $\Rightarrow$ $\hat{\rho}_0$ and $\hat{\rho}_1$ (KE) are dynamically equivalent iff $\exists\ \hat{U} \in U(N)$ such that

  $$\boxed{\hat{\rho}_1 = \hat{U}\hat{\rho}_0\hat{U}^\dagger} \quad \text{and} \quad \boxed{\hat{U}^T \hat{J} \hat{U} = \hat{J}}$$

  $\Leftrightarrow$ $\hat{\rho}_0$, $\hat{\rho}_1$ dynamically equivalent (DE) iff

  $$\boxed{\hat{\rho}_1 = \hat{U}\hat{\rho}_0\hat{U}^\dagger} \quad \text{and} \quad \boxed{(\hat{J}\hat{\rho}_1\hat{J}^\dagger)^* = \hat{U}(\hat{J}\hat{\rho}_0\hat{J}^\dagger)^*\hat{U}^\dagger}$$

System with dynamical Lie group $Sp(2)$

Consider a four-level system with $\hat{H} = \hat{H}_0 + f(t)\hat{H}_1$,

$$\hat{H}_0 = \begin{pmatrix} -\frac{3}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & +\frac{1}{2} & 0 \\ 0 & 0 & 0 & +\frac{3}{2} \end{pmatrix}, \qquad \hat{H}_1 = \begin{pmatrix} 0 & +1 & 0 & 0 \\ +1 & 0 & +1 & 0 \\ 0 & +1 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

The dynamical Lie algebra $\mathcal{L}$ generated by $i\hat{H}_0$ and $i\hat{H}_1$ has dimension 10 and both $i\hat{H}_0$ and $i\hat{H}_1$ satisfy

$$\boxed{\hat{x}^T \hat{J} = -\hat{J}\hat{x}} \qquad \text{for} \qquad \hat{J} = \begin{pmatrix} 0 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

$\Rightarrow \mathcal{L} = sp(2)$ and the dynamical Lie group $S = Sp(2)$.

Non-Reachable States for $Sp(2)$ Example

Let $0 \leq a, b \leq 1$, $a \neq b$, $a + b = \frac{1}{2}$. Consider the kinematically equivalent states

$$\hat{\rho}_0 = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & a & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & b \end{pmatrix}, \; \hat{\rho}_1 = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & a \end{pmatrix}, \; \hat{\rho}_2 = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & a & 0 \\ 0 & 0 & 0 & b \end{pmatrix},$$

$\hat{\rho}_0$ and $\hat{\rho}_2$ are NOT dynamically equivalent since

$$\boxed{\tilde{\rho}_2 = (\hat{J}\hat{\rho}_2\hat{J}^\dagger)^* = \hat{\rho}_2} \quad \text{but} \quad \boxed{\tilde{\rho}_0 = (\hat{J}\hat{\rho}_0\hat{J}^\dagger)^* \neq \hat{\rho}_0}$$

There cannot be a unitary operator such that $\hat{\rho}_2 = \hat{U}\hat{\rho}_0\hat{U}^\dagger = \hat{U}\tilde{\rho}_0\hat{U}^\dagger$ if $\hat{\rho}_0 \neq \tilde{\rho}_0$.

Similarly, $\hat{\rho}_1$ and $\hat{\rho}_2$ are NOT dynamically equivalent since

$$\boxed{\tilde{\rho}_2 = (\hat{J}\hat{\rho}_2\hat{J}^\dagger)^* = \hat{\rho}_2} \quad \text{but} \quad \boxed{\tilde{\rho}_1 = (\hat{J}\hat{\rho}_1\hat{J}^\dagger)^* \neq \hat{\rho}_1}$$

Finally, $\hat{\rho}_0$ and $\hat{\rho}_1$ are NOT dynamically equivalent since the equations (1)

$$\boxed{\hat{\rho}_1 = \hat{U}\hat{\rho}_0\hat{U}^\dagger} \quad \text{and} \quad \boxed{\tilde{\rho}_1 = \hat{U}\tilde{\rho}_0\hat{U}^\dagger}$$

for $\tilde{\rho} = (\hat{J}\hat{\rho}\hat{J}^\dagger)^*$ cannot be simultaneously solved.

To see this, note that the associated linear equations (2)

$$\boxed{\hat{U}\hat{\rho}_0 - \hat{\rho}_1\hat{U} = 0} \quad \text{and} \quad \boxed{\hat{U}\tilde{\rho}_0 - \tilde{\rho}_1\hat{U} = 0}$$

can be re-written in matrix form (3)

$$\boxed{\underline{R}\mathbf{U} = 0}$$

where $\underline{R}$ is a $2N^2$ by N^2 matrix and $\mathbf{U}$ is a column vector of length N^2. The null space of the matrix $\underline{R}$ is empty. Thus, there is no solution $\mathbf{U}$ to the linear system of equations (3), and therefore, no unitary operator $\hat{U}$ that solves (1).

