Quantum Control: Applications & Limitations

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Relationship between quantum control & quantum computation

- Quantum computation requires:
  - Preparation of the quantum computer in a desired initial state.
    - The ability to create arbitrary superpositions for single qubits
    - Entanglement between pairs of qubits.
  - Implementation of quantum logic operations (unitary operators)
  - Means to protect and store quantum information.
  - The ability to extract quantum information.
- Quantum control addresses problems such as:
  - Preparation of a quantum system in a desired quantum state.
  - Control of unitary evolution (implementation of unitary operators).
  - Control of dissipative processes (decay, decoherence).
  - Optimal measurements of quantum systems.

Requirements for quantum control

1. Accurate models: Modelling realistic quantum systems and their interaction with control fields, the environment and a measurement apparatus.
2. Controllability: Assessing the feasibility of control objectives by studying the degree of controllability of the systems to be manipulated.
3. Control Field Design: Developing means to design control fields to achieve various control objectives (which have been shown to be feasible).
4. Applications: Application of control techniques to specific problems in quantum computing, quantum optics, quantum chemistry, etc.

Modelling quantum systems

Control of quantum systems requires a basic mathematical model.

Describing any dynamical system requires three basic ingredients:

	State space	Dynamical law	Observables
	set of possible states of the system	determining the time evolution of states	quantities we can measure
CM	position, momentum $\mathbf{x}$, $\mathbf{p}$,	Newton's laws $\mathbf{F} = m\ddot{\mathbf{x}}$	state of the system $\mathbf{x}$, $\mathbf{p}$
PQM	wavefunctions $\lvert\Psi(t)\rangle$	Schrodinger equation $i\hbar\frac{\partial}{\partial t}\lvert\Psi(t)\rangle = \hat{H}\lvert\Psi(t)\rangle$	expectation values $\langle\hat{A}\rangle = \langle\Psi(t)\lvert\hat{A}\rvert\Psi(t)\rangle$
QSM	density operators $\hat{\rho}(t)$	Quantum Liouville eq. $i\hbar\frac{\partial}{\partial t}\hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)]$	ensemble averages $\langle\hat{A}(t)\rangle = \mathrm{Tr}(\hat{A}\hat{\rho}(t))$

Manipulating the dynamics

- The evolution of an unperturbed quantum system is determined by its free Hamiltonian $\hat{H}_0$.
- Application of external control fields — e.g., derived from lasers — perturbs the evolution of the system ⇒ new total Hamiltonian

$$\hat{H} = \hat{H}_0 + \sum_{m=1}^{M} f_m(t)\hat{H}_m$$

- $\hat{H}_m$, $m > 0$, describes the interaction of the system with field f_m.
- The controls are classical fields, i.e., bounded, measurable, real-valued functions defined for some time interval $[t_0, t_F]$.

$$\mathbf{f}(t) = (f_1(t), f_2(t), \ldots, f_M(t)) \qquad M < \infty$$

The effect of the environment

- Ideal: The quantum system interacts only with the control fields.
  ⇒ The evolution of an ideal quantum control system is unitary.
- Reality: Most quantum systems also interact in uncontrollable ways with the environment.
  ⇒ The evolution of the system is non-unitary due to:
  - Phase decoherence, which destroys the off-diagonal elements (coherences) of the density operator.
  - Population relaxation, which changes populations (diagonal elements of the density operator) and leads to phase decoherence.
- Phase decoherence and population decay necessitate the introduction of a dissipation super operator $\mathcal{D}$ determined by the phase and population relaxation rates γ_{km}^d and γ_{km}:

$$\mathcal{D}_{km,km} = -\gamma_{km}^d,$$
$$\mathcal{D}_{kk,mm} = \gamma_{km},$$
$$\mathcal{D}_{kk,kk} = -\sum_{m \neq k} \gamma_{mk}.$$

Liouville Equation for Dissipative Systems

Combining the effect of the controls and the dissipation, leads to the quantum Liouville equation for dissipative systems:

$$\frac{\partial}{\partial t}\hat{\rho}(t) = -\frac{i}{\hbar}\left[\mathcal{L}_0 + \sum_{m=1}^{M} f_m(t)\mathcal{L}_m\right]\hat{\rho}(t) + \mathcal{D}\hat{\rho}(t)$$

$\mathcal{L}_m\hat{\rho}(t) \equiv [\hat{H}_m, \hat{\rho}]$ for $0 \leq m \leq M$ and $\mathcal{D}$ can always be written as

$$\mathcal{D}[V_k]\hat{\rho} = \tfrac{1}{2}\sum_k [\hat{V}_k\hat{\rho}, \hat{V}_k^\dagger] + [\hat{V}_k, \hat{\rho}\hat{V}_k^\dagger]$$

where the $\hat{V}_k$ are arbitrary bounded operators [Lindblad].

Unitary evolution & Magnus expansion

- The evolution of a Hamiltonian quantum control system is given by

$$\hat{U}(t, t_0) = \exp_+\left[-\frac{i}{\hbar}\int_{t_0}^{t} \hat{H}[\mathbf{f}(\tau)]\, d\tau\right]$$

- The time-ordered exponential is unitary and can be expressed in terms of an ordinary exponential via the Magnus expansion

$$\exp_+\left[-\frac{i}{\hbar}\int_{t_0}^{t} \hat{H}(\tau)\, d\tau\right] = \exp\left[\sum_{n=1}^{\infty} \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \hat{A}_n\right]$$

where $\hat{H}(\tau) = \hat{H}[\mathbf{f}(\tau)]$ and the operators $\hat{A}_n$ are defined by

$$\hat{A}_1 = \int_{t_0}^{t} \hat{H}(\tau_1)\, d\tau_1, \qquad \hat{A}_2 = \int_{t_0}^{t}\int_{t_0}^{\tau_2} [\hat{H}(\tau_2), \hat{H}(\tau_1)]\, d\tau_1\, d\tau_2$$
$$\hat{A}_3 = \int_{t_0}^{t}\int_{t_0}^{\tau_3}\int_{t_0}^{\tau_2} [\hat{H}(\tau_3), [\hat{H}(\tau_2), \hat{H}(\tau_1)]] + [[\hat{H}(\tau_3), \hat{H}(\tau_2)], \hat{H}(\tau_1)]\, d\tau_1 d\tau_2 d\tau_3, \ldots$$

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 & Samelson (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 occurring 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

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

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

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

Let $0 \le a, b \le 1$, $a \ne b$, $a + b = \frac{1}{2}$. 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

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

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 $\hat{\rho}_0 \ne \tilde{\rho}_0$.

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

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

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
    $\hat{\rho}_1 = \hat{U}\hat{\rho}_0\hat{U}^\dagger$ 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-symmetric 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

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

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

Controllability of Hamiltonian systems

Even for Hamiltonian quantum control systems, there are various notions of controllability:

- CC Complete controllability: any unitary evolution is dynamically realizable, i.e., given any unitary operator $\hat{U}$, there exists $t_F > 0$ and an admissible control-trajectory pair $(\mathbf{f}, \hat{U}(t, t_0))$ such that $\hat{U} = \hat{U}(t_F, t_0)$.
- OC Observable controllability: kinematical bounds for any observable $\hat{A}$ dynamically realizable, i.e., there exists $t_F > 0$ and an admissible control-trajectory pair $(\mathbf{f}, \hat{U}(t, t_0))$ such that $\langle \hat{A}(t)\rangle$ assumes its kinematical upper or lower bound at $t = t_F$.
- DC Density matrix controllability: given any two (kinematically equivalent) density matrices $\hat{\rho}_0$, $\hat{\rho}_1$, there exists $t_F > 0$ and an admissible control-trajectory pair $(\mathbf{f}, \hat{U}(t, t_0))$ such that $\hat{\rho}_1 = \hat{U}(t_F, t_0)\hat{\rho}_0\hat{U}(t_F, t_0)^\dagger$.
- PC Pure-state controllability: given any two pure states (wavefunctions) $|\Psi_0\rangle$, $|\Psi_1\rangle$, there exists $t_F > 0$ and an admissible control-trajectory pair $(\mathbf{f}, \hat{U}(t, t_0))$ such that $|\Psi_1\rangle = \hat{U}(t_F, t_0)|\Psi_0\rangle$.

Lie algebraic criteria for controllability

The Magnus expansion shows that the evolution of a control-linear system is determined by the operators of the form $\exp(\hat{x})$ where $\hat{x}$ is an element of the dynamical Lie algebra L generated by the operators $i\hat{H}_m$, $0 \le m \le M$.

Theorem: [Abertini, D'Alessandro / Schirmer, Solomon, Leahy] If $\dim \mathcal{H} = N$ then L is a subalgebra of $u(N)$ and the system is

- Completely controllable ⇔ $L \simeq u(N)$.
- Observable controllable ⇔ $L \simeq u(N)$ or $L \simeq su(N)$.
- Density matrix controllable ⇔ $L \simeq u(N)$ or $L \simeq su(N)$.
- Pure-state controllable ⇔ $L \simeq u(N)$, $L \simeq su(N)$, or, if $N = 2\ell$, $sp(\ell)$, $sp(\ell) \oplus u(1)$.

Thus we have CC ⇒ OC ⇔ DC ⇒ PC.

We shall call a system controllable if its dynamical Lie algebra is $su(N)$ or $u(N)$.

Results about controllability

Consider a quantum system subject to a single control field $(M = 1)$ with $N < \infty$ energy levels E_n with $E_n \le E_{n+1}$ and transition frequencies $\omega_{mn} = E_n - E_m$.

Theorem: [Altafini / Turinici] If the energy levels are non-degenerate and the transition frequencies are unique, i.e., $\omega_{mn} \neq \omega_{ab}$ unless $(m, n) = (a, b)$, let the eigenstates $|n\rangle$ be the vertices of a graph and the transitions $|n\rangle \to |m\rangle$ with non-zero dipole moment be the edges. If the graph is connected then the system is controllable.

Theorem: [Schirmer, Fu, Solomon] Given a system with nearest-neighbor interaction, i.e., $d_{mn} = 0$ unless $n = m \pm 1$ and $d_{n,n+1} = d_{n+1,n} \neq 0$, let $v_n \equiv 2d_{n,n+1}^2 - d_{n-1,n}^2 - d_{n+1,n+2}^2$. The system is controllable if either

1. $\exists p$ such that $\omega_{n,n+1} \neq \omega_{p,p+1}$ for $n \neq p$, or
2. $\omega_{n,n+1} = \omega$ for all n but $\exists p$ s.t. $v_n \neq v_p$ for $n \neq p$,

and $d_{p-k}^2 \neq d_{p+k}^2$ for some $k \neq 0$ in case $N = 2p$.

Conclusion

In this first talk we introduced some of the ideas of quantum control:

- The relationship between quantum control and computing
- Environmental effects
- Dynamical Group approach to non-dissipative systems
- Degrees of controllability of Hamiltonian quantum systems

In the following talk we will describe how we can implement quantum control, and discuss at greater length the effects of dissipation.