Dynamical Equivalence of States for $S \simeq SO(N)$

- $SO(N)$ transitive only on trivial KEC of completely random ensembles
- Any other KEC is partitioned into subclasses of dynamically equivalent states
- Criteria for dynamical equivalence of states:
  Method 1: Use $\hat{J}$ matrix.
  - For any $S \simeq SO(N)$ there exists $\hat{J}$ such that $\hat{U}^T \hat{J} \hat{U} = \hat{J}$ for any $\hat{U} \in S$
  - KE states $\hat{\rho}_0$, $\hat{\rho}_1$ dynamically equivalent iff
    $$\hat{\rho}_1 = \hat{U} \hat{\rho}_0 \hat{U}^\dagger \text{ and } (\hat{J} \hat{\rho}_1 \hat{J}^\dagger)^* = \hat{U} (\hat{J} \hat{\rho}_0 \hat{J}^\dagger)^* \hat{U}^\dagger$$

  Method 2: Change of basis.
  - Dynamical Lie algebra $\mathcal{L}$ is a representation of $so(N)$ in terms of skew-Hermitian operators since $i\hat{H}_m$ skew-Hermitian
  - Find unitary basis transformation B such that $B(i\hat{H}_m)B^\dagger$ are real, skew-symmetric matrices
  - Real orthogonal transformations cannot map matrices with real entries onto matrices with non-real entries.

System with dynamical Lie group $SO(5)$

Consider a five-level system with $\hat{H} = \hat{H}_0 + f(t)\hat{H}_1$,

$$\hat{H}_0 = \begin{pmatrix} -2 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix}, \qquad \hat{H}_1 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 \\ 0 & 2 & 0 & 2 & 0 \\ 0 & 0 & 2 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

The skew-Hermitian matrices $i\hat{H}_0$ and $i\hat{H}_1$ generate the Lie algebra $so(5)$, or rather, a skew-Hermitian representation of $so(5)$.

However, the unitary transformation

$$B = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & \sqrt{2} & 0 & 0 \\ i & 0 & 0 & 0 & -i \\ 1 & i & 0 & i & 0 \end{pmatrix}$$

maps $i\hat{H}_0$ and $i\hat{H}_1$ onto real, anti-symmetic matrices

$$\tilde{H}_0 = B(i\hat{H}_0)B^\dagger = \begin{pmatrix} 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{H}_1 = B(i\hat{H}_1)B^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2\sqrt{2} \\ 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & -2\sqrt{2} & 0 & 0 \end{pmatrix}$$

which generate a representation of $so(5)$ in terms of real, skew-symmetric matrices.

$\Rightarrow$ associated Lie group $\tilde{S}$ consists of real orthogonal transformations!

Non-Reachable States for $SO(5)$ Example

- Basis change B maps the pure states

$$\hat{\rho}_0 = |1\rangle\langle 1| \text{ and } \hat{\rho}_1 = \tfrac{1}{2}(|1\rangle + |5\rangle)(\langle 1| + \langle 5|)$$

to $\tilde{\rho}_0 = B\hat{\rho}_0 B^\dagger$ and $\tilde{\rho}_1 = B\hat{\rho}_1 B^\dagger$, where

$$\tilde{\rho}_0 = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ i & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad \tilde{\rho}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

- $\tilde{\rho}_0$ has non-real entries, while $\tilde{\rho}_1$ has only real entries

$\Rightarrow$ There is no real orthogonal transformation $\hat{U}$ such that $\tilde{\rho}_1 = \hat{U}\tilde{\rho}_0\hat{U}^\dagger$ [Note $\hat{U}^\dagger = U^T$]

$\Rightarrow$ $\hat{\rho}_0$ and $\hat{\rho}_1$ not dynamically equivalent!

Summary

- The constraint of unitary evolution partitions density operators into kinematical equalence classes.
- The action of the dynamical Lie group of the system partitions the KEC into subclasses of dynamically equivalent states.
- The set of dynamically reachable states is equal to the KEC iff the dynamical Lie group acts transitively on the KEC.
- $U(N)$ and $SU(N)$ act transitively on all KEC.
- $Sp(\frac{N}{2})$ and $Sp(\frac{N}{2}) \times U(1)$ are the only proper subgroups of $SU(N)$ that act transitively on the KEC of pure states.
- Any other dynamical Lie group acts transitively only on the trivial KEC of completely random ensembles.